



Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 02:41 PM EST

PDB ID : 8UXM
EMDB ID : EMD-42769
Title : Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium and calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.56 Å(reported)
Based on initial model : 7UA5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

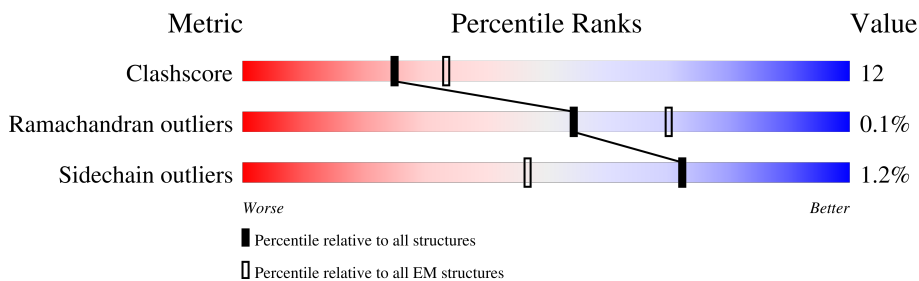
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






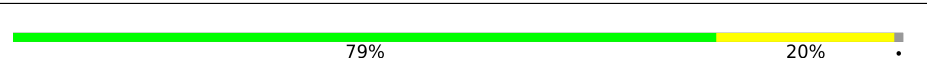
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	149	
1	J	149	
1	K	149	
1	L	149	
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	

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Mol	Chain	Length	Quality of chain
3	E	108	 80% 19% ..
3	F	108	 80% 19% ..
3	G	108	 80% 19% ..
3	H	108	 79% 20% .

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 143464 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	143	1131	694	182	246	9	0	0
1	J	143	1131	694	182	246	9	0	0
1	L	143	1131	694	182	246	9	0	0
1	K	143	1131	694	182	246	9	0	0

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	4231	33849	21572	5764	6283	230	2	0
2	B	4231	33849	21572	5764	6283	230	2	0
2	C	4231	33849	21572	5764	6283	230	2	0
2	D	4231	33849	21572	5764	6283	230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

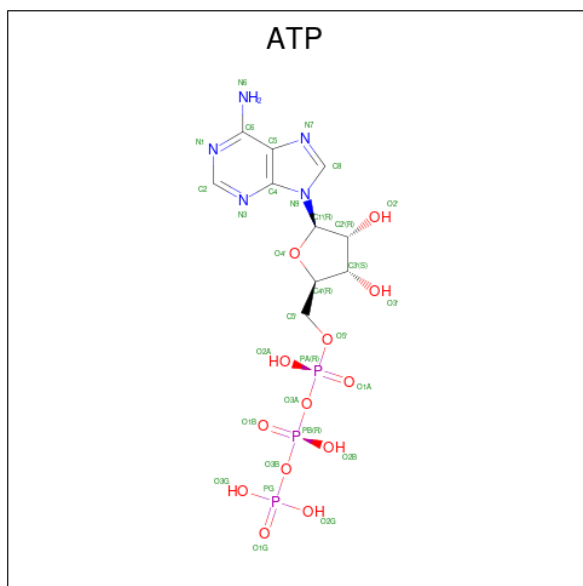
Mol	Chain	Residues	Atoms		AltConf
4	I	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	J	4	Total	Ca	0
			4	4	
4	L	4	Total	Ca	0
			4	4	
4	K	4	Total	Ca	0
			4	4	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

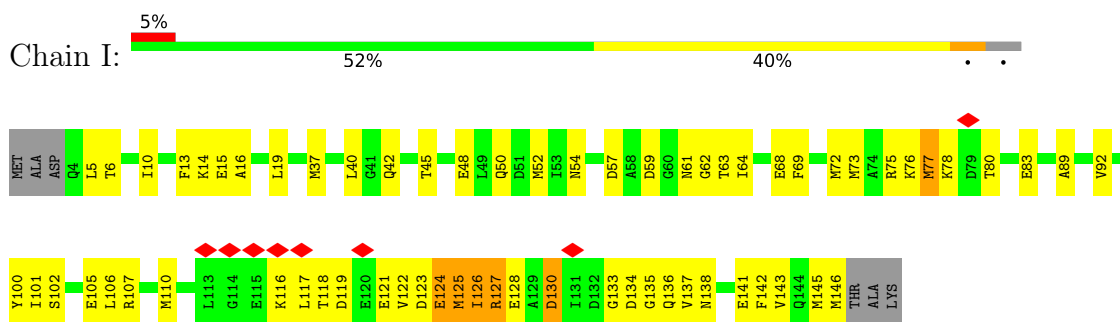


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

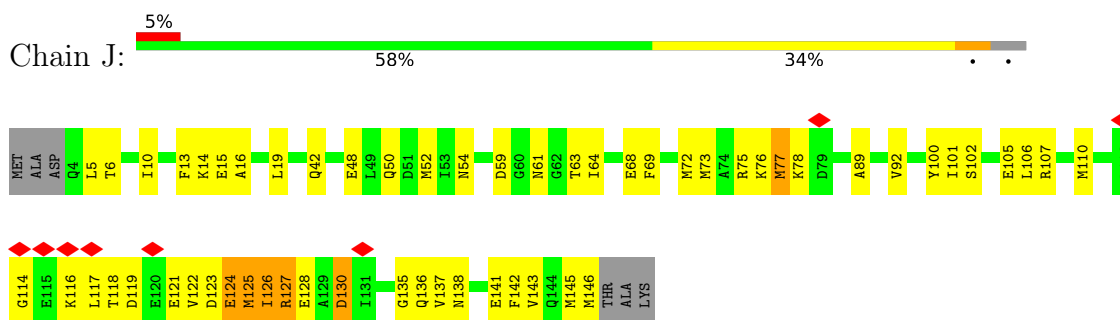
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

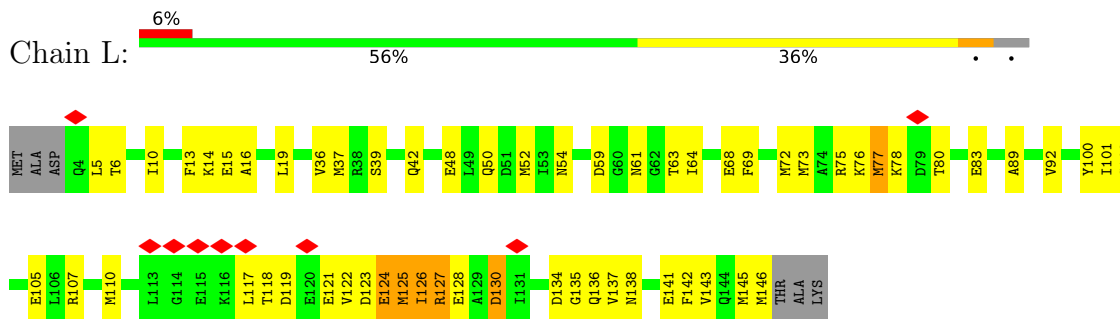
- Molecule 1: Calmodulin-1



- Molecule 1: Calmodulin-1



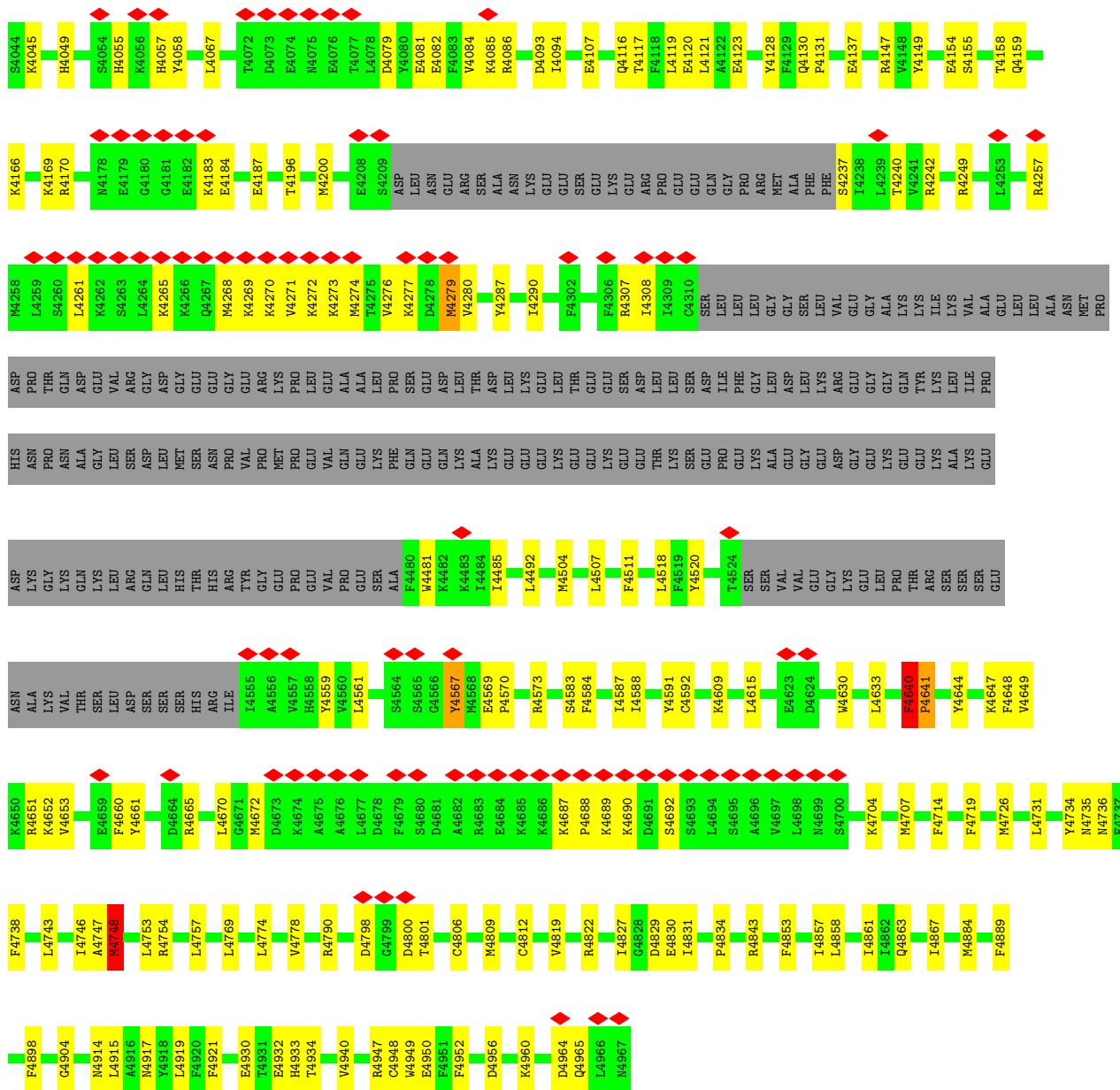
- Molecule 1: Calmodulin-1



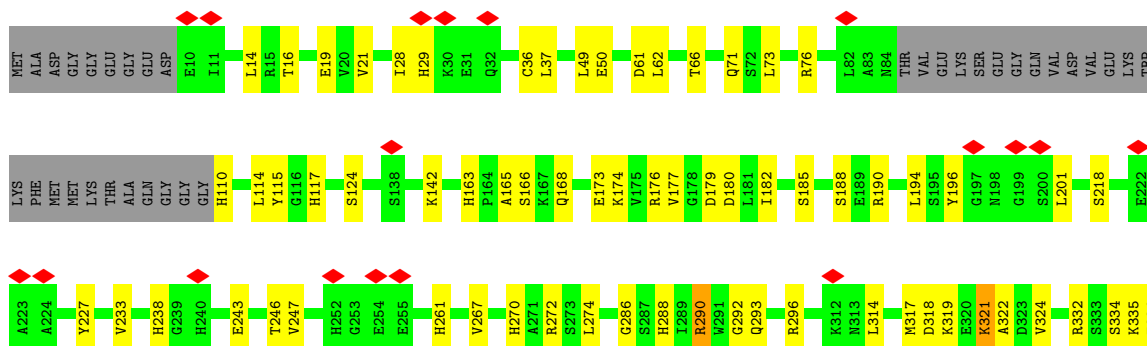
- Molecule 1: Calmodulin-1

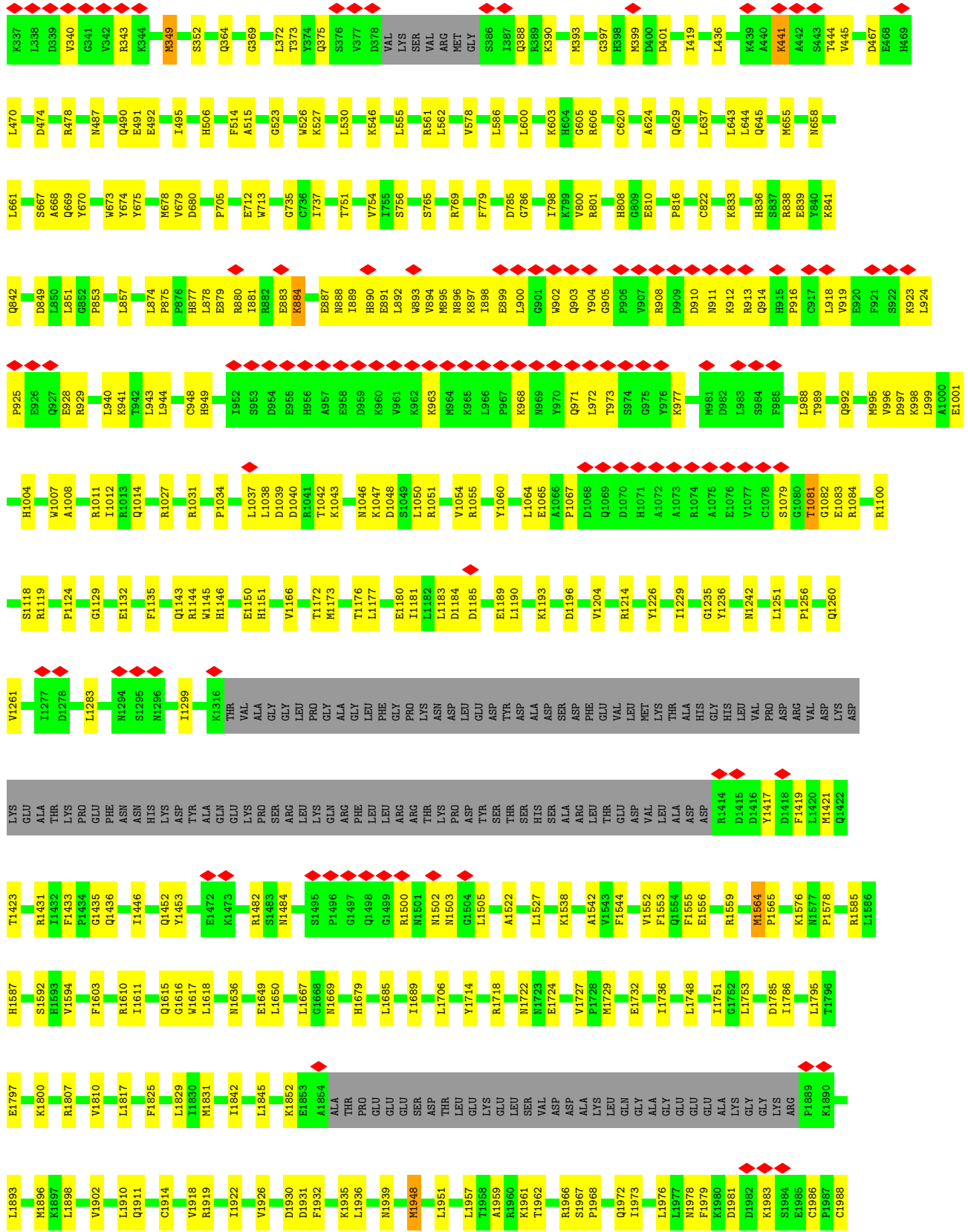


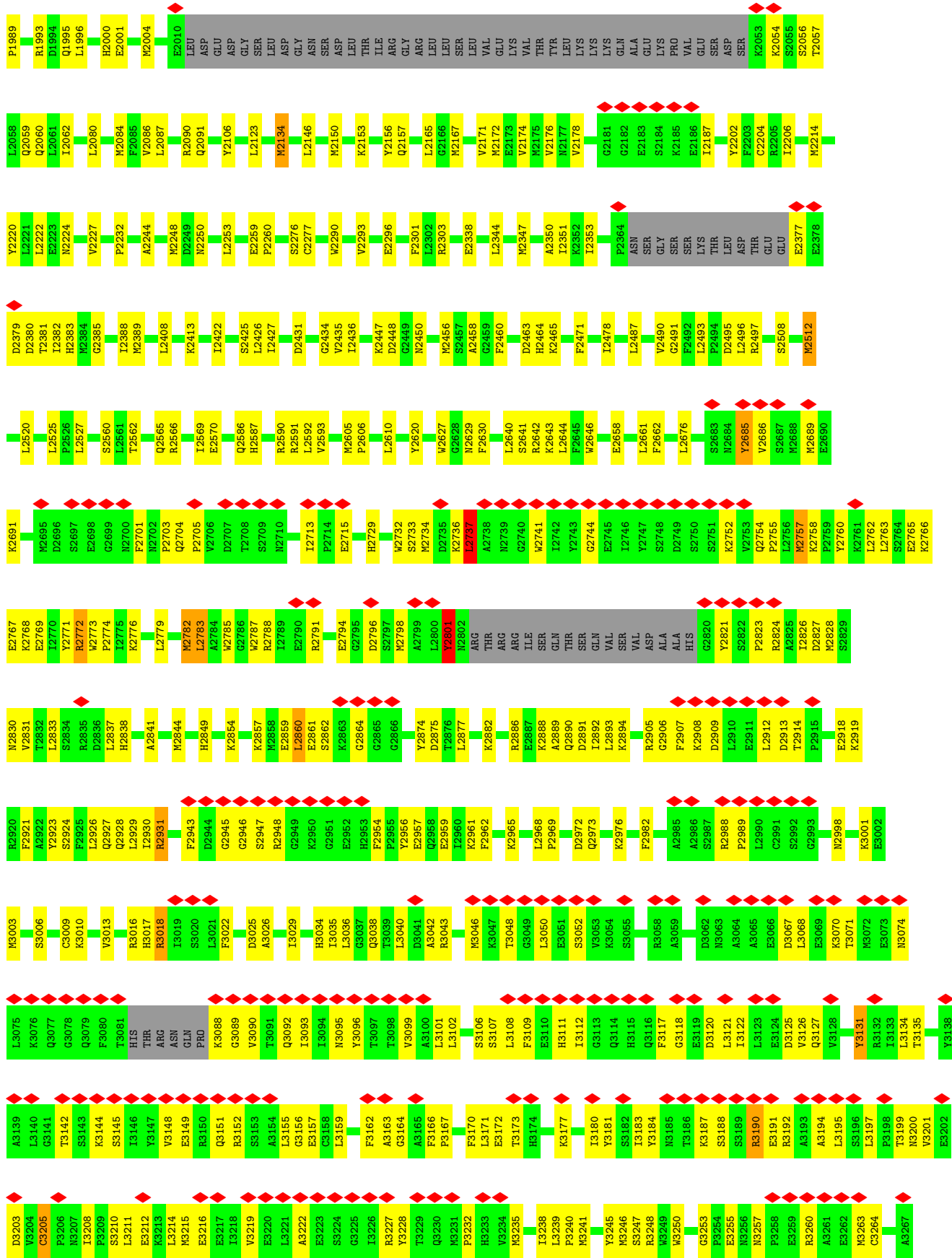
R2824	R2825	L2826	D2827	M2828	S2829	M2830	V2831	L2833	S2834	R2835	D2836	L2837	H2838	A2841	M2844	H2849	K2854	K2857	L2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	L2871	D2875	T2876	L2877	E2881	R2886	K2888	A2889	D2891	L2892	L2893	K2894	L2898	R2905	G2906	F2907										
Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	E2769	I2770	Y2771	R2772	W2773	P2774	K2775	K2776	L2779	M2782	L2783	A2784	W2785	G2786	W2787	R2788	R2791	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	M2802	ARG	THR	ARG	THR	ILE	SER	GLN	THR	SER	GLN	THR	VAL	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	
M2684	Y2685	Y2686	M2687	S2688	M2689	K2690	K2691	M2695	D2696	S2697	G2698	G2699	M2700	F2701	M2702	P2703	Q2704	P2705	V2706	D2707	T2708	S2709	M2710	I2713	P2714	E2715	H2729	W2732	S2733	D2735	K2736	L2737	A2738	M2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	F2662	L2747	S2748	D2749	S2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759
D2495	L2496	R2497	S2508	M2512	L2520	L2525	P2526	L2527	L2548	S2550	L2561	T2562	Q2565	R2566	L2569	Q2586	H2587	R2590	R2591	L2592	V2593	P2606	L2610	Y2620	W2627	G2628	N2629	F2630	L2640	S2641	R2642	K2643	L2644	F2645	W2646	E2658	L2661	F2662	L2676	S2683															
ASP	THR	GLU	E2377	D2378	D2379	D2380	T2381	I2382	H2383	G2384	G2385	I2388	M2389	L2408	K2413	I2422	S2425	L2426	I2427	D2431	G2434	V2435	I2436	K2447	D2448	G2449	N2450	M2456	S2457	A2458	G2459	F2460	D2463	H2464	K2465	F2471	I2478	L2487	L2488	E2489	S2490	G2491	F2492	L2493	P2494										
GLU	SER	ASP	K2063	K2054	S2055	K1890	T2067	L2068	Q2069	Q2060	L2061	L2062	L2080	M2084	F2085	V2086	L2087	R2090	Q2091	Y2106	L2123	M2134	L2146	M2150	K2153	Y2156	Q2157	L2165	G2166	M2167	V2171	M2172	E2173	V2174	M2175	L2176	N2177	V2178	G2181	C2182	E2183	S2184	E2185	E2186	I2187										
K1980	D1981	L1982	K1983	S1984	I1985	C1986	F1987	C1988	P1989	R1993	D1994	Q1995	L1996	H2000	E2001	M2004	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	ASN	SER	L1935	L1936	N1939	M1943	L1951	L1957	T1958	A1959	F1960	K1961	T1962	R1966	S1967	P1968	Q1972	I1973	L1976	L1977	N1978	F1979								
K1980	D1981	L1982	K1983	S1984	I1985	C1986	F1987	C1988	P1989	R1993	D1994	Q1995	L1996	H2000	E2001	M2004	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	ASN	SER	L1935	L1936	N1939	M1943	L1951	L1957	T1958	A1959	F1960	K1961	T1962	R1966	S1967	P1968	Q1972	I1973	L1976	L1977	N1978	F1979								
GLU	SER	ASP	K2063	K2054	S2055	K1890	T2067	L2068	Q2069	Q2060	L2061	L2062	L2080	M2084	F2085	V2086	L2087	R2090	Q2091	Y2106	L2123	M2134	L2146	M2150	K2153	Y2156	Q2157	L2165	G2166	M2167	V2171	M2172	E2173	V2174	M2175	L2176	N2177	V2178	G2181	C2182	E2183	S2184	E2185	E2186	I2187										
Y2202	F2203	C2204	R2205	L2206	W2214	Y2220	L2221	L2222	E2223	N2224	V2227	P2232	A2244	M2248	D2249	N2250	L2253	E2259	P2260	W2290	V2293	E2296	F2301	L2302	K2303	E2338	L2344	W2347	A2350	I2351	K2352	L2353	P2364	ASN	SER	GLY	SER	SER	THR	LEU															
ASP	THR	GLU	E2377	D2378	D2379	D2380	T2381	I2382	H2383	G2384	G2385	I2388	M2389	L2408	K2413	I2422	S2425	L2426	I2427	D2431	G2434	V2435	I2436	K2447	D2448	G2449	N2450	M2456	S2457	A2458	G2459	F2460	D2463	H2464	K2465	F2471	I2478	L2487	L2488	E2489	S2490	G2491	F2492	L2493	P2494										
D2495	L2496	R2497	S2508	M2512	L2520	L2525	P2526	L2527	L2548	S2550	L2561	T2562	Q2565	R2566	L2569	Q2586	H2587	R2590	R2591	L2592	V2593	P2606	L2610	Y2620	W2627	G2628	N2629	F2630	L2640	S2641	R2642	K2643	L2644	F2645	W2646	E2658	L2661	F2662	L2676	S2683															
M2684	Y2685	Y2686	M2687	S2688	M2689	K2690	K2691	M2695	D2696	S2697	G2698	G2699	M2700	F2701	M2702	P2703	Q2704	P2705	V2706	D2707	T2708	S2709	M2710	I2713	P2714	E2715	H2729	W2732	S2733	D2735	K2736	L2737	A2738	M2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	F2662	L2747	S2748	D2749	S2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759
Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	E2769	I2770	Y2771	R2772	W2773	P2774	K2775	K2776	L2779	M2782	L2783	A2784	W2785	G2786	W2787	R2788	R2791	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	M2802	ARG	THR	ARG	THR	ILE	SER	GLN	THR	SER	GLN	THR	VAL	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	
ASP	ARG	VAL	ASP	ASP	ASP	LYS	GLU	ALA	THR	LYS	PRO	GLU	PHE	LEU	LEU	LEU	GLN	ARG	ARG	ARG	ARG	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	LEU	ARG	THR	LYS	PRO	ASP	TYR	SER	THR	SER	HIS	SER	ALA	ALA	ASP	VAL	VAL	ASP	LEU	LEU	ALA	ASP	R1414	D1415	D1416	
Y1417	D1418	F1419	L1420	M1421	G1422	T1423	R1431	I1432	F1433	P1434	G1435	Q1436	I1446	Q1452	Y1453	E1472	K1473	R1482	S1483	N1484	S1485	P1486	G1487	Q1498	S1499	R1499	M1501	N1502	N1503	G1504	L1505	D1512	S1515	A1522	L1527	K1538	A1542	V1543	F1544	M1550	V1552	F1553	Q1554	F1555	E1556										

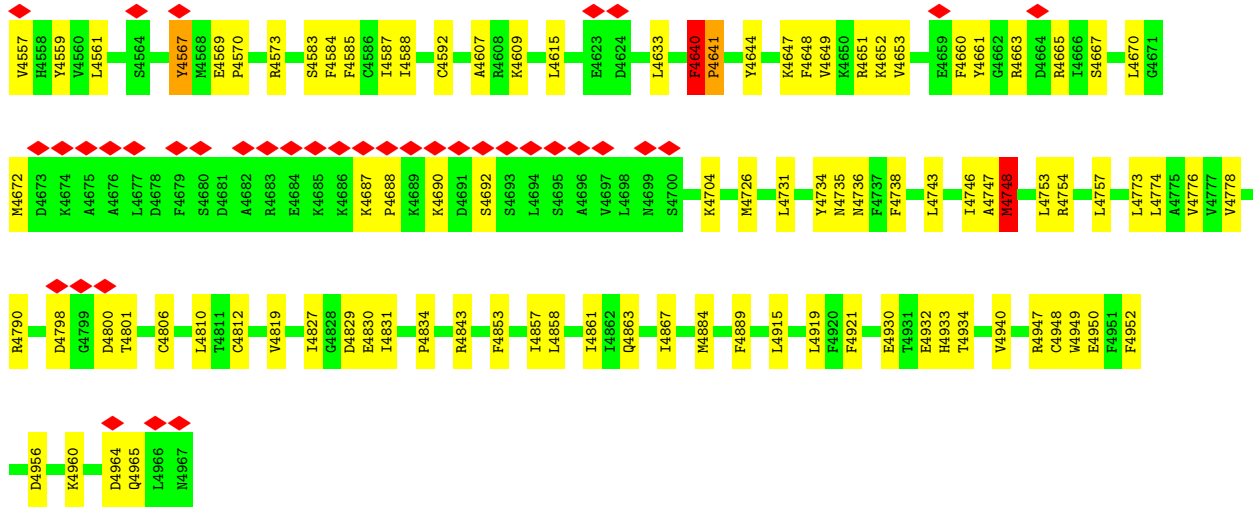


• Molecule 2: Ryanodine receptor 2

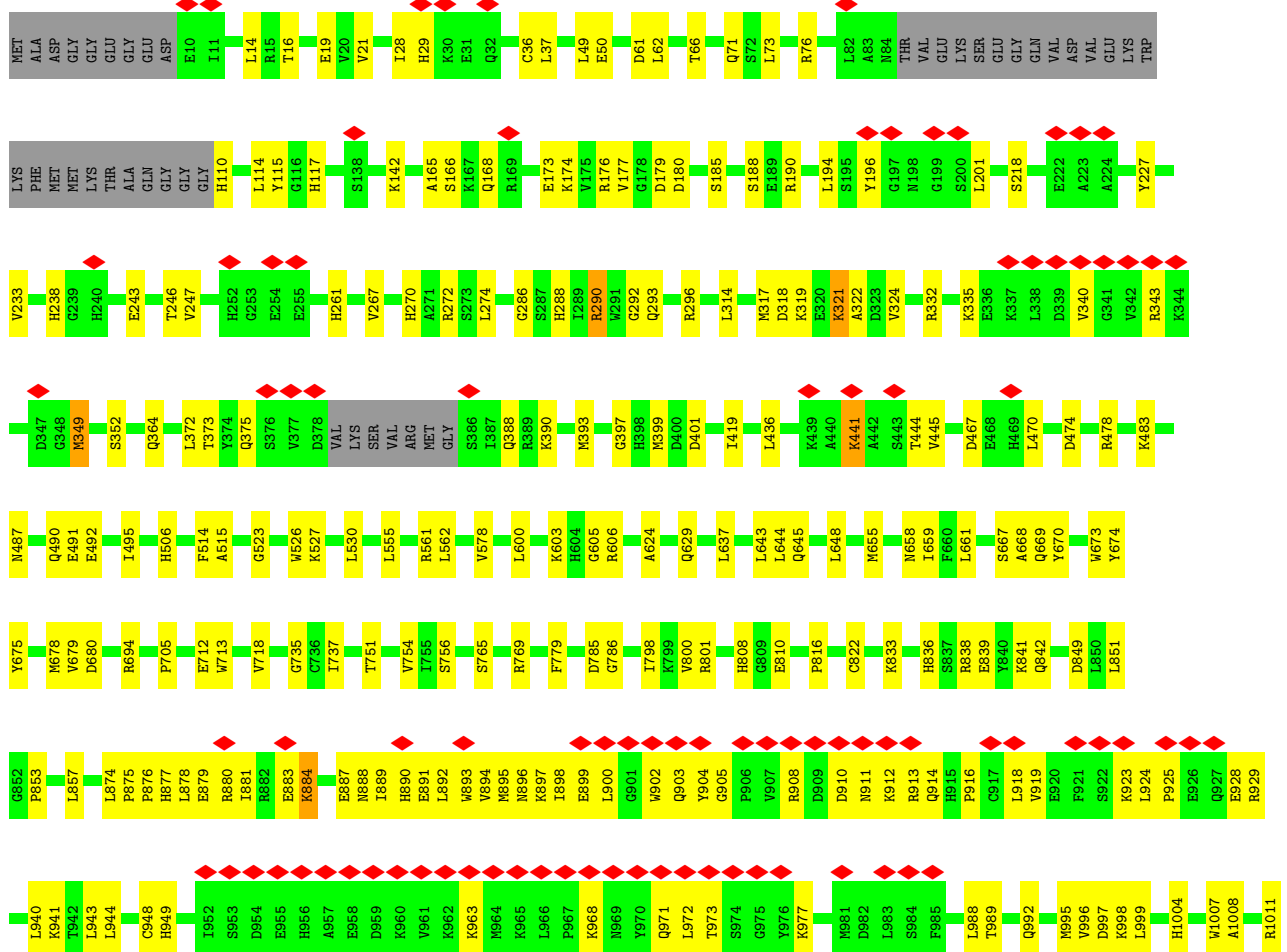




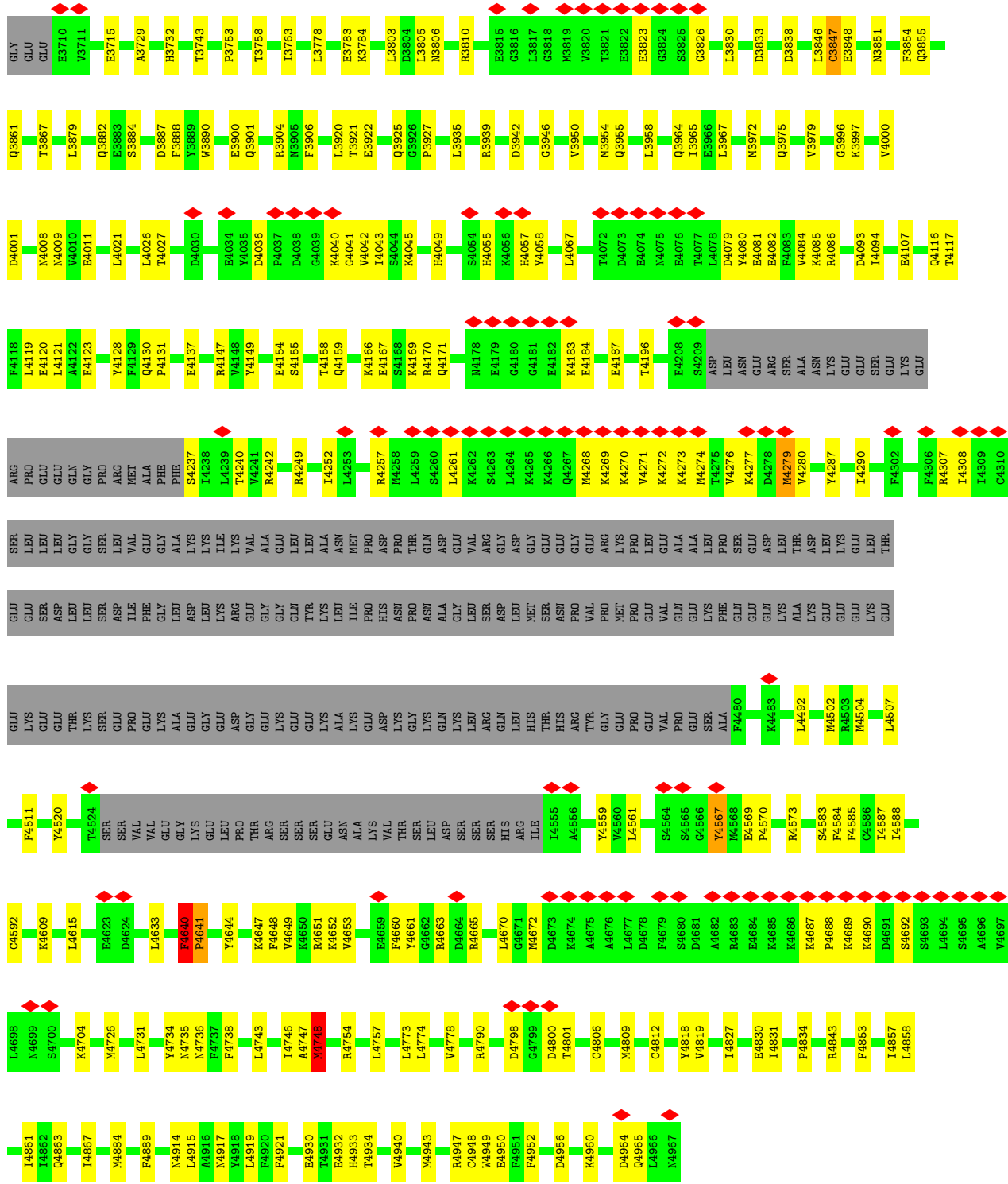




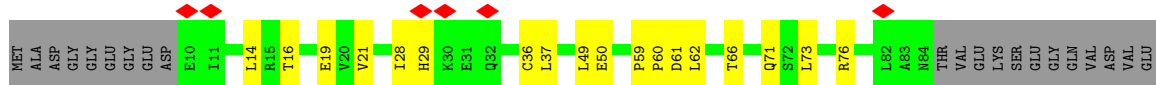
• Molecule 2: Ryanodine receptor 2

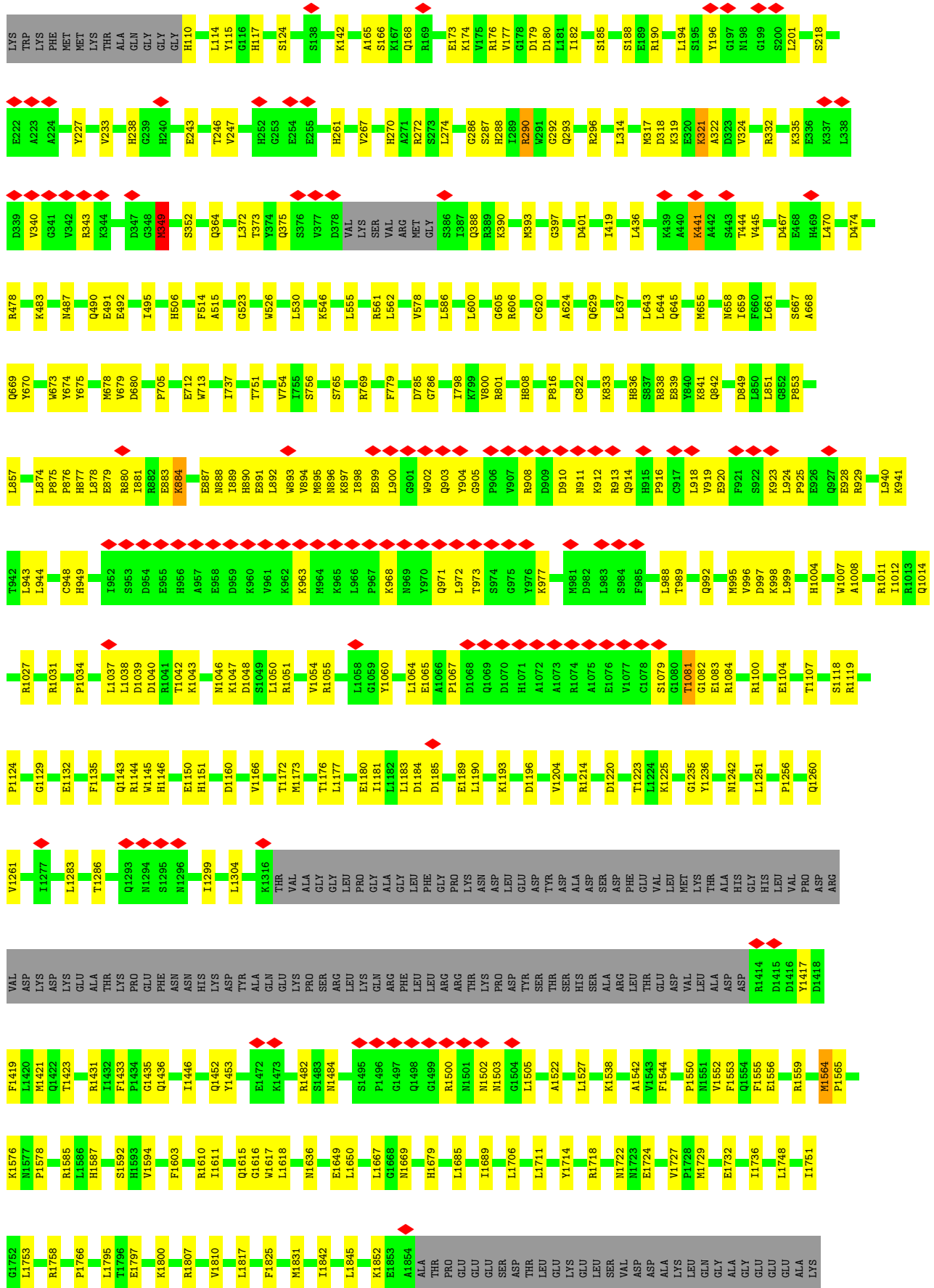


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T2562	G2384	V2227	M2084	H2000	L1910	V1810	I1611	Q1436	PHE	S1295	E1132	Q1014
Q2565	G2385	P2232	V2085	E2001	Q1911	V1817	Q1615	I1446	ASN	F1296	F1135	R1027
R2566	M2388	A2244	L2086	M2004	C1914	L1817	W1616	Q1452	HIS	I1299	Q1143	R1031
T2569	I2422	M2248	L2087	E2010	V1918	F1825	L1618	Y1453	ASP	L1299	R1144	P1034
Q2586	S2425	M2249	Q2091	LEU	R1919	M1831	M1636	E1472	ALA	K1316	R1146	L1037
H2587	L2426	N2250	Y2106	ASP	R1919	I1842	E1649	K1473	VAL	THR	H1146	L1038
L2427	I2427	L2283	L2123	GLY	L1845	L1845	L1650	R1482	GLY	VAL	H1146	D1039
R2590	D2431	E2259	M2134	SER	K1852	K1852	L1482	S1483	LEU	ALA	E1150	D1040
R2591	G2434	P2260	L2146	ASP	D1930	E1853	L1667	N1484	ARG	ALA	H1151	T1042
V2593	V2435	Q2287	M2150	GLY	D1931	A1854	G1668	M1669	PRO	LYS	T1172	R1043
P2606	I2436	N2287	L2157	ASN	F1932	ALA	M1669	P1496	ALA	ALA	M1173	K1043
L2610	K2447	W2290	K2153	SER	K1935	THR	H1679	G1497	GLY	GLY	T1176	M1046
Y2620	D2448	W2290	Y2156	ASP	L1936	PRO	L1685	Q1498	LEU	LEU	T1176	K1047
G2628	M2450	V2293	Q2157	THR	L1936	GLU	L1685	Q1499	PHE	LEU	T1176	D1048
N2629	M2456	E2296	Q2157	ILE	M1939	GLU	I1689	R1500	ARG	PRO	I1181	S1049
F2630	M2457	F2301	L2165	ARG	M1948	SER	L1697	N1501	THR	ASN	L1183	R1051
L2640	A2458	R2302	G2166	LEU	L1951	THR	L1706	G1504	LEU	ASP	D1184	V1054
S2641	G2459	R2303	M2167	LEU	L1957	GLU	Y1714	L1505	LEU	LEU	E1189	R1055
R2642	F2460	E2338	T2170	SER	T1958	LYS	Y1714	A1522	TYR	ASP	L1190	Y1060
K2643	D2463	L2344	V2171	VAL	K1959	GLU	R1718	L1527	THR	ASP	L1064	L1064
L2644	H2464	L2344	M2172	GLU	A1960	GLU	R1718	L1527	SER	ALA	E1065	E1065
F2645	K2465	M2347	E2173	LYS	K1961	LEU	M1722	L1527	HIS	ASP	A1066	A1066
W2646	F2471	M2347	V2174	VAL	T1962	SER	M1722	L1527	SER	SER	P1067	P1067
E2658	I2478	A2350	M2175	THR	R1966	ASP	M1723	K1538	ALA	ASP	V1204	D1068
Q2659	I2478	L2351	V2176	THR	S1967	ASP	E1724	A1542	ARG	PHE	Q1069	Q1069
E2660	L2487	K2352	V2177	LEU	P1968	ALA	V1727	A1542	LEU	LEU	D1070	D1070
F2662	L2487	L2353	V2178	LYS	Q1972	LEU	F1728	F1544	THR	VAL	H1071	H1071
L2676	V2490	S2363	G2181	LYS	I1973	GLN	M1729	V1552	ASP	MET	A1072	A1072
S2683	G2491	P2364	G2182	ALA	L1976	GLY	E1732	F1553	LEU	THR	R1074	R1074
N2684	F2492	N2364	E2183	GLU	L1977	GLY	I1736	Q1554	ALA	ALA	A1075	A1075
T2685	L2493	ASN	S2184	PRO	M1978	LYS	I1736	F1555	HIS	HIS	E1076	E1076
V2686	D2495	GLY	K2185	VAL	F1979	GLU	L1748	E1556	GLY	GLY	V1077	V1077
S2687	L2496	SER	E2186	GLU	K1980	GLU	I1751	R1559	HIS	HIS	C1078	C1078
M2688	R2497	LYS	I2187	SER	D1981	ALA	I1751	R1559	LEU	VAL	S1079	S1079
N2689	S2508	THR	Y2202	ASP	D1982	GLY	G1752	M1564	VAL	VAL	G1080	G1080
E2690	M2512	LEU	F2203	SER	K1983	GLY	L1753	P1565	ASP	PRO	T1081	T1081
K2691	C2204	ASP	R2205	K2054	S1984	LYS	R1758	P1565	ARG	ARG	G1082	G1082
L2820	L2206	GLU	C1986	S2055	C1986	LYS	F1768	M1577	VAL	VAL	E1083	E1083
L2525	I2206	GLU	P1987	Q2056	P1987	ARG	P1578	Q1422	ASP	LYS	R1084	R1084
P2526	M2214	THR	C1988	T2057	C1988	P1889	L1795	Q1422	ASP	ASP	R1100	R1100
E2697	E2377	Q2059	P1989	L2058	P1989	L1893	E1797	T1423	LYS	LYS	E1104	E1104
F2698	E2378	Q2060	R1993	L2059	R1993	M1896	E1797	I1432	GLU	GLU	S1118	S1118
Q2699	D2379	Q2060	M1896	Q2060	M1896	K1897	E1797	I1432	ALA	ALA	R1119	R1119
W2700	D2380	L2221	K1897	L2061	K1897				THR	THR	P1124	P1124
F2701	T2381	L2222							LYS	LYS		



• Molecule 2: Ryanodine receptor 2





Gly	Gly	Lys	Arg	P1889	K1890	L1893	M1896	K1897	L1898	V1902	L1910	Q1911	C1914	V1918	R1919	I1922	V1926	D1930	D1931	F1932	K1935	L1936	M1939	M1948	L1951	L1957	T1958	A1959	K1961	T1962	R1966	S1967	P1968	Q1972	I1973	L1976	L1977	N1978	F1979	K1980	D1981															
D1982	K1983	S1984	E1985	C1986	P1987	P1988	P1989	R1983	L1994	Q1995	L1996	H2000	E2001	M2004	E2010	ASP	LEU	ASP	GLU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	LEU	LEU	SER	VAL	GLU	LYS	VAL	THR	TYR	LEU	LYS	LYS	GLN	ALA	GLU	LYS	PRO	F1979	VAL	GLU	SER						
ASP	SER	K2053	K2054	S2055	S2056	T2057	L2058	Q2059	Q2060	L2061	L2062	L2080	M2084	P2085	V2086	L2087	R2090	Q2091	Y2106	M2123	M2134	L2146	M2150	K2153	Y2156	Q2157	G2165	M2167	T2170	V2171	M2172	E2173	V2174	M2175	V2176	N2177	V2178	G2181	G2182	E2183	S2184	K2185	F2186	L2187												
Y2202	F2203	C2204	R2205	I2206	M2214	Y2220	L2221	L2222	E2223	M2224	G2227	G2228	L2229	P2232	L2240	A2244	M2248	H2249	M2250	L2253	E2259	P2280	S2276	C2277	D2287	W2290	V2293	E2296	F2301	L2302	R2303	R2327	P2328	E2329	E2338	L2344	M2347	A2350	L2351																	
K2352	I2353	S2363	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	T2381	I2382	H2383	K2384	G2385	I2388	M2389	L2408	K2413	I2422	S2425	L2426	L2427	D2431	G2434	V2435	I2436	K2447	D2448	G2449	N2450	A2458	G2459	F2460	D2463	H2464	K2465	F2471										
L2478	L2487	L2488	E2489	V2490	G2491	F2492	L2493	P2494	D2495	L2496	R2497	S2508	M2512	L2520	L2525	L2527	L2548	S2560	L2561	T2562	Q2565	R2566	I2569	Q2586	H2587	R2590	R2591	L2592	V2593	P2606	L2610	Y2620	W2627	G2628	M2629	F2630	L2640	S2641	R2642	K2643	L2644															
F2645	W2646	E2658	Q2659	E2660	L2661	F2662	L2676	S2683	L2684	Y2685	V2686	S2687	M2688	M2689	E2690	K2691	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	L2706	D2707	T2708	S2709	N2710	L2713	P2714	E2715	H2729	W2732	S2733	M2734	D2735	K2736	L2737	N2738	A2739	G2740	W2741	I2742	Y2743	G2744	E2745	L2746	S2747	D2749						
S2750	S2751	K2752	W2753	Q2754	P2755	L2756	K2757	K2758	P2759	Y2760	L2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	E2769	I2770	Y2771	W2772	P2773	L2774	L2775	K2776	L2779	M2782	L2783	Q2784	W2785	G2786	W2787	R2788	K2791	E2794	G2795	D2796	S2797	M2798	A2799	L2800	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL		
SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829	N2830	Y2831	L2832	L2833	L2837	H2838	A2841	M2844	H2849	K2854	K2857	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	L2871	Y2874	D2875	T2876	L2877	K2882	R2886	E2887	K2888	A2889	Q2890	D2891							
L2892	L2893	K2894	R2905	G2906	F2907	K2908	D2909	L2910	P2911	L2912	D2913	T2914	P2915	E2918	K2919	R2920	F2921	Y2923	S2924	F2925	L2926	Q2927	Q2928	L2929	I2930	R2931	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	P2955	Y2956	E2957	Q2958	E2959	L2960	K2961	F2962	K2965	L2968	P2969	D2972	Q2973					
K2976	F2982	A2985	A2986	S2987	R2988	P2989	L2990	P2991	C2991	S2992	G2994	H2995	N2998	K3001	E3002	M3003	S3006	G3009	K3010	V3013	R3016	H3017	R3018	I3019	ARG	THR	ASN	GLN	PRO	D3025	A3026	I3029	H3034	L3035	L3036	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	Y3045	M3046	K3047	T3048	G3049	E3051							
S3052	V3053	K3054	S3055	R3058	A3059	D3062	N3063	A3064	A3065	E3066	D3067	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	Q3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	I3093	I3094	N3095	Q3096	T3097	K3098	V3099	A3100	L3101	L3102	P3103	M3104	L3105	S3106	S3107	F3109	E3110	H3111	I3112	G3113
Q3114	H3115	F3116	F3117	G3118	E3119	D3120	L3121	L3122	L3123	F3124	D3125	V3126	Q3127	Y3131	R3132	L3133	L3134	T3135	A3139	L3140	G3141	T3142	S3143	K3144	Q3145	L3146	L3147	V3148	E3149	R3150	Q3151	R3152	S3153	A3154	L3155	G3156	E3157	G3158	L3159	F3162	A3163	G3164	A3165	F3166	P3167	F3170	L3171	E3172	T3173	H3174	K3177	L3180	Y3181			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.594	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.30	0/1143	0.58	1/1534 (0.1%)
1	J	0.30	0/1143	0.58	1/1534 (0.1%)
1	K	0.30	0/1143	0.58	1/1534 (0.1%)
1	L	0.30	0/1143	0.58	1/1534 (0.1%)
2	A	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	B	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	C	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	D	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
3	E	0.29	0/834	0.54	0/1123
3	F	0.28	0/834	0.53	0/1123
3	G	0.28	0/834	0.54	0/1123
3	H	0.28	0/834	0.54	0/1123
All	All	0.68	28/146284 (0.0%)	0.51	36/197520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3205	CYS	CB-SG	105.30	3.61	1.82
2	B	3205	CYS	CB-SG	105.27	3.61	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3205	CYS	CB-SG	105.27	3.61	1.82
2	C	3205	CYS	CB-SG	105.21	3.61	1.82
2	B	3131	TYR	CD2-CE2	29.66	1.83	1.39
2	A	3131	TYR	CD2-CE2	29.65	1.83	1.39
2	D	3131	TYR	CD2-CE2	29.64	1.83	1.39
2	C	3131	TYR	CD2-CE2	29.62	1.83	1.39
2	B	3131	TYR	CD1-CE1	28.64	1.82	1.39
2	C	3131	TYR	CD1-CE1	28.64	1.82	1.39
2	A	3131	TYR	CD1-CE1	28.61	1.82	1.39
2	D	3131	TYR	CD1-CE1	28.58	1.82	1.39
2	B	3131	TYR	CE2-CZ	21.85	1.67	1.38
2	C	3131	TYR	CE2-CZ	21.85	1.67	1.38
2	A	3131	TYR	CE2-CZ	21.80	1.66	1.38
2	D	3131	TYR	CE2-CZ	21.78	1.66	1.38
2	D	3131	TYR	CE1-CZ	21.53	1.66	1.38
2	A	3131	TYR	CE1-CZ	21.49	1.66	1.38
2	B	3131	TYR	CE1-CZ	21.46	1.66	1.38
2	C	3131	TYR	CE1-CZ	21.44	1.66	1.38
2	B	3131	TYR	CG-CD2	16.68	1.60	1.39
2	D	3131	TYR	CG-CD2	16.68	1.60	1.39
2	C	3131	TYR	CG-CD2	16.67	1.60	1.39
2	A	3131	TYR	CG-CD2	16.64	1.60	1.39
2	A	3131	TYR	CG-CD1	16.39	1.60	1.39
2	D	3131	TYR	CG-CD1	16.38	1.60	1.39
2	B	3131	TYR	CG-CD1	16.38	1.60	1.39
2	C	3131	TYR	CG-CD1	16.34	1.60	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3205	CYS	CA-CB-SG	12.07	135.73	114.00
2	A	3205	CYS	CA-CB-SG	12.06	135.71	114.00
2	D	3205	CYS	CA-CB-SG	12.05	135.68	114.00
2	B	3205	CYS	CA-CB-SG	12.04	135.68	114.00
2	D	2737	LEU	CA-CB-CG	7.16	131.77	115.30
2	A	2737	LEU	CA-CB-CG	7.16	131.76	115.30
2	C	2737	LEU	CA-CB-CG	7.15	131.75	115.30
2	B	2737	LEU	CA-CB-CG	7.15	131.74	115.30
2	D	2860	LEU	CA-CB-CG	6.15	129.44	115.30
2	B	2860	LEU	CA-CB-CG	6.15	129.44	115.30
2	A	2860	LEU	CA-CB-CG	6.14	129.42	115.30
2	C	2860	LEU	CA-CB-CG	6.12	129.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4567	TYR	CB-CG-CD1	6.09	124.65	121.00
2	A	4567	TYR	CB-CG-CD1	6.05	124.63	121.00
2	C	4567	TYR	CB-CG-CD1	6.04	124.62	121.00
2	B	4567	TYR	CB-CG-CD1	5.97	124.58	121.00
1	J	77	MET	CB-CG-SD	5.78	129.75	112.40
1	I	77	MET	CB-CG-SD	5.78	129.74	112.40
1	L	77	MET	CB-CG-SD	5.78	129.73	112.40
1	K	77	MET	CB-CG-SD	5.78	129.74	112.40
2	D	4640	PHE	C-N-CD	-5.38	108.77	120.60
2	A	4640	PHE	C-N-CD	-5.36	108.80	120.60
2	C	4640	PHE	C-N-CD	-5.36	108.81	120.60
2	B	4640	PHE	C-N-CD	-5.35	108.83	120.60
2	B	4748	MET	CB-CG-SD	5.34	128.43	112.40
2	C	4748	MET	CB-CG-SD	5.33	128.39	112.40
2	A	4748	MET	CB-CG-SD	5.33	128.38	112.40
2	D	4748	MET	CB-CG-SD	5.32	128.35	112.40
2	B	4567	TYR	CA-CB-CG	5.13	123.15	113.40
2	C	4567	TYR	CA-CB-CG	5.13	123.14	113.40
2	A	4567	TYR	CA-CB-CG	5.12	123.13	113.40
2	D	4567	TYR	CA-CB-CG	5.12	123.13	113.40
2	C	349	MET	CB-CG-SD	5.09	127.67	112.40
2	D	349	MET	CB-CG-SD	5.09	127.68	112.40
2	A	349	MET	CB-CG-SD	5.08	127.65	112.40
2	B	349	MET	CB-CG-SD	5.08	127.63	112.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2801	TYR	Peptide
2	A	4640	PHE	Peptide
2	B	2801	TYR	Peptide
2	B	4640	PHE	Peptide
2	C	2801	TYR	Peptide
2	C	4640	PHE	Peptide
2	D	2801	TYR	Peptide
2	D	4640	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1131	0	1058	50	0
1	J	1131	0	1058	45	0
1	K	1131	0	1058	47	0
1	L	1131	0	1058	46	0
2	A	33849	0	33549	793	0
2	B	33849	0	33549	790	0
2	C	33849	0	33549	767	0
2	D	33849	0	33549	795	0
3	E	818	0	821	11	0
3	F	818	0	821	11	0
3	G	818	0	821	13	0
3	H	818	0	821	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	62	0	24	1	0
6	B	62	0	24	1	0
6	C	62	0	24	1	0
6	D	62	0	24	1	0
All	All	143464	0	141808	3297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (3297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3131:TYR:CD1	2:D:3131:TYR:CE1	1.82	1.68
2:A:3131:TYR:CD1	2:A:3131:TYR:CE1	1.82	1.63
2:C:3131:TYR:CD2	2:C:3131:TYR:CE2	1.83	1.61
2:C:3131:TYR:CE1	2:C:3131:TYR:CD1	1.82	1.61
2:D:3131:TYR:CE2	2:D:3131:TYR:CD2	1.83	1.61
2:B:3131:TYR:CD2	2:B:3131:TYR:CE2	1.83	1.58
2:B:3131:TYR:CD1	2:B:3131:TYR:CE1	1.82	1.58
2:A:3131:TYR:CE2	2:A:3131:TYR:CD2	1.83	1.58
1:J:127:ARG:NH1	1:J:135:GLY:CA	1.70	1.53
1:K:127:ARG:NH1	1:K:135:GLY:CA	1.70	1.53
1:L:127:ARG:NH1	1:L:135:GLY:CA	1.70	1.50
1:I:127:ARG:NH1	1:I:135:GLY:CA	1.70	1.48
2:A:3131:TYR:CZ	2:A:3205:CYS:SG	2.37	1.17
2:B:3131:TYR:CZ	2:B:3205:CYS:SG	2.37	1.17
2:C:3131:TYR:CZ	2:C:3205:CYS:SG	2.37	1.17
2:A:3131:TYR:CE2	2:A:3205:CYS:SG	2.38	1.17
2:B:3131:TYR:CE2	2:B:3205:CYS:SG	2.38	1.17
2:C:3131:TYR:CE2	2:C:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CE2	2:D:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CZ	2:D:3205:CYS:SG	2.37	1.17
2:A:3848:GLU:OE1	2:A:3922:GLU:CD	1.87	1.13
2:B:3131:TYR:CE1	2:B:3205:CYS:SG	2.42	1.13
2:C:3848:GLU:OE1	2:C:3922:GLU:CD	1.87	1.12
2:A:3131:TYR:CE1	2:A:3205:CYS:SG	2.42	1.12
2:C:3131:TYR:CE1	2:C:3205:CYS:SG	2.42	1.11
2:D:3131:TYR:CE1	2:D:3205:CYS:SG	2.42	1.11
2:A:3131:TYR:CD2	2:A:3205:CYS:SG	2.44	1.11
2:B:3131:TYR:CD2	2:B:3205:CYS:SG	2.43	1.11
2:B:3848:GLU:OE1	2:B:3922:GLU:CD	1.87	1.11
2:D:3848:GLU:OE1	2:D:3922:GLU:CD	1.87	1.11
2:C:3131:TYR:CD2	2:C:3205:CYS:SG	2.43	1.11
2:D:3131:TYR:CD2	2:D:3205:CYS:SG	2.44	1.10
2:C:3131:TYR:CD1	2:C:3205:CYS:SG	2.46	1.09
2:D:3131:TYR:CD1	2:D:3205:CYS:SG	2.46	1.09
2:A:3131:TYR:CD1	2:A:3205:CYS:SG	2.46	1.08
2:B:3131:TYR:CD1	2:B:3205:CYS:SG	2.46	1.08
1:L:127:ARG:NH1	1:L:135:GLY:HA2	0.74	1.07
1:I:127:ARG:NH1	1:I:135:GLY:HA2	0.74	1.07
1:J:127:ARG:NH1	1:J:135:GLY:HA2	0.74	1.06
1:K:127:ARG:NH1	1:K:135:GLY:HA2	0.74	1.06
1:K:127:ARG:CZ	1:K:135:GLY:HA2	1.88	1.03
1:J:127:ARG:CZ	1:J:135:GLY:HA2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ARG:CZ	1:I:135:GLY:HA2	1.88	1.02
1:L:127:ARG:CZ	1:L:135:GLY:HA2	1.88	1.01
2:C:3131:TYR:CG	2:C:3205:CYS:SG	2.53	1.01
2:B:3131:TYR:CG	2:B:3205:CYS:SG	2.53	1.01
2:D:3131:TYR:CG	2:D:3205:CYS:SG	2.53	1.01
2:A:3131:TYR:CG	2:A:3205:CYS:SG	2.53	1.01
2:C:3131:TYR:CZ	2:C:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CZ	2:A:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CE1	2:A:3205:CYS:CB	2.51	0.94
2:B:3131:TYR:CE1	2:B:3205:CYS:CB	2.51	0.94
2:C:3131:TYR:CE2	2:C:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE1	2:D:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CE2	2:A:3205:CYS:CB	2.51	0.93
2:B:3131:TYR:CZ	2:B:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE2	2:D:3205:CYS:CB	2.51	0.93
1:I:127:ARG:HH11	1:I:135:GLY:HA2	1.27	0.93
2:D:3131:TYR:CZ	2:D:3205:CYS:CB	2.51	0.93
1:K:127:ARG:HH11	1:K:135:GLY:HA2	1.27	0.93
2:C:3131:TYR:CD2	2:C:3205:CYS:CB	2.52	0.93
2:C:3131:TYR:CE1	2:C:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CD2	2:A:3205:CYS:CB	2.52	0.92
2:B:3131:TYR:CE2	2:B:3205:CYS:CB	2.51	0.92
1:J:127:ARG:HH11	1:J:135:GLY:HA2	1.27	0.92
2:B:3131:TYR:CD2	2:B:3205:CYS:CB	2.52	0.92
2:D:3131:TYR:CD2	2:D:3205:CYS:CB	2.52	0.91
2:B:3131:TYR:CD1	2:B:3205:CYS:CB	2.54	0.91
2:C:3131:TYR:CD1	2:C:3205:CYS:CB	2.54	0.91
2:A:3131:TYR:CD1	2:A:3205:CYS:CB	2.54	0.90
2:D:3131:TYR:CD1	2:D:3205:CYS:CB	2.54	0.90
1:L:127:ARG:HH11	1:L:135:GLY:HA2	1.27	0.90
2:C:3131:TYR:CG	2:C:3205:CYS:CB	2.56	0.89
2:D:3131:TYR:CG	2:D:3205:CYS:CB	2.56	0.89
2:B:3131:TYR:CG	2:B:3205:CYS:CB	2.56	0.89
2:C:4834:PRO:HB3	2:C:4843:ARG:HD3	1.55	0.88
2:A:3131:TYR:CG	2:A:3205:CYS:CB	2.56	0.88
2:A:4834:PRO:HB3	2:A:4843:ARG:HD3	1.55	0.88
2:D:4834:PRO:HB3	2:D:4843:ARG:HD3	1.55	0.86
2:B:4834:PRO:HB3	2:B:4843:ARG:HD3	1.55	0.85
2:C:2425:SER:O	2:D:142:LYS:NZ	2.08	0.85
2:A:142:LYS:NZ	2:D:2425:SER:O	2.11	0.84
2:D:2512:MET:HA	2:D:2512:MET:HE2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2788:ARG:NH1	2:B:2905:ARG:O	2.12	0.83
2:A:2788:ARG:NH1	2:A:2905:ARG:O	2.12	0.82
2:A:888:ASN:ND2	2:A:1060:TYR:OH	2.13	0.82
2:C:2788:ARG:NH1	2:C:2905:ARG:O	2.12	0.82
2:D:888:ASN:ND2	2:D:1060:TYR:OH	2.13	0.82
2:D:2788:ARG:NH1	2:D:2905:ARG:O	2.12	0.81
2:C:888:ASN:ND2	2:C:1060:TYR:OH	2.13	0.81
2:C:3890:TRP:HB3	2:D:76:ARG:HG2	1.61	0.81
2:D:2773:TRP:HE3	2:D:2776:LYS:HZ3	1.27	0.81
2:B:888:ASN:ND2	2:B:1060:TYR:OH	2.13	0.80
2:C:1559:ARG:HD2	2:C:1565:PRO:HD3	1.64	0.80
2:B:1559:ARG:HD2	2:B:1565:PRO:HD3	1.64	0.80
2:B:2773:TRP:HE3	2:B:2776:LYS:HZ3	1.28	0.79
2:C:2773:TRP:HE3	2:C:2776:LYS:HZ3	1.27	0.79
2:A:76:ARG:HG2	2:D:3890:TRP:HB3	1.64	0.79
2:A:2773:TRP:HE3	2:A:2776:LYS:HZ3	1.28	0.79
2:D:1559:ARG:HD2	2:D:1565:PRO:HD3	1.64	0.78
2:A:1559:ARG:HD2	2:A:1565:PRO:HD3	1.64	0.78
2:B:3183:ILE:HG23	2:B:3184:TYR:HD1	1.49	0.78
3:G:12:ASP:OD2	3:G:15:THR:OG1	2.03	0.77
2:A:3183:ILE:HG23	2:A:3184:TYR:HD1	1.49	0.77
2:C:3183:ILE:HG23	2:C:3184:TYR:HD1	1.49	0.77
2:C:3122:ILE:HD11	2:C:3167:PRO:HD3	1.67	0.77
2:D:3122:ILE:HD11	2:D:3167:PRO:HD3	1.67	0.77
2:D:3183:ILE:HG23	2:D:3184:TYR:HD1	1.49	0.76
3:E:12:ASP:OD2	3:E:15:THR:OG1	2.03	0.76
3:H:12:ASP:OD2	3:H:15:THR:OG1	2.03	0.76
2:A:2512:MET:HE2	2:A:2512:MET:HA	1.68	0.76
2:C:3783:GLU:OE1	2:C:3784:LYS:NZ	2.18	0.76
2:B:2957:GLU:OE1	2:B:2961:LYS:NZ	2.18	0.76
2:B:3122:ILE:HD11	2:B:3167:PRO:HD3	1.67	0.76
3:F:12:ASP:OD2	3:F:15:THR:OG1	2.02	0.76
2:B:2923:TYR:O	2:B:2927:GLN:NE2	2.19	0.76
2:C:2512:MET:HE2	2:C:2512:MET:HA	1.67	0.76
2:C:2923:TYR:O	2:C:2927:GLN:NE2	2.19	0.76
2:D:2923:TYR:O	2:D:2927:GLN:NE2	2.19	0.75
2:A:2923:TYR:O	2:A:2927:GLN:NE2	2.19	0.75
2:A:3122:ILE:HD11	2:A:3167:PRO:HD3	1.67	0.75
2:B:3050:LEU:HD23	2:B:3052:SER:H	1.51	0.75
2:D:3050:LEU:HD23	2:D:3052:SER:H	1.51	0.75
2:C:3050:LEU:HD23	2:C:3052:SER:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2957:GLU:OE1	2:A:2961:LYS:NZ	2.18	0.74
2:A:3222:ALA:O	2:A:3282:LYS:NZ	2.20	0.74
2:B:3783:GLU:OE1	2:B:3784:LYS:NZ	2.18	0.74
2:C:4237:SER:N	2:C:4240:THR:HG1	1.85	0.74
2:A:3050:LEU:HD23	2:A:3052:SER:H	1.51	0.74
2:B:4641:PRO:HB3	2:B:4644:TYR:HB3	1.69	0.74
2:C:4641:PRO:HB3	2:C:4644:TYR:HB3	1.69	0.74
2:D:2957:GLU:OE1	2:D:2961:LYS:NZ	2.18	0.74
2:D:3222:ALA:O	2:D:3282:LYS:NZ	2.20	0.74
2:D:4641:PRO:HB3	2:D:4644:TYR:HB3	1.69	0.74
2:C:2957:GLU:OE1	2:C:2961:LYS:NZ	2.18	0.73
2:B:2512:MET:HE2	2:B:2512:MET:HA	1.68	0.73
2:A:4641:PRO:HB3	2:A:4644:TYR:HB3	1.69	0.73
1:K:117:LEU:HD22	1:K:122:VAL:HG23	1.71	0.73
2:C:3131:TYR:CG	2:C:3205:CYS:HB3	2.23	0.73
1:K:72:MET:HA	1:K:75:ARG:HG2	1.71	0.72
2:D:3131:TYR:CG	2:D:3205:CYS:HB3	2.24	0.72
2:D:1079:SER:OG	2:D:1084:ARG:NH2	2.22	0.72
2:A:3131:TYR:CG	2:A:3205:CYS:HB3	2.23	0.72
2:C:2830:ASN:HB3	2:D:1435:GLY:HA3	1.71	0.72
2:C:3067:ASP:HA	2:C:3070:LYS:HZ3	1.55	0.72
2:C:1079:SER:OG	2:C:1084:ARG:NH2	2.22	0.72
1:L:117:LEU:HD22	1:L:122:VAL:HG23	1.71	0.72
2:B:1079:SER:OG	2:B:1084:ARG:NH2	2.22	0.72
2:C:3222:ALA:O	2:C:3282:LYS:NZ	2.20	0.72
1:J:117:LEU:HD22	1:J:122:VAL:HG23	1.71	0.72
1:L:72:MET:HA	1:L:75:ARG:HG2	1.71	0.72
1:K:137:VAL:HG13	1:K:141:GLU:HB2	1.72	0.71
2:D:3184:TYR:HB3	2:D:3192:ARG:HH21	1.55	0.71
2:A:3783:GLU:OE1	2:A:3784:LYS:NZ	2.18	0.71
2:B:3131:TYR:CG	2:B:3205:CYS:HB3	2.23	0.71
2:D:3131:TYR:CE1	2:D:3205:CYS:HB2	2.25	0.71
2:D:3247:SER:HA	2:D:3250:TRP:HD1	1.56	0.71
2:A:1079:SER:OG	2:A:1084:ARG:NH2	2.22	0.71
2:A:2703:PRO:O	2:A:2854:LYS:NZ	2.23	0.71
1:J:137:VAL:HG13	1:J:141:GLU:HB2	1.72	0.71
2:B:3067:ASP:HA	2:B:3070:LYS:HZ3	1.56	0.71
2:B:3131:TYR:CE1	2:B:3205:CYS:HB2	2.25	0.71
2:D:2703:PRO:O	2:D:2854:LYS:NZ	2.23	0.71
1:J:72:MET:HA	1:J:75:ARG:HG2	1.71	0.71
2:A:3184:TYR:HB3	2:A:3192:ARG:HH21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:VAL:HG13	1:I:141:GLU:HB2	1.72	0.70
2:A:3247:SER:HA	2:A:3250:TRP:HD1	1.56	0.70
2:C:3184:TYR:HB3	2:C:3192:ARG:HH21	1.55	0.70
2:B:188:SER:HB2	2:B:190:ARG:HH11	1.56	0.70
1:I:117:LEU:HD22	1:I:122:VAL:HG23	1.71	0.70
2:C:3247:SER:HA	2:C:3250:TRP:HD1	1.56	0.70
2:A:3131:TYR:CE1	2:A:3205:CYS:HB2	2.25	0.70
2:B:2703:PRO:O	2:B:2854:LYS:NZ	2.23	0.70
1:I:72:MET:HA	1:I:75:ARG:HG2	1.71	0.70
2:B:3222:ALA:O	2:B:3282:LYS:NZ	2.20	0.70
2:B:3247:SER:HA	2:B:3250:TRP:HD1	1.56	0.70
2:A:2998:ASN:ND2	2:A:3048:THR:OG1	2.25	0.70
2:C:3131:TYR:CE1	2:C:3205:CYS:HB2	2.25	0.70
2:A:188:SER:HB2	2:A:190:ARG:HH11	1.57	0.70
1:L:137:VAL:HG13	1:L:141:GLU:HB2	1.72	0.69
2:B:875:PRO:HD2	2:B:878:LEU:HD12	1.74	0.69
2:C:188:SER:HB2	2:C:190:ARG:HH11	1.57	0.69
2:D:2389:MET:HE1	2:D:2460:PHE:HA	1.74	0.69
2:D:2998:ASN:ND2	2:D:3048:THR:OG1	2.25	0.69
2:B:2998:ASN:ND2	2:B:3048:THR:OG1	2.25	0.69
2:B:3184:TYR:HB3	2:B:3192:ARG:HH21	1.55	0.69
2:C:2703:PRO:O	2:C:2854:LYS:NZ	2.23	0.69
2:D:4237:SER:N	2:D:4240:THR:HG1	1.90	0.69
2:C:2998:ASN:ND2	2:C:3048:THR:OG1	2.25	0.69
2:D:188:SER:HB2	2:D:190:ARG:HH11	1.57	0.69
2:D:3067:ASP:HA	2:D:3070:LYS:HZ3	1.57	0.69
2:D:4687:LYS:HD2	2:D:4688:PRO:HD2	1.75	0.69
2:C:288:HIS:O	2:C:290:ARG:NH1	2.26	0.69
2:D:3783:GLU:OE1	2:D:3784:LYS:NZ	2.18	0.69
2:D:875:PRO:HD2	2:D:878:LEU:HD12	1.74	0.68
2:D:4747:ALA:HB1	2:D:4757:LEU:HD11	1.75	0.68
2:B:4687:LYS:HD2	2:B:4688:PRO:HD2	1.75	0.68
2:C:875:PRO:HD2	2:C:878:LEU:HD12	1.74	0.68
2:C:4687:LYS:HD2	2:C:4688:PRO:HD2	1.75	0.68
2:A:3067:ASP:HA	2:A:3070:LYS:HZ2	1.58	0.68
2:C:988:LEU:HD13	2:C:1055:ARG:HE	1.59	0.68
2:C:2389:MET:HE1	2:C:2460:PHE:HA	1.76	0.68
2:A:4687:LYS:HD2	2:A:4688:PRO:HD2	1.75	0.68
2:B:988:LEU:HD13	2:B:1055:ARG:HE	1.59	0.68
2:A:288:HIS:O	2:A:290:ARG:NH1	2.26	0.68
2:B:2389:MET:HE1	2:B:2460:PHE:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4747:ALA:HB1	2:C:4757:LEU:HD11	1.75	0.68
2:A:875:PRO:HD2	2:A:878:LEU:HD12	1.74	0.67
2:B:679:VAL:HG22	2:B:800:VAL:HG12	1.76	0.67
2:B:3890:TRP:HB3	2:C:76:ARG:HG2	1.76	0.67
2:A:3118:GLY:HA2	2:A:3121:LEU:HB3	1.76	0.67
2:A:1435:GLY:H	2:A:1500:ARG:HH22	1.43	0.67
2:C:4640:PHE:CD2	2:C:4641:PRO:HD3	2.30	0.67
2:D:4640:PHE:CD2	2:D:4641:PRO:HD3	2.30	0.67
2:A:988:LEU:HD13	2:A:1055:ARG:HE	1.59	0.67
2:B:4237:SER:N	2:B:4240:THR:HG1	1.92	0.67
2:C:679:VAL:HG22	2:C:800:VAL:HG12	1.77	0.67
2:C:4831:ILE:HG13	2:C:4843:ARG:HH21	1.59	0.67
1:J:137:VAL:HG21	2:B:3587:TRP:CH2	2.30	0.67
2:B:288:HIS:O	2:B:290:ARG:NH1	2.26	0.67
2:B:897:LYS:HD2	2:B:902:TRP:NE1	2.10	0.67
2:A:4237:SER:N	2:A:4240:THR:HG1	1.92	0.67
2:A:4270:LYS:HA	2:A:4273:LYS:HE2	1.77	0.67
2:A:4640:PHE:CD2	2:A:4641:PRO:HD3	2.30	0.67
2:B:4831:ILE:HG13	2:B:4843:ARG:HH21	1.59	0.67
2:D:988:LEU:HD13	2:D:1055:ARG:HE	1.59	0.67
2:D:3253:GLY:HA2	2:D:3264:CYS:HB3	1.77	0.67
2:A:2389:MET:HE1	2:A:2460:PHE:HA	1.77	0.67
2:A:4747:ALA:HB1	2:A:4757:LEU:HD11	1.75	0.67
2:C:897:LYS:HD2	2:C:902:TRP:NE1	2.10	0.67
2:C:3118:GLY:HA2	2:C:3121:LEU:HB3	1.76	0.67
2:D:4651:ARG:NH2	2:D:4672:MET:SD	2.68	0.67
2:A:3253:GLY:HA2	2:A:3264:CYS:HB3	1.77	0.67
2:B:1435:GLY:H	2:B:1500:ARG:HH22	1.43	0.67
2:B:4747:ALA:HB1	2:B:4757:LEU:HD11	1.75	0.67
2:C:3253:GLY:HA2	2:C:3264:CYS:HB3	1.77	0.67
2:D:288:HIS:O	2:D:290:ARG:NH1	2.26	0.67
2:D:3118:GLY:HA2	2:D:3121:LEU:HB3	1.76	0.67
1:I:101:ILE:N	1:I:137:VAL:O	2.25	0.67
2:A:679:VAL:HG22	2:A:800:VAL:HG12	1.77	0.67
2:A:2760:TYR:HA	2:A:2763:LEU:HD13	1.78	0.67
2:D:897:LYS:HD2	2:D:902:TRP:NE1	2.10	0.67
2:D:1435:GLY:H	2:D:1500:ARG:HH22	1.43	0.67
2:D:3142:THR:O	2:D:3144:LYS:NZ	2.28	0.67
2:A:897:LYS:HD2	2:A:902:TRP:NE1	2.10	0.66
2:C:2760:TYR:HA	2:C:2763:LEU:HD13	1.77	0.66
2:D:3848:GLU:OE1	2:D:3922:GLU:OE2	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3142:THR:O	2:C:3144:LYS:NZ	2.28	0.66
2:C:4818:TYR:OH	2:D:4847:ASP:OD2	2.08	0.66
2:D:679:VAL:HG22	2:D:800:VAL:HG12	1.77	0.66
2:A:4120:GLU:HA	2:A:4123:GLU:HG2	1.78	0.66
2:B:4270:LYS:HA	2:B:4273:LYS:HE2	1.77	0.66
2:D:4831:ILE:HG13	2:D:4843:ARG:HH21	1.60	0.66
2:B:4640:PHE:CD2	2:B:4641:PRO:HD3	2.30	0.66
2:C:3250:TRP:HZ2	2:C:3309:LYS:HE3	1.60	0.66
2:A:3848:GLU:OE1	2:A:3922:GLU:OE2	2.13	0.66
2:B:3253:GLY:HA2	2:B:3264:CYS:HB3	1.77	0.66
2:C:2824:ARG:NH2	2:D:1502:ASN:HB3	2.10	0.66
2:C:4270:LYS:HA	2:C:4273:LYS:HE2	1.77	0.66
2:C:4651:ARG:NH2	2:C:4672:MET:SD	2.68	0.66
2:A:185:SER:HG	2:A:188:SER:HG	1.42	0.66
2:A:1172:THR:HB	2:A:1190:LEU:HD11	1.78	0.66
2:A:4831:ILE:HG13	2:A:4843:ARG:HH21	1.59	0.66
2:B:606:ARG:HH11	2:B:644:LEU:HD21	1.61	0.66
2:B:897:LYS:HD2	2:B:902:TRP:CE2	2.31	0.66
2:B:1172:THR:HB	2:B:1190:LEU:HD11	1.78	0.66
2:B:2760:TYR:HA	2:B:2763:LEU:HD13	1.77	0.66
2:B:4651:ARG:NH2	2:B:4672:MET:SD	2.68	0.66
2:C:2928:GLN:OE1	2:C:2931:ARG:NH2	2.29	0.66
2:A:897:LYS:HD2	2:A:902:TRP:CE2	2.31	0.66
2:B:3118:GLY:HA2	2:B:3121:LEU:HB3	1.76	0.66
2:B:3848:GLU:OE1	2:B:3922:GLU:OE2	2.13	0.66
2:C:1172:THR:HB	2:C:1190:LEU:HD11	1.78	0.66
2:C:1242:ASN:HB3	2:C:1807:ARG:HG3	1.77	0.66
2:D:1172:THR:HB	2:D:1190:LEU:HD11	1.78	0.66
2:A:4651:ARG:NH2	2:A:4672:MET:SD	2.68	0.66
2:D:3250:TRP:HZ2	2:D:3309:LYS:HE3	1.60	0.66
2:B:2830:ASN:HB3	2:C:1435:GLY:HA3	1.76	0.66
2:C:3848:GLU:OE1	2:C:3922:GLU:OE2	2.13	0.66
1:J:101:ILE:N	1:J:137:VAL:O	2.25	0.66
2:B:3997:LYS:NZ	2:B:4001:ASP:OD2	2.29	0.66
2:C:606:ARG:HH11	2:C:644:LEU:HD21	1.61	0.66
2:D:606:ARG:HH11	2:D:644:LEU:HD21	1.61	0.66
2:D:2760:TYR:HA	2:D:2763:LEU:HD13	1.78	0.66
2:D:4270:LYS:HA	2:D:4273:LYS:HE2	1.77	0.66
2:A:2928:GLN:OE1	2:A:2931:ARG:NH2	2.29	0.65
2:C:185:SER:HG	2:C:188:SER:HG	1.41	0.65
2:C:1435:GLY:H	2:C:1500:ARG:HH22	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1242:ASN:HB3	2:B:1807:ARG:HG3	1.77	0.65
2:B:2928:GLN:OE1	2:B:2931:ARG:NH2	2.29	0.65
2:C:874:LEU:HD13	2:C:940:LEU:HD13	1.79	0.65
2:D:897:LYS:HD2	2:D:902:TRP:CE2	2.31	0.65
2:A:606:ARG:HH11	2:A:644:LEU:HD21	1.61	0.65
2:A:1910:LEU:HD13	2:A:2062:ILE:HG12	1.79	0.65
1:K:101:ILE:N	1:K:137:VAL:O	2.25	0.65
2:B:3847:CYS:HB3	2:B:3855:GLN:HG3	1.78	0.65
2:C:897:LYS:HD2	2:C:902:TRP:CE2	2.31	0.65
2:D:16:THR:HG1	2:D:110:HIS:N	1.94	0.65
2:D:4120:GLU:HA	2:D:4123:GLU:HG2	1.78	0.65
2:B:1910:LEU:HD13	2:B:2062:ILE:HG12	1.79	0.65
2:B:3250:TRP:HZ2	2:B:3309:LYS:HE3	1.60	0.65
2:B:4120:GLU:HA	2:B:4123:GLU:HG2	1.78	0.65
2:B:16:THR:HG1	2:B:110:HIS:N	1.95	0.65
2:D:2928:GLN:OE1	2:D:2931:ARG:NH2	2.29	0.65
1:L:101:ILE:N	1:L:137:VAL:O	2.25	0.65
2:C:3847:CYS:HB3	2:C:3855:GLN:HG3	1.78	0.65
2:C:3848:GLU:OE2	2:C:3922:GLU:OE1	2.03	0.65
2:B:1936:LEU:HD11	2:B:1976:LEU:HD22	1.79	0.65
2:B:2831:VAL:HB	2:B:2894:LYS:HE3	1.79	0.65
2:C:1910:LEU:HD13	2:C:2062:ILE:HG12	1.79	0.65
2:A:1242:ASN:HB3	2:A:1807:ARG:HG3	1.78	0.65
2:B:185:SER:HG	2:B:188:SER:HG	1.44	0.65
2:C:4120:GLU:HA	2:C:4123:GLU:HG2	1.78	0.65
2:D:185:SER:HG	2:D:188:SER:HG	1.42	0.65
2:A:4822:ARG:NH1	2:B:4829:ASP:OD1	2.29	0.65
2:B:2187:ILE:HG13	2:B:2227:VAL:HG13	1.79	0.65
2:B:2801:TYR:OH	2:C:1496:PRO:O	2.14	0.65
2:D:1910:LEU:HD13	2:D:2062:ILE:HG12	1.79	0.65
2:D:3246:MET:HG2	2:D:3309:LYS:NZ	2.12	0.65
2:A:1936:LEU:HD11	2:A:1976:LEU:HD22	1.79	0.64
2:A:3250:TRP:HZ2	2:A:3309:LYS:HE3	1.60	0.64
2:D:1242:ASN:HB3	2:D:1807:ARG:HG3	1.77	0.64
2:A:874:LEU:HD13	2:A:940:LEU:HD13	1.79	0.64
2:A:3142:THR:O	2:A:3144:LYS:NZ	2.28	0.64
2:C:16:THR:HG1	2:C:110:HIS:N	1.94	0.64
2:C:2831:VAL:HB	2:C:2894:LYS:HE3	1.79	0.64
2:D:2831:VAL:HB	2:D:2894:LYS:HE3	1.79	0.64
2:B:874:LEU:HD13	2:B:940:LEU:HD13	1.79	0.64
2:D:1936:LEU:HD11	2:D:1976:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:THR:HG1	2:A:110:HIS:N	1.95	0.64
2:C:2187:ILE:HG13	2:C:2227:VAL:HG13	1.79	0.64
2:C:3997:LYS:NZ	2:C:4001:ASP:OD2	2.29	0.64
2:A:2187:ILE:HG13	2:A:2227:VAL:HG13	1.79	0.64
2:A:3848:GLU:OE1	2:A:3848:GLU:HA	1.97	0.64
2:B:902:TRP:CD1	2:B:918:LEU:HD12	2.33	0.64
2:B:3246:MET:HG2	2:B:3309:LYS:NZ	2.12	0.64
2:C:4690:LYS:HE3	2:C:4692:SER:HB2	1.80	0.64
2:A:2831:VAL:HB	2:A:2894:LYS:HE3	1.79	0.64
2:A:3246:MET:HG2	2:A:3309:LYS:NZ	2.12	0.64
2:D:2187:ILE:HG13	2:D:2227:VAL:HG13	1.79	0.64
2:A:3260:ARG:HG2	2:A:3263:MET:HB3	1.80	0.64
2:C:3246:MET:HG2	2:C:3309:LYS:NZ	2.12	0.64
2:A:3847:CYS:HB3	2:A:3855:GLN:HG3	1.78	0.64
2:D:3260:ARG:HG2	2:D:3263:MET:HB3	1.80	0.64
2:D:3848:GLU:OE1	2:D:3848:GLU:HA	1.97	0.64
2:D:3997:LYS:NZ	2:D:4001:ASP:OD2	2.29	0.64
2:A:902:TRP:CD1	2:A:918:LEU:HD12	2.33	0.64
2:B:4889:PHE:HD2	2:B:4915:LEU:HD21	1.63	0.64
2:D:3847:CYS:HB3	2:D:3855:GLN:HG3	1.78	0.64
2:A:3997:LYS:NZ	2:A:4001:ASP:OD2	2.29	0.64
2:C:801:ARG:NH1	2:C:1615:GLN:O	2.30	0.64
2:C:3848:GLU:OE1	2:C:3848:GLU:HA	1.97	0.64
2:A:801:ARG:NH1	2:A:1615:GLN:O	2.30	0.63
2:A:4753:LEU:HD23	2:B:4773:LEU:HD13	1.80	0.63
2:B:3142:THR:O	2:B:3144:LYS:NZ	2.28	0.63
2:C:3172:GLU:HG2	2:C:3211:LEU:HD12	1.81	0.63
2:A:3172:GLU:HG2	2:A:3211:LEU:HD12	1.80	0.63
2:B:3260:ARG:HG2	2:B:3263:MET:HB3	1.80	0.63
2:C:1936:LEU:HD11	2:C:1976:LEU:HD22	1.79	0.63
2:D:4690:LYS:HE3	2:D:4692:SER:HB2	1.80	0.63
2:C:3260:ARG:HG2	2:C:3263:MET:HB3	1.80	0.63
2:D:902:TRP:CD1	2:D:918:LEU:HD12	2.33	0.63
2:C:902:TRP:CD1	2:C:918:LEU:HD12	2.33	0.63
2:C:4276:VAL:O	2:C:4279:MET:HG3	1.99	0.63
2:D:4889:PHE:HD2	2:D:4915:LEU:HD21	1.63	0.63
2:B:3172:GLU:HG2	2:B:3211:LEU:HD12	1.81	0.63
2:D:3172:GLU:HG2	2:D:3211:LEU:HD12	1.80	0.63
2:A:4276:VAL:O	2:A:4279:MET:HG3	1.99	0.63
2:B:3848:GLU:OE1	2:B:3848:GLU:HA	1.97	0.63
2:C:655:MET:HE1	2:C:836:HIS:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:893:TRP:O	2:C:897:LYS:HG2	1.99	0.63
2:A:4889:PHE:HD2	2:A:4915:LEU:HD21	1.63	0.62
2:C:2758:LYS:HB2	2:C:2762:LEU:HD23	1.81	0.62
2:C:4045:LYS:HD2	2:C:4067:LEU:HD22	1.81	0.62
2:A:655:MET:HE1	2:A:836:HIS:HA	1.81	0.62
2:A:4690:LYS:HE3	2:A:4692:SER:HB2	1.80	0.62
2:B:4276:VAL:O	2:B:4279:MET:HG3	1.99	0.62
2:B:4690:LYS:HE3	2:B:4692:SER:HB2	1.80	0.62
2:B:4045:LYS:HD2	2:B:4067:LEU:HD22	1.81	0.62
2:D:874:LEU:HD13	2:D:940:LEU:HD13	1.79	0.62
2:D:3188:SER:OG	2:D:3190:ARG:NH1	2.32	0.62
2:B:999:LEU:HB3	2:B:1050:LEU:HD11	1.82	0.62
2:C:2969:PRO:O	2:C:2973:GLN:NE2	2.33	0.62
2:D:999:LEU:HB3	2:D:1050:LEU:HD11	1.82	0.62
2:A:2969:PRO:O	2:A:2973:GLN:NE2	2.33	0.62
2:A:3211:LEU:O	2:A:3215:MET:HG2	1.99	0.62
1:L:110:MET:HA	2:D:3590:LEU:HD21	1.82	0.62
2:B:655:MET:HE1	2:B:836:HIS:HA	1.81	0.62
2:B:2833:LEU:HB3	2:B:2837:LEU:HD11	1.82	0.62
2:C:999:LEU:HB3	2:C:1050:LEU:HD11	1.82	0.62
2:C:4889:PHE:HD2	2:C:4915:LEU:HD21	1.63	0.62
2:D:893:TRP:O	2:D:897:LYS:HG2	1.99	0.62
2:D:4276:VAL:O	2:D:4279:MET:HG3	1.99	0.62
2:A:999:LEU:HB3	2:A:1050:LEU:HD11	1.82	0.62
2:A:3188:SER:OG	2:A:3190:ARG:NH1	2.32	0.62
2:B:3188:SER:OG	2:B:3190:ARG:NH1	2.32	0.62
2:C:2833:LEU:HB3	2:C:2837:LEU:HD11	1.82	0.62
2:D:1048:ASP:HA	2:D:1051:ARG:HG2	1.81	0.62
2:A:2827:ASP:OD2	2:A:2830:ASN:ND2	2.32	0.62
2:B:2758:LYS:HB2	2:B:2762:LEU:HD23	1.81	0.62
2:B:2827:ASP:OD2	2:B:2830:ASN:ND2	2.32	0.62
2:B:3211:LEU:O	2:B:3215:MET:HG2	1.99	0.62
2:C:3188:SER:OG	2:C:3190:ARG:NH1	2.32	0.62
2:D:801:ARG:NH1	2:D:1615:GLN:O	2.30	0.62
2:D:1031:ARG:NH1	6:D:5004:ATP:O3G	2.33	0.62
2:D:2827:ASP:OD2	2:D:2830:ASN:ND2	2.32	0.62
2:D:2969:PRO:O	2:D:2973:GLN:NE2	2.33	0.62
2:A:174:LYS:O	2:A:176:ARG:NH1	2.33	0.62
2:A:1031:ARG:NH1	6:A:5004:ATP:O3G	2.33	0.62
2:B:896:ASN:OD1	2:B:897:LYS:N	2.33	0.62
2:B:3848:GLU:OE2	2:B:3922:GLU:OE1	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3211:LEU:O	2:D:3215:MET:HG2	1.99	0.62
2:B:893:TRP:O	2:B:897:LYS:HG2	1.99	0.62
2:D:655:MET:HE1	2:D:836:HIS:HA	1.80	0.62
2:D:896:ASN:OD1	2:D:897:LYS:N	2.33	0.62
2:A:1119:ARG:NH2	2:A:1196:ASP:OD1	2.33	0.61
2:A:1502:ASN:OD1	2:A:1503:ASN:N	2.33	0.61
2:A:2244:ALA:O	2:A:2248:MET:HB2	2.00	0.61
2:A:2758:LYS:HB2	2:A:2762:LEU:HD23	1.81	0.61
2:C:2827:ASP:OD2	2:C:2830:ASN:ND2	2.32	0.61
2:C:2857:LYS:HA	2:C:2860:LEU:HG	1.82	0.61
2:D:1119:ARG:NH2	2:D:1196:ASP:OD1	2.33	0.61
2:A:893:TRP:O	2:A:897:LYS:HG2	1.99	0.61
2:C:896:ASN:OD1	2:C:897:LYS:N	2.33	0.61
2:C:1048:ASP:HA	2:C:1051:ARG:HG2	1.81	0.61
2:C:1502:ASN:OD1	2:C:1503:ASN:N	2.33	0.61
2:D:4045:LYS:HD2	2:D:4067:LEU:HD22	1.81	0.61
2:A:896:ASN:OD1	2:A:897:LYS:N	2.33	0.61
2:B:1119:ARG:NH2	2:B:1196:ASP:OD1	2.33	0.61
2:A:1048:ASP:HA	2:A:1051:ARG:HG2	1.81	0.61
2:A:3803:LEU:HB2	2:A:3884:SER:HB2	1.83	0.61
2:A:4045:LYS:HD2	2:A:4067:LEU:HD22	1.81	0.61
1:J:137:VAL:HG21	2:B:3587:TRP:HH2	1.66	0.61
2:B:1048:ASP:HA	2:B:1051:ARG:HG2	1.81	0.61
2:B:3192:ARG:HA	2:B:3197:LEU:HD12	1.83	0.61
2:D:174:LYS:O	2:D:176:ARG:NH1	2.33	0.61
2:A:3034:HIS:CE1	2:A:3038:GLN:HE22	2.18	0.61
2:A:3192:ARG:HA	2:A:3197:LEU:HD12	1.83	0.61
2:C:878:LEU:HA	2:C:881:ILE:HG22	1.83	0.61
2:D:878:LEU:HA	2:D:881:ILE:HG22	1.83	0.61
2:B:878:LEU:HA	2:B:881:ILE:HG22	1.83	0.61
2:B:1502:ASN:OD1	2:B:1503:ASN:N	2.33	0.61
2:B:2232:PRO:HB3	2:B:2382:ILE:HD11	1.83	0.61
2:C:3192:ARG:HA	2:C:3197:LEU:HD12	1.83	0.61
2:C:3211:LEU:O	2:C:3215:MET:HG2	2.00	0.61
2:D:2857:LYS:HA	2:D:2860:LEU:HG	1.82	0.61
2:D:3803:LEU:HB2	2:D:3884:SER:HB2	1.83	0.61
2:A:2841:ALA:HB1	2:A:2889:ALA:HB1	1.83	0.61
2:B:2733:SER:O	2:B:2737:LEU:HG	2.01	0.61
2:B:2969:PRO:O	2:B:2973:GLN:NE2	2.33	0.61
2:C:2244:ALA:O	2:C:2248:MET:HB2	2.00	0.61
2:C:3034:HIS:CE1	2:C:3038:GLN:HE22	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2244:ALA:O	2:D:2248:MET:HB2	2.00	0.61
2:D:3034:HIS:CE1	2:D:3038:GLN:HE22	2.18	0.61
2:A:2773:TRP:HB3	2:A:2774:PRO:HD3	1.83	0.61
2:A:2833:LEU:HB3	2:A:2837:LEU:HD11	1.82	0.61
2:B:2841:ALA:HB1	2:B:2889:ALA:HB1	1.83	0.61
2:D:2232:PRO:HB3	2:D:2382:ILE:HD11	1.83	0.61
2:D:2465:LYS:NZ	2:D:2495:ASP:OD2	2.30	0.61
2:D:2758:LYS:HB2	2:D:2762:LEU:HD23	1.81	0.61
2:D:4748:MET:O	2:D:4754:ARG:NH2	2.34	0.61
2:B:3148:VAL:HG13	2:B:3151:GLN:HE21	1.66	0.61
2:C:373:THR:HG21	2:C:397:GLY:HA2	1.83	0.61
2:A:1129:GLY:HA3	2:A:1145:TRP:HB3	1.83	0.61
2:A:2478:ILE:HD13	2:A:2527:LEU:HD11	1.83	0.61
2:A:2857:LYS:HA	2:A:2860:LEU:HG	1.82	0.61
2:A:4187:GLU:OE2	2:A:4947:ARG:NH2	2.34	0.61
2:A:4930:GLU:HA	2:A:4933:HIS:HD2	1.66	0.61
2:B:2244:ALA:O	2:B:2248:MET:HB2	2.00	0.61
2:C:561:ARG:HH11	2:C:561:ARG:HG3	1.66	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:CD2	2.36	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:HD2	1.65	0.61
2:D:2833:LEU:HB3	2:D:2837:LEU:HD11	1.82	0.61
2:A:878:LEU:HA	2:A:881:ILE:HG22	1.83	0.60
2:A:3070:LYS:O	2:A:3074:ASN:ND2	2.34	0.60
2:A:3848:GLU:OE2	2:A:3922:GLU:OE1	2.03	0.60
2:A:4748:MET:O	2:A:4754:ARG:NH2	2.34	0.60
2:C:2733:SER:O	2:C:2737:LEU:HG	2.01	0.60
2:C:3848:GLU:OE1	2:C:3922:GLU:CG	2.49	0.60
2:D:1502:ASN:OD1	2:D:1503:ASN:N	2.33	0.60
2:B:1129:GLY:HA3	2:B:1145:TRP:HB3	1.83	0.60
2:B:3070:LYS:O	2:B:3074:ASN:ND2	2.34	0.60
2:C:174:LYS:O	2:C:176:ARG:NH1	2.33	0.60
2:C:3148:VAL:HG13	2:C:3151:GLN:HE21	1.66	0.60
2:D:2773:TRP:HB3	2:D:2774:PRO:HD3	1.83	0.60
2:D:3070:LYS:O	2:D:3074:ASN:ND2	2.34	0.60
2:D:3148:VAL:HG13	2:D:3151:GLN:HE21	1.66	0.60
2:A:2232:PRO:HB3	2:A:2382:ILE:HD11	1.83	0.60
1:J:110:MET:HA	2:B:3590:LEU:HD21	1.82	0.60
2:B:1031:ARG:NH1	6:B:5004:ATP:O3G	2.33	0.60
2:B:2773:TRP:HB3	2:B:2774:PRO:HD3	1.83	0.60
2:B:2857:LYS:HA	2:B:2860:LEU:HG	1.82	0.60
2:B:3183:ILE:HG23	2:B:3184:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3939:ARG:NH2	2:B:3942:ASP:OD2	2.34	0.60
2:B:4137:GLU:HG2	2:B:4147:ARG:HG2	1.83	0.60
2:C:2232:PRO:HB3	2:C:2382:ILE:HD11	1.83	0.60
2:D:561:ARG:HH11	2:D:561:ARG:HG3	1.66	0.60
2:D:2478:ILE:HD13	2:D:2527:LEU:HD11	1.83	0.60
2:B:561:ARG:HG3	2:B:561:ARG:HH11	1.66	0.60
2:B:2425:SER:O	2:C:142:LYS:NZ	2.33	0.60
2:C:3070:LYS:O	2:C:3074:ASN:ND2	2.34	0.60
2:C:4187:GLU:OE2	2:C:4947:ARG:NH2	2.34	0.60
2:C:1031:ARG:NH1	6:C:5004:ATP:O3G	2.33	0.60
2:C:3803:LEU:HB2	2:C:3884:SER:HB2	1.83	0.60
2:C:4049:HIS:HD2	2:C:4067:LEU:HD11	1.67	0.60
2:C:4137:GLU:HG2	2:C:4147:ARG:HG2	1.83	0.60
2:D:2733:SER:O	2:D:2737:LEU:HG	2.01	0.60
2:A:373:THR:HG21	2:A:397:GLY:HA2	1.83	0.60
2:A:3148:VAL:HG13	2:A:3151:GLN:HE21	1.66	0.60
2:A:4049:HIS:HD2	2:A:4067:LEU:HD11	1.67	0.60
2:A:4829:ASP:OD1	2:D:4822:ARG:NH1	2.35	0.60
2:B:174:LYS:O	2:B:176:ARG:NH1	2.33	0.60
2:B:3803:LEU:HB2	2:B:3884:SER:HB2	1.83	0.60
2:D:3192:ARG:HA	2:D:3197:LEU:HD12	1.83	0.60
2:D:4930:GLU:HA	2:D:4933:HIS:HD2	1.66	0.60
2:B:3034:HIS:CE1	2:B:3038:GLN:HE22	2.18	0.60
2:B:4187:GLU:OE2	2:B:4947:ARG:NH2	2.34	0.60
2:C:3183:ILE:HG23	2:C:3184:TYR:CD1	2.35	0.60
2:C:4748:MET:O	2:C:4754:ARG:NH2	2.34	0.60
2:D:373:THR:HG21	2:D:397:GLY:HA2	1.83	0.60
2:A:2465:LYS:NZ	2:A:2495:ASP:OD2	2.30	0.60
2:A:4930:GLU:HA	2:A:4933:HIS:CD2	2.36	0.60
2:B:2478:ILE:HD13	2:B:2527:LEU:HD11	1.83	0.60
2:B:4049:HIS:HD2	2:B:4067:LEU:HD11	1.67	0.60
2:C:1119:ARG:NH2	2:C:1196:ASP:OD1	2.33	0.60
2:C:2773:TRP:HB3	2:C:2774:PRO:HD3	1.83	0.60
2:D:3304:GLN:HA	2:D:3307:ILE:HG12	1.84	0.60
2:D:4187:GLU:OE2	2:D:4947:ARG:NH2	2.34	0.60
2:A:4137:GLU:HG2	2:A:4147:ARG:HG2	1.83	0.60
2:B:3304:GLN:HA	2:B:3307:ILE:HG12	1.84	0.60
2:C:1129:GLY:HA3	2:C:1145:TRP:HB3	1.83	0.60
2:A:4831:ILE:HG13	2:A:4843:ARG:NH2	2.17	0.60
2:B:4107:GLU:OE2	2:B:4149:TYR:OH	2.15	0.60
2:C:4818:TYR:OH	2:D:4843:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3848:GLU:OE1	2:D:3922:GLU:CG	2.49	0.60
2:A:2733:SER:O	2:A:2737:LEU:HG	2.01	0.59
2:A:3848:GLU:OE1	2:A:3922:GLU:CG	2.49	0.59
2:B:4831:ILE:HG13	2:B:4843:ARG:NH2	2.17	0.59
2:D:2841:ALA:HB1	2:D:2889:ALA:HB1	1.83	0.59
2:D:4831:ILE:HG13	2:D:4843:ARG:NH2	2.17	0.59
2:A:561:ARG:HH11	2:A:561:ARG:HG3	1.66	0.59
2:B:902:TRP:HD1	2:B:918:LEU:HD12	1.67	0.59
2:B:904:TYR:HB2	2:B:918:LEU:HD22	1.85	0.59
2:B:4748:MET:O	2:B:4754:ARG:NH2	2.34	0.59
2:C:2841:ALA:HB1	2:C:2889:ALA:HB1	1.83	0.59
2:C:4492:LEU:HD12	2:C:4592:CYS:SG	2.43	0.59
2:D:997:ASP:HA	2:D:1047:LYS:HE2	1.84	0.59
2:A:2641:SER:HB3	2:A:2676:LEU:HD21	1.84	0.59
2:A:3183:ILE:HG23	2:A:3184:TYR:CD1	2.35	0.59
2:A:4670:LEU:HB2	2:A:4672:MET:HE1	1.84	0.59
2:D:490:GLN:HG2	2:D:495:ILE:HD12	1.84	0.59
2:D:4930:GLU:HA	2:D:4933:HIS:CD2	2.36	0.59
2:A:902:TRP:HD1	2:A:918:LEU:HD12	1.67	0.59
2:A:2338:GLU:OE1	2:A:2338:GLU:N	2.36	0.59
2:B:801:ARG:NH1	2:B:1615:GLN:O	2.30	0.59
2:B:3848:GLU:OE1	2:B:3922:GLU:CG	2.49	0.59
1:L:5:LEU:HD23	1:L:10:ILE:HG13	1.84	0.59
1:K:5:LEU:HD23	1:K:10:ILE:HG13	1.85	0.59
2:C:490:GLN:HG2	2:C:495:ILE:HD12	1.84	0.59
2:D:2641:SER:HB3	2:D:2676:LEU:HD21	1.84	0.59
2:B:2641:SER:HB3	2:B:2676:LEU:HD21	1.85	0.59
2:C:3304:GLN:HA	2:C:3307:ILE:HG12	1.84	0.59
2:C:3317:THR:H	2:C:3320:LEU:HD23	1.67	0.59
2:D:2338:GLU:OE1	2:D:2338:GLU:N	2.36	0.59
2:D:3317:THR:H	2:D:3320:LEU:HD23	1.67	0.59
2:D:4049:HIS:HD2	2:D:4067:LEU:HD11	1.67	0.59
2:A:997:ASP:HA	2:A:1047:LYS:HE2	1.84	0.59
2:B:2338:GLU:OE1	2:B:2338:GLU:N	2.36	0.59
2:B:3317:THR:H	2:B:3320:LEU:HD23	1.67	0.59
2:B:4492:LEU:HD12	2:B:4592:CYS:SG	2.43	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:HD2	1.66	0.59
2:C:997:ASP:HA	2:C:1047:LYS:HE2	1.84	0.59
2:D:902:TRP:HD1	2:D:918:LEU:HD12	1.67	0.59
2:D:1129:GLY:HA3	2:D:1145:TRP:HB3	1.83	0.59
1:I:5:LEU:HD23	1:I:10:ILE:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3304:GLN:HA	2:A:3307:ILE:HG12	1.84	0.59
2:B:373:THR:HG21	2:B:397:GLY:HA2	1.83	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:CD2	2.36	0.59
2:C:2478:ILE:HD13	2:C:2527:LEU:HD11	1.83	0.59
2:C:3939:ARG:NH2	2:C:3942:ASP:OD2	2.34	0.59
2:B:894:VAL:O	2:B:898:ILE:HG12	2.03	0.59
2:B:997:ASP:HA	2:B:1047:LYS:HE2	1.84	0.59
2:B:3131:TYR:CD2	2:B:3205:CYS:HB3	2.38	0.59
2:C:902:TRP:HD1	2:C:918:LEU:HD12	1.67	0.59
2:C:904:TYR:HB2	2:C:918:LEU:HD22	1.85	0.59
2:A:904:TYR:HB2	2:A:918:LEU:HD22	1.85	0.59
2:A:4057:HIS:CE1	2:B:4660:PHE:HZ	2.21	0.59
2:A:4492:LEU:HD12	2:A:4592:CYS:SG	2.42	0.59
2:D:4137:GLU:HG2	2:D:4147:ARG:HG2	1.83	0.59
2:C:894:VAL:O	2:C:898:ILE:HG12	2.03	0.58
2:C:2338:GLU:N	2:C:2338:GLU:OE1	2.36	0.58
2:D:4492:LEU:HD12	2:D:4592:CYS:SG	2.43	0.58
2:A:884:LYS:HA	2:A:887:GLU:HG3	1.86	0.58
2:B:2926:LEU:O	2:B:2930:ILE:HD12	2.04	0.58
2:C:2465:LYS:NZ	2:C:2495:ASP:OD2	2.30	0.58
2:C:4818:TYR:HE1	2:D:4847:ASP:HB2	1.68	0.58
2:D:3939:ARG:NH2	2:D:3942:ASP:OD2	2.34	0.58
2:A:1722:ASN:O	2:A:1919:ARG:NH2	2.36	0.58
2:D:884:LYS:HA	2:D:887:GLU:HG3	1.86	0.58
2:D:1722:ASN:O	2:D:1919:ARG:NH2	2.36	0.58
2:D:3173:THR:O	2:D:3177:LYS:NZ	2.36	0.58
2:A:3317:THR:H	2:A:3320:LEU:HD23	1.67	0.58
1:J:5:LEU:HD23	1:J:10:ILE:HG13	1.85	0.58
2:B:1722:ASN:O	2:B:1919:ARG:NH2	2.36	0.58
2:D:894:VAL:O	2:D:898:ILE:HG12	2.03	0.58
2:D:1100:ARG:HH22	2:D:1235:GLY:HA3	1.69	0.58
2:A:3131:TYR:CD2	2:A:3205:CYS:HB3	2.38	0.58
2:B:2057:THR:OG1	2:B:2060:GLN:OE1	2.20	0.58
2:C:667:SER:HB2	2:C:669:GLN:HE22	1.69	0.58
2:C:884:LYS:HA	2:C:887:GLU:HG3	1.86	0.58
2:C:2982:PHE:O	2:C:3001:LYS:NZ	2.37	0.58
2:C:4831:ILE:HG13	2:C:4843:ARG:NH2	2.17	0.58
2:D:667:SER:HB2	2:D:669:GLN:HE22	1.69	0.58
2:D:904:TYR:HB2	2:D:918:LEU:HD22	1.85	0.58
2:A:490:GLN:HG2	2:A:495:ILE:HD12	1.84	0.58
2:A:2982:PHE:O	2:A:3001:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:GLN:HG2	2:B:495:ILE:HD12	1.84	0.58
2:B:903:GLN:H	2:B:913:ARG:HE	1.52	0.58
2:C:2202:TYR:O	2:C:2206:ILE:HG12	2.04	0.58
2:C:2641:SER:HB3	2:C:2676:LEU:HD21	1.84	0.58
2:D:2202:TYR:O	2:D:2206:ILE:HG12	2.04	0.58
2:D:2736:LYS:HB3	2:D:2741:TRP:HB2	1.86	0.58
2:D:2982:PHE:O	2:D:3001:LYS:NZ	2.37	0.58
2:A:963:LYS:HB3	2:A:977:LYS:HE2	1.86	0.58
2:A:2973:GLN:HA	2:A:2976:LYS:HZ2	1.67	0.58
1:L:42:GLN:HE21	2:D:1957:LEU:HD21	1.68	0.58
2:B:2982:PHE:O	2:B:3001:LYS:NZ	2.37	0.58
2:C:903:GLN:H	2:C:913:ARG:HE	1.52	0.58
2:C:2926:LEU:O	2:C:2930:ILE:HD12	2.04	0.58
2:A:335:LYS:NZ	2:A:401:ASP:OD2	2.37	0.58
2:A:4271:VAL:HG12	2:A:4274:MET:HE3	1.85	0.58
2:A:4518:LEU:HG	2:B:4810:LEU:HD13	1.85	0.58
2:D:903:GLN:H	2:D:913:ARG:HE	1.52	0.58
2:D:905:GLY:HA3	2:D:914:GLN:HB3	1.86	0.58
2:A:1898:LEU:HD22	2:A:1902:VAL:HG11	1.86	0.58
2:A:2736:LYS:HB3	2:A:2741:TRP:HB2	1.86	0.58
2:B:884:LYS:HA	2:B:887:GLU:HG3	1.86	0.58
2:C:1722:ASN:O	2:C:1919:ARG:NH2	2.36	0.58
2:D:247:VAL:O	2:D:272:ARG:NH1	2.37	0.58
2:D:963:LYS:HB3	2:D:977:LYS:HE2	1.86	0.58
2:D:3112:ILE:HG23	2:D:3118:GLY:HA3	1.86	0.58
2:A:247:VAL:O	2:A:272:ARG:NH1	2.37	0.57
2:B:667:SER:HB2	2:B:669:GLN:HE22	1.69	0.57
2:B:963:LYS:HB3	2:B:977:LYS:HE2	1.86	0.57
2:B:1100:ARG:HH22	2:B:1235:GLY:HA3	1.69	0.57
2:C:1100:ARG:HH22	2:C:1235:GLY:HA3	1.69	0.57
2:D:335:LYS:NZ	2:D:401:ASP:OD2	2.37	0.57
2:A:270:HIS:CD2	2:A:491:GLU:HG3	2.39	0.57
2:A:891:GLU:O	2:A:894:VAL:HG22	2.04	0.57
2:A:894:VAL:O	2:A:898:ILE:HG12	2.03	0.57
2:A:3677:THR:O	2:A:3679:LYS:NZ	2.37	0.57
2:B:270:HIS:CD2	2:B:491:GLU:HG3	2.39	0.57
2:B:2465:LYS:NZ	2:B:2495:ASP:OD2	2.30	0.57
2:C:247:VAL:O	2:C:272:ARG:NH1	2.37	0.57
2:C:2123:LEU:HD13	2:C:2167:MET:HG2	1.87	0.57
2:C:3321:PRO:O	2:C:3325:LYS:HG2	2.04	0.57
2:A:903:GLN:H	2:A:913:ARG:HE	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4719:PHE:CE2	2:D:4294:LEU:HD22	2.39	0.57
1:J:106:LEU:HD22	2:B:3587:TRP:HE1	1.70	0.57
2:B:670:TYR:O	2:B:673:TRP:NE1	2.38	0.57
2:B:891:GLU:O	2:B:894:VAL:HG22	2.04	0.57
2:C:891:GLU:O	2:C:894:VAL:HG22	2.04	0.57
2:C:905:GLY:HA3	2:C:914:GLN:HB3	1.86	0.57
2:C:2972:ASP:HA	2:C:3035:ILE:HD11	1.87	0.57
2:C:3112:ILE:HG23	2:C:3118:GLY:HA3	1.86	0.57
2:D:1898:LEU:HD22	2:D:1902:VAL:HG11	1.86	0.57
2:B:335:LYS:NZ	2:B:401:ASP:OD2	2.37	0.57
2:B:2202:TYR:O	2:B:2206:ILE:HG12	2.04	0.57
2:D:2972:ASP:HA	2:D:3035:ILE:HD11	1.87	0.57
2:A:667:SER:HB2	2:A:669:GLN:HE22	1.69	0.57
2:A:1100:ARG:HH22	2:A:1235:GLY:HA3	1.69	0.57
2:A:2972:ASP:HA	2:A:3035:ILE:HD11	1.87	0.57
2:A:3321:PRO:O	2:A:3325:LYS:HG2	2.04	0.57
2:B:247:VAL:O	2:B:272:ARG:NH1	2.37	0.57
2:B:3321:PRO:O	2:B:3325:LYS:HG2	2.04	0.57
2:C:968:LYS:NZ	2:C:971:GLN:O	2.38	0.57
2:C:2057:THR:OG1	2:C:2060:GLN:OE1	2.20	0.57
2:D:2123:LEU:HD13	2:D:2167:MET:HG2	1.86	0.57
2:A:924:LEU:HD12	2:A:925:PRO:HD2	1.86	0.57
2:A:2926:LEU:O	2:A:2930:ILE:HD12	2.04	0.57
2:B:1898:LEU:HD22	2:B:1902:VAL:HG11	1.86	0.57
2:C:670:TYR:O	2:C:673:TRP:NE1	2.38	0.57
2:C:3677:THR:O	2:C:3679:LYS:NZ	2.37	0.57
2:D:670:TYR:O	2:D:673:TRP:NE1	2.38	0.57
2:D:2627:TRP:HB2	2:D:2630:PHE:HB2	1.87	0.57
2:D:3321:PRO:O	2:D:3325:LYS:HG2	2.04	0.57
1:I:102:SER:HA	1:I:136:GLN:HG3	1.87	0.57
2:A:2202:TYR:O	2:A:2206:ILE:HG12	2.04	0.57
2:B:1989:PRO:O	2:B:1993:ARG:HG3	2.05	0.57
2:C:1989:PRO:O	2:C:1993:ARG:HG3	2.05	0.57
2:D:2926:LEU:O	2:D:2930:ILE:HD12	2.04	0.57
2:D:3677:THR:O	2:D:3679:LYS:NZ	2.37	0.57
2:A:4583:SER:O	2:A:4587:ILE:HD12	2.05	0.57
2:B:3677:THR:O	2:B:3679:LYS:NZ	2.37	0.57
2:C:1898:LEU:HD22	2:C:1902:VAL:HG11	1.86	0.57
2:C:3958:LEU:HD22	2:C:3964:GLN:HG3	1.87	0.57
2:D:2973:GLN:HA	2:D:2976:LYS:HZ2	1.69	0.57
2:D:3183:ILE:HG23	2:D:3184:TYR:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3112:ILE:HG23	2:A:3118:GLY:HA3	1.86	0.57
2:A:3173:THR:O	2:A:3177:LYS:NZ	2.36	0.57
2:B:2972:ASP:HA	2:B:3035:ILE:HD11	1.87	0.57
2:C:924:LEU:HD12	2:C:925:PRO:HD2	1.86	0.57
2:C:963:LYS:HB3	2:C:977:LYS:HE2	1.86	0.57
2:C:3163:ALA:HB1	2:C:3245:TYR:HD1	1.70	0.57
2:D:4583:SER:O	2:D:4587:ILE:HD12	2.05	0.57
2:A:3131:TYR:CZ	2:A:3205:CYS:O	2.58	0.57
2:B:1951:LEU:HD11	2:B:1961:LYS:HE3	1.87	0.57
2:C:335:LYS:NZ	2:C:401:ASP:OD2	2.37	0.57
2:D:3163:ALA:HB1	2:D:3245:TYR:HD1	1.70	0.57
2:A:4827:ILE:O	2:A:4831:ILE:HG12	2.05	0.56
2:B:924:LEU:HD12	2:B:925:PRO:HD2	1.86	0.56
2:B:968:LYS:NZ	2:B:971:GLN:O	2.38	0.56
2:B:3958:LEU:HD22	2:B:3964:GLN:HG3	1.87	0.56
2:C:3173:THR:O	2:C:3177:LYS:NZ	2.36	0.56
2:C:4040:LYS:NZ	2:C:4042:VAL:O	2.38	0.56
2:D:924:LEU:HD12	2:D:925:PRO:HD2	1.86	0.56
2:D:968:LYS:NZ	2:D:971:GLN:O	2.38	0.56
2:D:2146:LEU:O	2:D:2150:MET:HG2	2.05	0.56
2:D:3823:GLU:HG3	2:D:3826:GLY:H	1.70	0.56
2:A:670:TYR:O	2:A:673:TRP:NE1	2.38	0.56
2:A:3920:LEU:HD22	2:A:3935:LEU:HD11	1.87	0.56
2:B:1795:LEU:HD23	2:B:1842:ILE:HD11	1.87	0.56
2:B:2610:LEU:HD13	2:B:2644:LEU:HD21	1.87	0.56
2:B:3026:ALA:HA	2:B:3029:ILE:HD12	1.87	0.56
2:C:1732:GLU:HB3	2:C:1753:LEU:HD21	1.87	0.56
2:C:1795:LEU:HD23	2:C:1842:ILE:HD11	1.87	0.56
2:D:3920:LEU:HD22	2:D:3935:LEU:HD11	1.87	0.56
2:D:4040:LYS:NZ	2:D:4042:VAL:O	2.38	0.56
2:A:705:PRO:HD3	2:A:857:LEU:HD13	1.87	0.56
2:A:905:GLY:HA3	2:A:914:GLN:HB3	1.86	0.56
2:A:1435:GLY:HA3	2:D:2830:ASN:HB3	1.87	0.56
2:A:1732:GLU:HB3	2:A:1753:LEU:HD21	1.87	0.56
2:A:2123:LEU:HD13	2:A:2167:MET:HG2	1.87	0.56
2:A:2627:TRP:HB2	2:A:2630:PHE:HB2	1.87	0.56
2:A:3823:GLU:HG3	2:A:3826:GLY:H	1.70	0.56
1:L:102:SER:HA	1:L:136:GLN:HG3	1.87	0.56
1:L:102:SER:OG	1:L:105:GLU:OE1	2.22	0.56
2:B:905:GLY:HA3	2:B:914:GLN:HB3	1.86	0.56
2:B:4827:ILE:O	2:B:4831:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:HIS:CD2	2:C:491:GLU:HG3	2.39	0.56
2:C:3823:GLU:HG3	2:C:3826:GLY:H	1.70	0.56
2:C:4827:ILE:O	2:C:4831:ILE:HG12	2.05	0.56
2:D:270:HIS:CD2	2:D:491:GLU:HG3	2.39	0.56
2:D:3026:ALA:HA	2:D:3029:ILE:HD12	1.87	0.56
2:A:3163:ALA:HB1	2:A:3245:TYR:HD1	1.70	0.56
2:B:2123:LEU:HD13	2:B:2167:MET:HG2	1.87	0.56
2:B:3253:GLY:C	2:B:3255:GLU:H	2.09	0.56
2:B:3823:GLU:HG3	2:B:3826:GLY:H	1.70	0.56
2:C:1951:LEU:HD11	2:C:1961:LYS:HE3	1.87	0.56
2:C:4819:VAL:HG12	2:C:4830:GLU:HG3	1.88	0.56
2:D:3131:TYR:CZ	2:D:3205:CYS:O	2.58	0.56
2:A:3939:ARG:NH2	2:A:3942:ASP:OD2	2.34	0.56
2:B:1732:GLU:HB3	2:B:1753:LEU:HD21	1.87	0.56
2:B:3246:MET:HG2	2:B:3309:LYS:HZ2	1.68	0.56
2:B:4040:LYS:NZ	2:B:4042:VAL:O	2.38	0.56
2:C:4583:SER:O	2:C:4587:ILE:HD12	2.05	0.56
2:D:891:GLU:O	2:D:894:VAL:HG22	2.04	0.56
2:A:968:LYS:NZ	2:A:971:GLN:O	2.38	0.56
2:B:4583:SER:O	2:B:4587:ILE:HD12	2.05	0.56
2:C:705:PRO:HD3	2:C:857:LEU:HD13	1.87	0.56
2:C:3846:LEU:HB3	2:C:3854:PHE:CE2	2.41	0.56
2:D:3152:ARG:HD2	2:D:3232:PRO:HB2	1.87	0.56
2:A:2610:LEU:HD13	2:A:2644:LEU:HD21	1.87	0.56
2:A:3152:ARG:HD2	2:A:3232:PRO:HB2	1.87	0.56
2:A:4040:LYS:NZ	2:A:4042:VAL:O	2.38	0.56
1:K:102:SER:OG	1:K:105:GLU:OE1	2.22	0.56
2:B:1500:ARG:HG3	2:B:1505:LEU:HB2	1.88	0.56
2:B:2172:MET:HA	2:B:2172:MET:HE3	1.88	0.56
2:B:2736:LYS:HB3	2:B:2741:TRP:HB2	1.86	0.56
2:B:3112:ILE:HG23	2:B:3118:GLY:HA3	1.86	0.56
2:B:3163:ALA:HB1	2:B:3245:TYR:HD1	1.70	0.56
2:B:3846:LEU:HB3	2:B:3854:PHE:CE2	2.41	0.56
2:C:2627:TRP:HB2	2:C:2630:PHE:HB2	1.87	0.56
2:C:2736:LYS:HB3	2:C:2741:TRP:HB2	1.86	0.56
2:D:2610:LEU:HD13	2:D:2644:LEU:HD21	1.87	0.56
2:D:3958:LEU:HD22	2:D:3964:GLN:HG3	1.87	0.56
1:J:102:SER:HA	1:J:136:GLN:HG3	1.87	0.56
1:K:102:SER:HA	1:K:136:GLN:HG3	1.87	0.56
2:B:705:PRO:HD3	2:B:857:LEU:HD13	1.87	0.56
2:B:4819:VAL:HG12	2:B:4830:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2610:LEU:HD13	2:C:2644:LEU:HD21	1.87	0.56
2:C:3152:ARG:HD2	2:C:3232:PRO:HB2	1.87	0.56
2:C:3235:MET:HB2	2:C:3239:LEU:HD12	1.88	0.56
2:A:2146:LEU:O	2:A:2150:MET:HG2	2.05	0.56
2:A:3026:ALA:HA	2:A:3029:ILE:HD12	1.87	0.56
1:J:122:VAL:O	1:J:126:ILE:HG23	2.06	0.56
1:K:122:VAL:O	1:K:126:ILE:HG23	2.06	0.56
2:B:3173:THR:O	2:B:3177:LYS:NZ	2.36	0.56
2:C:1500:ARG:HG3	2:C:1505:LEU:HB2	1.88	0.56
2:C:3729:ALA:HA	2:C:3732:HIS:CD2	2.41	0.56
2:A:3253:GLY:C	2:A:3255:GLU:H	2.09	0.56
2:A:3729:ALA:HA	2:A:3732:HIS:CD2	2.41	0.56
2:B:3013:VAL:O	2:B:3018:ARG:NH2	2.40	0.56
2:C:3920:LEU:HD22	2:C:3935:LEU:HD11	1.87	0.56
2:D:3192:ARG:HD3	2:D:3199:THR:HG22	1.87	0.56
2:D:3235:MET:HB2	2:D:3239:LEU:HD12	1.88	0.56
2:D:3846:LEU:HB3	2:D:3854:PHE:CE2	2.41	0.56
1:I:5:LEU:HB3	1:I:10:ILE:HD11	1.88	0.55
2:A:1989:PRO:O	2:A:1993:ARG:HG3	2.05	0.55
2:A:3013:VAL:O	2:A:3018:ARG:NH2	2.39	0.55
2:A:3846:LEU:HB3	2:A:3854:PHE:CE2	2.41	0.55
3:F:83:TYR:HB3	3:F:87:GLY:HA2	1.88	0.55
1:J:5:LEU:HB3	1:J:10:ILE:HD11	1.88	0.55
2:B:16:THR:OG1	2:B:110:HIS:N	2.39	0.55
2:B:2146:LEU:O	2:B:2150:MET:HG2	2.05	0.55
1:I:122:VAL:O	1:I:126:ILE:HG23	2.06	0.55
2:A:1951:LEU:HD11	2:A:1961:LYS:HE3	1.87	0.55
2:A:2057:THR:OG1	2:A:2060:GLN:OE1	2.20	0.55
2:A:2512:MET:HA	2:A:2512:MET:CE	2.35	0.55
2:B:514:PHE:CD2	2:B:526:TRP:HB2	2.41	0.55
2:B:2627:TRP:HB2	2:B:2630:PHE:HB2	1.87	0.55
2:B:3131:TYR:CZ	2:B:3205:CYS:O	2.58	0.55
2:C:2961:LYS:HB2	2:C:2965:LYS:NZ	2.21	0.55
2:C:3192:ARG:HD3	2:C:3199:THR:HG22	1.87	0.55
2:C:3253:GLY:C	2:C:3255:GLU:H	2.09	0.55
2:D:705:PRO:HD3	2:D:857:LEU:HD13	1.87	0.55
2:D:1795:LEU:HD23	2:D:1842:ILE:HD11	1.87	0.55
2:D:1989:PRO:O	2:D:1993:ARG:HG3	2.05	0.55
2:D:2961:LYS:HB2	2:D:2965:LYS:NZ	2.21	0.55
2:D:3729:ALA:HA	2:D:3732:HIS:CD2	2.41	0.55
2:D:3848:GLU:OE2	2:D:3922:GLU:OE1	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3958:LEU:HD22	2:A:3964:GLN:HG3	1.87	0.55
2:B:2961:LYS:HB2	2:B:2965:LYS:NZ	2.21	0.55
2:C:798:ILE:HD12	2:C:800:VAL:HG22	1.88	0.55
2:A:1795:LEU:HD23	2:A:1842:ILE:HD11	1.87	0.55
2:A:2961:LYS:HB2	2:A:2965:LYS:NZ	2.21	0.55
3:G:83:TYR:HB3	3:G:87:GLY:HA2	1.89	0.55
3:H:83:TYR:HB3	3:H:87:GLY:HA2	1.88	0.55
1:L:122:VAL:O	1:L:126:ILE:HG23	2.06	0.55
1:K:107:ARG:NH2	1:K:119:ASP:OD2	2.40	0.55
2:C:3131:TYR:CZ	2:C:3205:CYS:O	2.58	0.55
2:D:514:PHE:CD2	2:D:526:TRP:HB2	2.41	0.55
2:D:3591:LEU:HB3	2:D:3595:ARG:NH1	2.22	0.55
2:D:4271:VAL:HG12	2:D:4274:MET:HE3	1.86	0.55
2:A:3131:TYR:CD1	2:A:3205:CYS:HB2	2.41	0.55
2:B:2512:MET:HA	2:B:2512:MET:CE	2.35	0.55
2:C:514:PHE:CD2	2:C:526:TRP:HB2	2.41	0.55
2:C:4271:VAL:HG12	2:C:4274:MET:HE3	1.89	0.55
2:D:1732:GLU:HB3	2:D:1753:LEU:HD21	1.87	0.55
2:B:3152:ARG:HD2	2:B:3232:PRO:HB2	1.87	0.55
2:B:3591:LEU:HB3	2:B:3595:ARG:NH1	2.22	0.55
2:B:3920:LEU:HD22	2:B:3935:LEU:HD11	1.87	0.55
2:C:2146:LEU:O	2:C:2150:MET:HG2	2.05	0.55
2:D:798:ILE:HD12	2:D:800:VAL:HG22	1.88	0.55
2:D:3013:VAL:O	2:D:3018:ARG:NH2	2.40	0.55
1:L:107:ARG:NH2	1:L:119:ASP:OD2	2.40	0.55
1:K:5:LEU:HB3	1:K:10:ILE:HD11	1.88	0.55
2:B:3192:ARG:HD3	2:B:3199:THR:HG22	1.87	0.55
2:C:2448:ASP:OD2	2:C:2450:ASN:ND2	2.40	0.55
2:C:4670:LEU:HB2	2:C:4672:MET:HE1	1.87	0.55
2:D:4819:VAL:HG12	2:D:4830:GLU:HG3	1.88	0.55
2:D:4827:ILE:O	2:D:4831:ILE:HG12	2.05	0.55
2:A:1500:ARG:HG3	2:A:1505:LEU:HB2	1.88	0.55
2:A:2923:TYR:HA	2:A:3003:MET:HE1	1.89	0.55
2:C:3026:ALA:HA	2:C:3029:ILE:HD12	1.87	0.55
2:C:3227:ARG:HD2	2:C:3228:TYR:H	1.72	0.55
2:D:2448:ASP:OD2	2:D:2450:ASN:ND2	2.40	0.55
2:D:2732:TRP:O	2:D:2736:LYS:HG3	2.07	0.55
2:A:514:PHE:CD2	2:A:526:TRP:HB2	2.41	0.55
2:A:1007:TRP:O	2:A:1011:ARG:HG2	2.07	0.55
2:A:2448:ASP:OD2	2:A:2450:ASN:ND2	2.40	0.55
2:B:3729:ALA:HA	2:B:3732:HIS:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2512:MET:HA	2:C:2512:MET:CE	2.35	0.55
2:C:2923:TYR:HA	2:C:3003:MET:HE1	1.87	0.55
2:C:3322:LEU:HD12	2:C:3323:MET:HG3	1.89	0.55
2:D:1951:LEU:HD11	2:D:1961:LYS:HE3	1.87	0.55
2:A:246:THR:HG21	2:A:267:VAL:HG11	1.89	0.55
2:A:3131:TYR:OH	2:A:3205:CYS:O	2.23	0.55
2:A:4819:VAL:HG12	2:A:4830:GLU:HG3	1.88	0.55
1:J:102:SER:OG	1:J:105:GLU:OE1	2.22	0.55
1:J:107:ARG:NH2	1:J:119:ASP:OD2	2.40	0.55
2:B:2732:TRP:O	2:B:2736:LYS:HG3	2.07	0.55
2:B:3227:ARG:HD2	2:B:3228:TYR:H	1.72	0.55
2:B:3235:MET:HB2	2:B:3239:LEU:HD12	1.88	0.55
2:C:2436:ILE:HG22	2:C:2491:GLY:HA3	1.89	0.55
2:D:1007:TRP:O	2:D:1011:ARG:HG2	2.07	0.55
2:D:2918:GLU:HA	2:D:2923:TYR:CD1	2.42	0.55
2:D:3227:ARG:HD2	2:D:3228:TYR:H	1.72	0.55
1:I:102:SER:OG	1:I:105:GLU:OE1	2.22	0.54
2:A:629:GLN:OE1	2:A:1669:ASN:ND2	2.37	0.54
2:A:2732:TRP:O	2:A:2736:LYS:HG3	2.07	0.54
2:A:2918:GLU:HA	2:A:2923:TYR:CD1	2.42	0.54
2:A:4169:LYS:HE3	2:A:4170:ARG:HH22	1.72	0.54
3:E:83:TYR:HB3	3:E:87:GLY:HA2	1.89	0.54
2:B:4271:VAL:HG12	2:B:4274:MET:HE3	1.87	0.54
2:A:16:THR:OG1	2:A:110:HIS:N	2.39	0.54
2:A:849:ASP:OD1	2:A:1214:ARG:NE	2.37	0.54
2:A:3192:ARG:HD3	2:A:3199:THR:HG22	1.87	0.54
2:B:2918:GLU:HA	2:B:2923:TYR:CD1	2.42	0.54
2:C:2171:VAL:HA	2:C:2174:VAL:HG22	1.89	0.54
2:C:3591:LEU:HB3	2:C:3595:ARG:NH1	2.22	0.54
2:D:4169:LYS:HE3	2:D:4170:ARG:HH22	1.72	0.54
2:A:562:LEU:HG	2:A:600:LEU:HD13	1.89	0.54
2:A:2436:ILE:HG22	2:A:2491:GLY:HA3	1.89	0.54
2:A:3591:LEU:HB3	2:A:3595:ARG:NH1	2.22	0.54
1:L:5:LEU:HB3	1:L:10:ILE:HD11	1.88	0.54
2:B:296:ARG:HH21	2:B:324:VAL:HA	1.73	0.54
2:B:839:GLU:HB3	2:B:851:LEU:HD12	1.88	0.54
2:C:3901:GLN:OE1	2:C:3904:ARG:NH1	2.40	0.54
2:D:1500:ARG:HG3	2:D:1505:LEU:HB2	1.88	0.54
2:D:2057:THR:OG1	2:D:2060:GLN:OE1	2.20	0.54
2:D:3253:GLY:C	2:D:3255:GLU:H	2.09	0.54
2:D:3322:LEU:HD12	2:D:3323:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:ASP:OD1	2:A:3298:ARG:NH1	2.39	0.54
2:A:555:LEU:HD21	2:A:578:VAL:HG11	1.90	0.54
2:A:798:ILE:HD12	2:A:800:VAL:HG22	1.88	0.54
2:A:3322:LEU:HD12	2:A:3323:MET:HG3	1.89	0.54
2:A:4107:GLU:OE2	2:A:4149:TYR:OH	2.15	0.54
2:B:246:THR:HG21	2:B:267:VAL:HG11	1.89	0.54
2:B:555:LEU:HD21	2:B:578:VAL:HG11	1.90	0.54
2:B:798:ILE:HD12	2:B:800:VAL:HG22	1.88	0.54
2:B:2436:ILE:HG22	2:B:2491:GLY:HA3	1.90	0.54
2:B:3322:LEU:HD12	2:B:3323:MET:HG3	1.89	0.54
2:B:4169:LYS:HE3	2:B:4170:ARG:HH22	1.72	0.54
2:D:2171:VAL:HA	2:D:2174:VAL:HG22	1.89	0.54
2:D:2436:ILE:HG22	2:D:2491:GLY:HA3	1.89	0.54
2:A:839:GLU:HB3	2:A:851:LEU:HD12	1.88	0.54
2:A:3235:MET:HB2	2:A:3239:LEU:HD12	1.88	0.54
2:A:3312:PRO:HA	2:A:3315:LEU:HB2	1.89	0.54
2:B:2171:VAL:HA	2:B:2174:VAL:HG22	1.89	0.54
2:B:2923:TYR:HA	2:B:3003:MET:HE1	1.89	0.54
2:C:16:THR:OG1	2:C:110:HIS:N	2.39	0.54
2:C:562:LEU:HG	2:C:600:LEU:HD13	1.89	0.54
2:C:3283:ILE:O	2:C:3287:ASN:HB2	2.08	0.54
2:C:4169:LYS:HE3	2:C:4170:ARG:HH22	1.72	0.54
2:D:1842:ILE:HD12	2:D:1845:LEU:HD12	1.90	0.54
2:A:1124:PRO:HD2	2:A:1594:VAL:HG23	1.90	0.54
2:A:2171:VAL:HA	2:A:2174:VAL:HG22	1.89	0.54
1:J:100:TYR:CD1	1:J:138:ASN:HB3	2.43	0.54
2:B:238:HIS:HB3	2:B:243:GLU:HG3	1.90	0.54
2:B:562:LEU:HG	2:B:600:LEU:HD13	1.89	0.54
2:D:16:THR:OG1	2:D:110:HIS:N	2.39	0.54
2:D:839:GLU:HB3	2:D:851:LEU:HD12	1.88	0.54
2:D:4633:LEU:O	2:D:4704:LYS:NZ	2.41	0.54
2:B:1007:TRP:O	2:B:1011:ARG:HG2	2.07	0.54
2:B:2448:ASP:OD2	2:B:2450:ASN:ND2	2.40	0.54
2:B:3901:GLN:OE1	2:B:3904:ARG:NH1	2.41	0.54
2:C:2918:GLU:HA	2:C:2923:TYR:CD1	2.42	0.54
2:D:842:GLN:HB2	2:D:1603:PHE:HB2	1.90	0.54
2:D:3283:ILE:O	2:D:3287:ASN:HB2	2.08	0.54
2:D:3950:VAL:O	2:D:3954:MET:HB2	2.08	0.54
2:A:296:ARG:HH21	2:A:324:VAL:HA	1.72	0.54
2:C:238:HIS:HB3	2:C:243:GLU:HG3	1.90	0.54
2:C:849:ASP:OD1	2:C:1214:ARG:NE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2732:TRP:O	2:C:2736:LYS:HG3	2.07	0.54
2:C:3131:TYR:CD2	2:C:3205:CYS:HB3	2.38	0.54
2:C:3950:VAL:O	2:C:3954:MET:HB2	2.08	0.54
1:I:107:ARG:NH2	1:I:119:ASP:OD2	2.40	0.54
2:A:3227:ARG:HD2	2:A:3228:TYR:H	1.72	0.54
2:B:842:GLN:HB2	2:B:1603:PHE:HB2	1.90	0.54
2:A:1435:GLY:H	2:A:1500:ARG:NH2	2.06	0.54
2:A:3950:VAL:O	2:A:3954:MET:HB2	2.08	0.54
1:K:100:TYR:CD1	1:K:138:ASN:HB3	2.43	0.54
2:C:296:ARG:HH21	2:C:324:VAL:HA	1.72	0.54
2:C:839:GLU:HB3	2:C:851:LEU:HD12	1.89	0.54
2:C:1124:PRO:HD2	2:C:1594:VAL:HG23	1.90	0.54
2:C:1842:ILE:HD12	2:C:1845:LEU:HD12	1.90	0.54
2:D:296:ARG:HH21	2:D:324:VAL:HA	1.72	0.54
2:D:562:LEU:HG	2:D:600:LEU:HD13	1.89	0.54
2:D:996:VAL:HG22	2:D:1054:VAL:HG21	1.89	0.54
2:D:2172:MET:HA	2:D:2172:MET:HE3	1.90	0.54
2:D:2593:VAL:HG12	2:D:2644:LEU:HB2	1.90	0.54
2:D:3901:GLN:OE1	2:D:3904:ARG:NH1	2.41	0.54
1:I:19:LEU:HD11	2:A:3595:ARG:HH21	1.73	0.53
2:A:605:GLY:HA2	2:A:1585:ARG:HD2	1.91	0.53
2:A:2172:MET:HA	2:A:2172:MET:HE3	1.90	0.53
2:A:3901:GLN:OE1	2:A:3904:ARG:NH1	2.41	0.53
2:B:713:TRP:HH2	2:B:1251:LEU:HD21	1.73	0.53
2:C:246:THR:HG21	2:C:267:VAL:HG11	1.89	0.53
2:C:555:LEU:HD21	2:C:578:VAL:HG11	1.90	0.53
2:C:842:GLN:HB2	2:C:1603:PHE:HB2	1.90	0.53
2:C:3312:PRO:HA	2:C:3315:LEU:HB2	1.89	0.53
2:D:2562:THR:O	2:D:2566:ARG:HG3	2.08	0.53
2:A:238:HIS:HB3	2:A:243:GLU:HG3	1.90	0.53
2:B:1979:PHE:CD1	2:B:1993:ARG:HG2	2.44	0.53
2:B:3283:ILE:O	2:B:3287:ASN:HB2	2.08	0.53
2:C:436:LEU:HG	2:C:445:VAL:HG11	1.91	0.53
2:C:713:TRP:HH2	2:C:1251:LEU:HD21	1.73	0.53
2:D:238:HIS:HB3	2:D:243:GLU:HG3	1.90	0.53
2:D:555:LEU:HD21	2:D:578:VAL:HG11	1.90	0.53
2:D:605:GLY:HA2	2:D:1585:ARG:HD2	1.90	0.53
2:D:1256:PRO:HG3	2:D:1453:TYR:HB2	1.90	0.53
2:D:3900:GLU:OE2	2:D:3904:ARG:NH2	2.41	0.53
1:L:42:GLN:HE21	2:D:1957:LEU:CD2	2.21	0.53
1:L:100:TYR:CD1	1:L:138:ASN:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ILE:HG22	2:B:29:HIS:HD2	1.73	0.53
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.37	0.53
2:B:1842:ILE:HD12	2:B:1845:LEU:HD12	1.90	0.53
2:B:4633:LEU:O	2:B:4704:LYS:NZ	2.41	0.53
2:C:801:ARG:HG2	2:C:1618:LEU:HA	1.91	0.53
2:C:1979:PHE:CD1	2:C:1993:ARG:HG2	2.44	0.53
2:C:3216:GLU:HA	2:C:3219:VAL:HG22	1.90	0.53
2:A:28:ILE:HG22	2:A:29:HIS:HD2	1.73	0.53
2:A:996:VAL:HG22	2:A:1054:VAL:HG21	1.90	0.53
2:A:1256:PRO:HG3	2:A:1453:TYR:HB2	1.90	0.53
2:A:1936:LEU:HD21	2:A:1976:LEU:HD13	1.91	0.53
2:B:1124:PRO:HD2	2:B:1594:VAL:HG23	1.90	0.53
2:C:2562:THR:O	2:C:2566:ARG:HG3	2.08	0.53
2:C:3900:GLU:OE2	2:C:3904:ARG:NH2	2.41	0.53
2:D:71:GLN:HB3	2:D:73:LEU:HD23	1.90	0.53
2:D:246:THR:HG21	2:D:267:VAL:HG11	1.89	0.53
1:I:100:TYR:CD1	1:I:138:ASN:HB3	2.43	0.53
2:A:3246:MET:HG2	2:A:3309:LYS:HZ1	1.72	0.53
2:A:3900:GLU:OE2	2:A:3904:ARG:NH2	2.41	0.53
2:B:996:VAL:HG22	2:B:1054:VAL:HG21	1.89	0.53
2:B:3312:PRO:HA	2:B:3315:LEU:HB2	1.89	0.53
2:C:4049:HIS:CD2	2:C:4067:LEU:HD11	2.43	0.53
2:C:4633:LEU:O	2:C:4704:LYS:NZ	2.41	0.53
2:D:1144:ARG:NE	2:D:1150:GLU:OE2	2.42	0.53
2:D:2512:MET:HA	2:D:2512:MET:CE	2.35	0.53
2:D:3131:TYR:CD2	2:D:3205:CYS:HB3	2.38	0.53
2:A:1144:ARG:NE	2:A:1150:GLU:OE2	2.42	0.53
2:A:2593:VAL:HG12	2:A:2644:LEU:HB2	1.90	0.53
1:K:134:ASP:OD1	2:C:3298:ARG:NH1	2.42	0.53
2:B:801:ARG:HG2	2:B:1618:LEU:HA	1.91	0.53
2:B:1936:LEU:HD21	2:B:1976:LEU:HD13	1.91	0.53
2:B:3861:GLN:H	2:B:3867:THR:HG23	1.74	0.53
2:B:3900:GLU:OE2	2:B:3904:ARG:NH2	2.41	0.53
2:B:3950:VAL:O	2:B:3954:MET:HB2	2.08	0.53
2:C:1007:TRP:O	2:C:1011:ARG:HG2	2.07	0.53
2:C:1256:PRO:HG3	2:C:1453:TYR:HB2	1.90	0.53
2:C:1957:LEU:HB2	2:C:3601:ALA:HB2	1.91	0.53
2:C:3013:VAL:O	2:C:3018:ARG:NH2	2.39	0.53
2:D:2779:LEU:O	2:D:2783:LEU:HD12	2.08	0.53
2:A:173:GLU:OE2	2:A:176:ARG:NH2	2.36	0.53
2:A:2290:TRP:CZ2	2:A:2388:ILE:HG12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4633:LEU:O	2:A:4704:LYS:NZ	2.41	0.53
2:B:71:GLN:HB3	2:B:73:LEU:HD23	1.90	0.53
2:B:436:LEU:HG	2:B:445:VAL:HG11	1.91	0.53
2:B:2493:LEU:HG	2:B:2497:ARG:HH21	1.74	0.53
2:B:2779:LEU:O	2:B:2783:LEU:HD12	2.08	0.53
2:D:801:ARG:HG2	2:D:1618:LEU:HA	1.91	0.53
2:D:849:ASP:OD1	2:D:1214:ARG:NE	2.37	0.53
2:D:1124:PRO:HD2	2:D:1594:VAL:HG23	1.90	0.53
2:D:2290:TRP:CZ2	2:D:2388:ILE:HG12	2.44	0.53
2:D:2779:LEU:HA	2:D:2782:MET:HG2	1.91	0.53
2:A:842:GLN:HB2	2:A:1603:PHE:HB2	1.90	0.53
2:A:3216:GLU:HA	2:A:3219:VAL:HG22	1.90	0.53
2:A:3283:ILE:O	2:A:3287:ASN:HB2	2.08	0.53
2:A:4049:HIS:CD2	2:A:4067:LEU:HD11	2.43	0.53
2:A:4559:TYR:OH	2:B:4790:ARG:NH2	2.42	0.53
2:B:185:SER:OG	2:B:188:SER:OG	2.20	0.53
2:B:1144:ARG:NE	2:B:1150:GLU:OE2	2.42	0.53
2:C:1144:ARG:NE	2:C:1150:GLU:OE2	2.42	0.53
2:D:1431:ARG:NH1	2:D:1556:GLU:OE2	2.42	0.53
2:D:2905:ARG:HE	2:D:2906:GLY:H	1.57	0.53
2:D:3125:ASP:HB2	2:D:3195:LEU:HD22	1.91	0.53
2:D:4049:HIS:CD2	2:D:4067:LEU:HD11	2.43	0.53
2:A:1979:PHE:CD1	2:A:1993:ARG:HG2	2.44	0.53
2:A:2493:LEU:HG	2:A:2497:ARG:HH21	1.74	0.53
2:A:2905:ARG:HE	2:A:2906:GLY:H	1.57	0.53
2:A:3125:ASP:HB2	2:A:3195:LEU:HD22	1.91	0.53
2:B:3102:LEU:HD21	2:B:3155:LEU:HD23	1.91	0.53
2:C:28:ILE:HG22	2:C:29:HIS:HD2	1.73	0.53
2:C:2779:LEU:O	2:C:2783:LEU:HD12	2.09	0.53
2:C:2905:ARG:HE	2:C:2906:GLY:H	1.57	0.53
2:D:658:ASN:ND2	2:D:833:LYS:HG2	2.24	0.53
2:D:3312:PRO:HA	2:D:3315:LEU:HB2	1.89	0.53
2:A:919:VAL:HB	2:A:923:LYS:HE3	1.91	0.53
2:A:2562:THR:O	2:A:2566:ARG:HG3	2.08	0.53
1:J:10:ILE:O	1:J:14:LYS:N	2.38	0.53
1:J:114:GLY:O	1:J:116:LYS:NZ	2.31	0.53
2:B:1256:PRO:HG3	2:B:1453:TYR:HB2	1.90	0.53
2:B:3125:ASP:HB2	2:B:3195:LEU:HD22	1.91	0.53
2:B:3131:TYR:CD1	2:B:3205:CYS:HB2	2.41	0.53
2:C:71:GLN:HB3	2:C:73:LEU:HD23	1.90	0.53
2:C:173:GLU:OE2	2:C:176:ARG:NH2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2859:GLU:O	2:C:2862:SER:OG	2.23	0.53
2:C:3125:ASP:HB2	2:C:3195:LEU:HD22	1.91	0.53
2:C:3861:GLN:H	2:C:3867:THR:HG23	1.74	0.53
2:D:233:VAL:HG12	2:D:274:LEU:HD22	1.91	0.53
2:D:1419:PHE:O	2:D:1423:THR:HB	2.09	0.53
2:D:1978:ASN:HB2	2:D:1986:CYS:HB3	1.91	0.53
1:I:69:PHE:O	1:I:73:MET:HG2	2.10	0.52
2:A:713:TRP:HH2	2:A:1251:LEU:HD21	1.73	0.52
2:A:801:ARG:HG2	2:A:1618:LEU:HA	1.91	0.52
2:A:3102:LEU:HD21	2:A:3155:LEU:HD23	1.91	0.52
2:A:3890:TRP:HB3	2:B:76:ARG:HG2	1.90	0.52
3:G:50:ARG:HH21	3:G:53:LYS:HZ2	1.57	0.52
2:B:605:GLY:HA2	2:B:1585:ARG:HD2	1.91	0.52
2:B:1611:ILE:HB	2:B:1615:GLN:HB2	1.91	0.52
2:B:2059:GLN:NE2	2:B:2091:GLN:O	2.42	0.52
2:B:2593:VAL:HG12	2:B:2644:LEU:HB2	1.90	0.52
2:B:3016:ARG:O	2:B:3018:ARG:NE	2.32	0.52
2:C:668:ALA:HB2	2:C:1012:ILE:HD11	1.92	0.52
2:C:996:VAL:HG22	2:C:1054:VAL:HG21	1.90	0.52
2:D:713:TRP:HH2	2:D:1251:LEU:HD21	1.73	0.52
2:A:28:ILE:HG22	2:A:29:HIS:CD2	2.44	0.52
2:A:1184:ASP:OD2	2:A:1193:LYS:NZ	2.38	0.52
2:A:1419:PHE:O	2:A:1423:THR:HB	2.09	0.52
2:B:28:ILE:HG22	2:B:29:HIS:CD2	2.45	0.52
2:B:919:VAL:HB	2:B:923:LYS:HE3	1.91	0.52
2:B:1957:LEU:HB2	2:B:3601:ALA:HB2	1.91	0.52
2:B:2905:ARG:HE	2:B:2906:GLY:H	1.57	0.52
2:C:629:GLN:OE1	2:C:1669:ASN:ND2	2.37	0.52
2:C:658:ASN:ND2	2:C:833:LYS:HG2	2.24	0.52
2:C:1419:PHE:O	2:C:1423:THR:HB	2.09	0.52
2:D:1435:GLY:H	2:D:1500:ARG:NH2	2.06	0.52
2:D:2859:GLU:O	2:D:2862:SER:OG	2.23	0.52
2:D:2923:TYR:HA	2:D:3003:MET:HE1	1.91	0.52
2:D:3861:GLN:H	2:D:3867:THR:HG23	1.74	0.52
2:A:233:VAL:HG12	2:A:274:LEU:HD22	1.91	0.52
1:K:69:PHE:O	1:K:73:MET:HG2	2.10	0.52
2:C:3246:MET:HG2	2:C:3309:LYS:HZ1	1.75	0.52
2:D:668:ALA:HB2	2:D:1012:ILE:HD11	1.92	0.52
2:D:1979:PHE:CD1	2:D:1993:ARG:HG2	2.44	0.52
2:A:71:GLN:HB3	2:A:73:LEU:HD23	1.90	0.52
2:A:1978:ASN:HB2	2:A:1986:CYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4790:ARG:HH22	2:D:4557:VAL:HG21	1.74	0.52
2:C:2831:VAL:CG2	2:D:1435:GLY:HA2	2.39	0.52
2:D:28:ILE:HG22	2:D:29:HIS:HD2	1.73	0.52
2:D:1936:LEU:HD21	2:D:1976:LEU:HD13	1.91	0.52
2:A:1957:LEU:HB2	2:A:3601:ALA:HB2	1.91	0.52
1:K:110:MET:HA	2:C:3590:LEU:HD21	1.92	0.52
2:B:3216:GLU:HA	2:B:3219:VAL:HG22	1.90	0.52
2:C:1431:ARG:NH1	2:C:1556:GLU:OE2	2.42	0.52
2:C:2290:TRP:CZ2	2:C:2388:ILE:HG12	2.44	0.52
2:C:3109:PHE:HB3	2:C:3162:PHE:HA	1.91	0.52
2:D:4081:GLU:O	2:D:4085:LYS:HG3	2.10	0.52
2:D:4520:TYR:CE2	2:D:4559:TYR:HB3	2.45	0.52
2:A:658:ASN:ND2	2:A:833:LYS:HG2	2.24	0.52
2:A:1842:ILE:HD12	2:A:1845:LEU:HD12	1.90	0.52
2:B:658:ASN:ND2	2:B:833:LYS:HG2	2.24	0.52
2:B:903:GLN:N	2:B:913:ARG:HE	2.07	0.52
2:B:2562:THR:O	2:B:2566:ARG:HG3	2.08	0.52
2:B:4049:HIS:CD2	2:B:4067:LEU:HD11	2.43	0.52
2:C:897:LYS:HD2	2:C:902:TRP:CD1	2.45	0.52
2:C:2593:VAL:HG12	2:C:2644:LEU:HB2	1.90	0.52
2:D:1611:ILE:HB	2:D:1615:GLN:HB2	1.91	0.52
2:A:2779:LEU:O	2:A:2783:LEU:HD12	2.08	0.52
2:A:3319:PHE:O	2:A:3322:LEU:HG	2.10	0.52
2:A:3861:GLN:H	2:A:3867:THR:HG23	1.74	0.52
2:B:467:ASP:HB3	2:B:470:LEU:HG	1.92	0.52
2:B:1038:LEU:O	2:B:1043:LYS:NZ	2.36	0.52
2:B:2973:GLN:HA	2:B:2976:LYS:HZ2	1.75	0.52
2:B:4518:LEU:HD12	2:C:4809:MET:HG3	1.92	0.52
2:C:1936:LEU:HD21	2:C:1976:LEU:HD13	1.91	0.52
2:C:3108:LEU:HA	2:C:3111:HIS:CD2	2.45	0.52
2:C:3134:LEU:HD22	2:C:3162:PHE:HE2	1.74	0.52
2:C:4081:GLU:O	2:C:4085:LYS:HG3	2.10	0.52
2:D:436:LEU:HG	2:D:445:VAL:HG11	1.91	0.52
2:D:919:VAL:HB	2:D:923:LYS:HE3	1.91	0.52
2:D:2059:GLN:NE2	2:D:2091:GLN:O	2.42	0.52
2:D:3319:PHE:O	2:D:3322:LEU:HG	2.10	0.52
2:A:37:LEU:HA	2:A:49:LEU:HD23	1.92	0.52
2:A:114:LEU:HB2	2:A:117:HIS:CE1	2.45	0.52
2:A:1431:ARG:NH1	2:A:1556:GLU:OE2	2.42	0.52
2:A:1611:ILE:HB	2:A:1615:GLN:HB2	1.91	0.52
2:A:4520:TYR:CE2	2:A:4559:TYR:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:24:VAL:HG22	3:E:48:LYS:HG2	1.92	0.52
2:B:114:LEU:HB2	2:B:117:HIS:CE1	2.45	0.52
2:B:173:GLU:OE2	2:B:176:ARG:NH2	2.36	0.52
2:B:1431:ARG:NH1	2:B:1556:GLU:OE2	2.42	0.52
2:B:2729:HIS:HB2	2:B:2771:TYR:HE2	1.75	0.52
2:B:2779:LEU:HA	2:B:2782:MET:HG2	1.91	0.52
2:B:3134:LEU:HD22	2:B:3162:PHE:HE2	1.74	0.52
2:B:3319:PHE:O	2:B:3322:LEU:HG	2.10	0.52
2:C:233:VAL:HG12	2:C:274:LEU:HD22	1.91	0.52
2:C:2059:GLN:NE2	2:C:2091:GLN:O	2.42	0.52
2:C:4584:PHE:O	2:C:4588:ILE:HG13	2.10	0.52
2:A:903:GLN:N	2:A:913:ARG:HE	2.07	0.52
2:A:2059:GLN:NE2	2:A:2091:GLN:O	2.42	0.52
2:A:2763:LEU:HD23	2:A:2767:GLU:HG2	1.92	0.52
2:B:4584:PHE:O	2:B:4588:ILE:HG13	2.10	0.52
2:C:605:GLY:HA2	2:C:1585:ARG:HD2	1.91	0.52
2:C:1435:GLY:H	2:C:1500:ARG:NH2	2.06	0.52
2:D:114:LEU:HB2	2:D:117:HIS:CE1	2.45	0.52
2:D:3216:GLU:HA	2:D:3219:VAL:HG22	1.90	0.52
2:A:1135:PHE:CE2	2:A:1146:HIS:CD2	2.98	0.52
2:A:3125:ASP:H	2:A:3183:ILE:HD11	1.75	0.52
2:B:3109:PHE:HB3	2:B:3162:PHE:HA	1.91	0.52
2:C:114:LEU:HB2	2:C:117:HIS:CE1	2.45	0.52
2:C:1135:PHE:CE2	2:C:1146:HIS:CD2	2.98	0.52
2:C:4520:TYR:CE2	2:C:4559:TYR:HB3	2.45	0.52
2:D:1957:LEU:HB2	2:D:3601:ALA:HB2	1.91	0.52
2:D:3109:PHE:HB3	2:D:3162:PHE:HA	1.91	0.52
2:A:436:LEU:HG	2:A:445:VAL:HG11	1.91	0.51
2:A:2729:HIS:HB2	2:A:2771:TYR:HE2	1.75	0.51
2:A:3925:GLN:NE2	2:A:4934:THR:HA	2.26	0.51
2:B:2290:TRP:CZ2	2:B:2388:ILE:HG12	2.44	0.51
2:B:2763:LEU:HD23	2:B:2767:GLU:HG2	1.92	0.51
2:C:925:PRO:HB2	2:C:928:GLU:OE1	2.10	0.51
2:C:3131:TYR:CD1	2:C:3205:CYS:HB2	2.41	0.51
2:D:467:ASP:HB3	2:D:470:LEU:HG	1.92	0.51
2:D:925:PRO:HB2	2:D:928:GLU:OE1	2.10	0.51
2:D:1685:LEU:O	2:D:1689:ILE:HG12	2.10	0.51
2:D:2729:HIS:HB2	2:D:2771:TYR:HE2	1.75	0.51
2:A:1685:LEU:O	2:A:1689:ILE:HG12	2.10	0.51
1:K:42:GLN:HE21	2:C:1957:LEU:HD21	1.75	0.51
2:B:1135:PHE:CE2	2:B:1146:HIS:CD2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1419:PHE:O	2:B:1423:THR:HB	2.09	0.51
2:C:3183:ILE:HD12	2:C:3187:LYS:HE3	1.93	0.51
2:D:185:SER:OG	2:D:188:SER:OG	2.20	0.51
2:D:897:LYS:HD2	2:D:902:TRP:CD1	2.45	0.51
2:A:897:LYS:HD2	2:A:902:TRP:CD1	2.45	0.51
2:A:3108:LEU:HA	2:A:3111:HIS:CD2	2.45	0.51
1:J:69:PHE:O	1:J:73:MET:HG2	2.10	0.51
2:B:1978:ASN:HB2	2:B:1986:CYS:HB3	1.91	0.51
2:C:919:VAL:HB	2:C:923:LYS:HE3	1.92	0.51
2:C:1611:ILE:HB	2:C:1615:GLN:HB2	1.91	0.51
2:C:2493:LEU:HG	2:C:2497:ARG:HH21	1.74	0.51
2:C:2779:LEU:HA	2:C:2782:MET:HG2	1.91	0.51
2:C:4252:ILE:HG21	2:D:4707:MET:HG2	1.92	0.51
2:D:3921:THR:O	2:D:3925:GLN:HG2	2.10	0.51
2:D:4026:LEU:HD13	2:D:4058:TYR:CE2	2.46	0.51
2:A:3183:ILE:HD12	2:A:3187:LYS:HE3	1.93	0.51
1:L:69:PHE:O	1:L:73:MET:HG2	2.10	0.51
2:B:233:VAL:HG12	2:B:274:LEU:HD22	1.91	0.51
2:B:3125:ASP:H	2:B:3183:ILE:HD11	1.75	0.51
2:C:2973:GLN:HA	2:C:2976:LYS:HZ2	1.76	0.51
2:C:3925:GLN:NE2	2:C:4934:THR:HA	2.26	0.51
2:D:37:LEU:HA	2:D:49:LEU:HD23	1.92	0.51
2:D:3102:LEU:HD21	2:D:3155:LEU:HD23	1.91	0.51
2:D:3108:LEU:HA	2:D:3111:HIS:CD2	2.45	0.51
2:A:2785:TRP:HD1	2:A:2905:ARG:HH22	1.59	0.51
2:A:3151:GLN:HE22	2:A:3155:LEU:HD11	1.76	0.51
2:A:4196:THR:HB	2:A:4919:LEU:HD11	1.93	0.51
2:A:4584:PHE:O	2:A:4588:ILE:HG13	2.10	0.51
2:A:4661:TYR:HB3	2:A:4665:ARG:NH2	2.26	0.51
2:B:1922:ILE:O	2:B:1926:VAL:HG23	2.11	0.51
2:B:3151:GLN:HE22	2:B:3155:LEU:HD11	1.76	0.51
2:B:3183:ILE:HD12	2:B:3187:LYS:HE3	1.93	0.51
2:C:28:ILE:HG22	2:C:29:HIS:CD2	2.44	0.51
2:C:1978:ASN:HB2	2:C:1986:CYS:HB3	1.91	0.51
2:D:2785:TRP:HD1	2:D:2905:ARG:HH22	1.59	0.51
2:D:3131:TYR:CD1	2:D:3205:CYS:HB2	2.41	0.51
2:D:3925:GLN:NE2	2:D:4934:THR:HA	2.26	0.51
2:D:4661:TYR:HB3	2:D:4665:ARG:NH2	2.26	0.51
2:A:2779:LEU:HA	2:A:2782:MET:HG2	1.91	0.51
2:A:3879:LEU:O	2:A:3882:GLN:HG3	2.11	0.51
2:B:4196:THR:HB	2:B:4919:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:903:GLN:N	2:C:913:ARG:HE	2.07	0.51
2:C:1685:LEU:O	2:C:1689:ILE:HG12	2.10	0.51
2:C:2729:HIS:HB2	2:C:2771:TYR:HE2	1.75	0.51
2:C:4011:GLU:HG2	2:C:4121:LEU:HD13	1.93	0.51
2:D:1135:PHE:CE2	2:D:1146:HIS:CD2	2.98	0.51
2:D:2134:MET:HG2	2:D:2178:VAL:HG22	1.93	0.51
2:D:3183:ILE:HD12	2:D:3187:LYS:HE3	1.93	0.51
2:D:4670:LEU:HB2	2:D:4672:MET:HE1	1.91	0.51
2:A:3134:LEU:HD22	2:A:3162:PHE:HE2	1.74	0.51
2:B:668:ALA:HB2	2:B:1012:ILE:HD11	1.92	0.51
2:B:925:PRO:HB2	2:B:928:GLU:OE1	2.10	0.51
2:B:4011:GLU:HG2	2:B:4121:LEU:HD13	1.93	0.51
2:D:62:LEU:O	2:D:66:THR:HG23	2.11	0.51
2:D:2493:LEU:HG	2:D:2497:ARG:HH21	1.74	0.51
2:D:2587:HIS:HA	2:D:2590:ARG:HG2	1.93	0.51
2:D:3134:LEU:HD22	2:D:3162:PHE:HE2	1.74	0.51
2:D:4196:THR:HB	2:D:4919:LEU:HD11	1.93	0.51
2:D:4584:PHE:O	2:D:4588:ILE:HG13	2.10	0.51
2:A:467:ASP:HB3	2:A:470:LEU:HG	1.92	0.51
2:A:891:GLU:C	2:A:895:MET:HE1	2.31	0.51
2:A:3921:THR:O	2:A:3925:GLN:HG2	2.10	0.51
2:B:897:LYS:HD2	2:B:902:TRP:CD1	2.45	0.51
2:B:2080:LEU:O	2:B:2084:MET:HG3	2.11	0.51
2:B:3108:LEU:HA	2:B:3111:HIS:CD2	2.45	0.51
2:B:4026:LEU:HD13	2:B:4058:TYR:CE2	2.46	0.51
2:B:4661:TYR:HB3	2:B:4665:ARG:NH2	2.26	0.51
2:C:62:LEU:O	2:C:66:THR:HG23	2.11	0.51
2:C:1922:ILE:O	2:C:1926:VAL:HG23	2.11	0.51
2:C:2134:MET:HG2	2:C:2178:VAL:HG22	1.93	0.51
2:C:2905:ARG:HG3	2:C:2907:PHE:H	1.76	0.51
2:D:903:GLN:N	2:D:913:ARG:HE	2.07	0.51
2:D:2250:ASN:HB3	2:D:2253:LEU:HB2	1.93	0.51
2:D:2758:LYS:NZ	2:D:2763:LEU:HA	2.26	0.51
2:D:3151:GLN:HE22	2:D:3155:LEU:HD11	1.76	0.51
2:A:668:ALA:HB2	2:A:1012:ILE:HD11	1.92	0.51
2:A:2587:HIS:HA	2:A:2590:ARG:HG2	1.93	0.51
2:A:2765:GLU:HG3	2:A:2769:GLU:OE2	2.11	0.51
2:A:3109:PHE:HB3	2:A:3162:PHE:HA	1.91	0.51
2:A:4081:GLU:O	2:A:4085:LYS:HG3	2.10	0.51
3:F:24:VAL:HG22	3:F:48:LYS:HG2	1.92	0.51
3:H:24:VAL:HG22	3:H:48:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2988:ARG:HB2	2:B:2989:PRO:HD3	1.93	0.51
2:C:2785:TRP:HD1	2:C:2905:ARG:HH22	1.59	0.51
2:C:3921:THR:O	2:C:3925:GLN:HG2	2.10	0.51
2:D:28:ILE:HG22	2:D:29:HIS:CD2	2.44	0.51
2:D:2763:LEU:HD23	2:D:2767:GLU:HG2	1.92	0.51
2:D:4011:GLU:HG2	2:D:4121:LEU:HD13	1.93	0.51
1:I:10:ILE:O	1:I:14:LYS:N	2.38	0.51
1:I:134:ASP:HA	2:A:3298:ARG:HG3	1.93	0.51
2:A:3805:LEU:HD11	2:A:3887:ASP:HB3	1.93	0.51
2:A:4026:LEU:HD13	2:A:4058:TYR:CE2	2.46	0.51
2:A:4569:GLU:HB3	2:A:4570:PRO:HD3	1.93	0.51
2:B:891:GLU:C	2:B:895:MET:HE1	2.32	0.51
2:B:3131:TYR:OH	2:B:3205:CYS:O	2.23	0.51
2:C:2080:LEU:O	2:C:2084:MET:HG3	2.11	0.51
2:C:2765:GLU:HG3	2:C:2769:GLU:OE2	2.11	0.51
2:C:3151:GLN:HE22	2:C:3155:LEU:HD11	1.76	0.51
2:C:4026:LEU:HD13	2:C:4058:TYR:CE2	2.46	0.51
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.37	0.51
2:D:891:GLU:C	2:D:895:MET:HE1	2.31	0.51
2:D:3805:LEU:HD11	2:D:3887:ASP:HB3	1.93	0.51
2:A:3215:MET:O	2:A:3219:VAL:HG13	2.11	0.50
2:A:4011:GLU:HG2	2:A:4121:LEU:HD13	1.93	0.50
2:B:37:LEU:HA	2:B:49:LEU:HD23	1.92	0.50
2:B:1435:GLY:H	2:B:1500:ARG:NH2	2.06	0.50
2:B:3925:GLN:NE2	2:B:4934:THR:HA	2.26	0.50
2:B:4520:TYR:CE2	2:B:4559:TYR:HB3	2.45	0.50
2:C:3016:ARG:O	2:C:3018:ARG:NE	2.32	0.50
2:C:3102:LEU:HD21	2:C:3155:LEU:HD23	1.91	0.50
2:C:3125:ASP:H	2:C:3183:ILE:HD11	1.75	0.50
2:C:3319:PHE:O	2:C:3322:LEU:HG	2.10	0.50
2:D:674:TYR:HE1	2:D:756:SER:HB3	1.76	0.50
2:A:925:PRO:HB2	2:A:928:GLU:OE1	2.10	0.50
2:A:2988:ARG:HB2	2:A:2989:PRO:HD3	1.93	0.50
3:G:24:VAL:HG22	3:G:48:LYS:HG2	1.92	0.50
2:B:1685:LEU:O	2:B:1689:ILE:HG12	2.10	0.50
2:B:1935:LYS:HE3	2:B:1995:GLN:HE22	1.76	0.50
2:B:3879:LEU:O	2:B:3882:GLN:HG3	2.11	0.50
2:C:4661:TYR:HB3	2:C:4665:ARG:NH2	2.26	0.50
2:D:2988:ARG:HB2	2:D:2989:PRO:HD3	1.93	0.50
2:D:3125:ASP:H	2:D:3183:ILE:HD11	1.76	0.50
2:D:4166:LYS:O	2:D:4170:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:674:TYR:HE1	2:A:756:SER:HB3	1.76	0.50
2:A:1922:ILE:O	2:A:1926:VAL:HG23	2.11	0.50
2:A:2758:LYS:NZ	2:A:2763:LEU:HA	2.26	0.50
2:B:2905:ARG:HG3	2:B:2907:PHE:H	1.76	0.50
2:B:3215:MET:O	2:B:3219:VAL:HG13	2.11	0.50
2:B:3921:THR:O	2:B:3925:GLN:HG2	2.10	0.50
2:B:4726:MET:O	2:B:4726:MET:HE3	2.11	0.50
2:C:1935:LYS:HE3	2:C:1995:GLN:HE22	1.76	0.50
2:C:3215:MET:O	2:C:3219:VAL:HG13	2.11	0.50
2:C:4154:GLU:O	2:C:4158:THR:HG23	2.12	0.50
2:D:3016:ARG:O	2:D:3018:ARG:NE	2.32	0.50
2:D:4055:HIS:CE1	2:D:4057:HIS:CD2	3.00	0.50
2:A:4057:HIS:HE1	2:B:4660:PHE:HZ	1.57	0.50
2:A:4154:GLU:O	2:A:4158:THR:HG23	2.12	0.50
2:B:1184:ASP:OD2	2:B:1193:LYS:NZ	2.38	0.50
2:B:4081:GLU:O	2:B:4085:LYS:HG3	2.10	0.50
2:B:4166:LYS:O	2:B:4170:ARG:HG2	2.11	0.50
2:C:2763:LEU:HD23	2:C:2767:GLU:HG2	1.92	0.50
2:D:1922:ILE:O	2:D:1926:VAL:HG23	2.11	0.50
2:D:4569:GLU:HB3	2:D:4570:PRO:HD3	1.94	0.50
2:A:62:LEU:O	2:A:66:THR:HG23	2.11	0.50
2:A:2134:MET:HG2	2:A:2178:VAL:HG22	1.93	0.50
2:A:2250:ASN:HB3	2:A:2253:LEU:HB2	1.93	0.50
2:A:4166:LYS:O	2:A:4170:ARG:HG2	2.11	0.50
2:B:2782:MET:HB2	2:B:2787:TRP:HE3	1.76	0.50
2:C:3292:GLU:O	2:C:3296:MET:HE2	2.12	0.50
2:C:4569:GLU:HB3	2:C:4570:PRO:HD3	1.94	0.50
2:D:1564:MET:SD	2:D:1565:PRO:HD2	2.52	0.50
2:A:4055:HIS:CE1	2:A:4057:HIS:CD2	3.00	0.50
1:J:106:LEU:HD22	2:B:3587:TRP:NE1	2.25	0.50
1:L:127:ARG:NH1	1:L:135:GLY:C	2.58	0.50
2:B:2758:LYS:NZ	2:B:2763:LEU:HA	2.26	0.50
2:B:2765:GLU:HG3	2:B:2769:GLU:OE2	2.11	0.50
2:B:2833:LEU:HB2	2:B:2838[A]:HIS:NE2	2.27	0.50
2:B:3677:THR:HB	2:B:3679:LYS:HZ2	1.77	0.50
2:B:4154:GLU:O	2:B:4158:THR:HG23	2.12	0.50
2:B:4569:GLU:HB3	2:B:4570:PRO:HD3	1.94	0.50
2:C:37:LEU:HA	2:C:49:LEU:HD23	1.92	0.50
2:C:891:GLU:C	2:C:895:MET:HE1	2.31	0.50
2:C:1014:GLN:O	2:C:1027:ARG:NH2	2.45	0.50
2:C:2054:LYS:HE2	2:C:2056:SER:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2250:ASN:HB3	2:C:2253:LEU:HB2	1.93	0.50
2:C:2782:MET:HB2	2:C:2787:TRP:HE3	1.76	0.50
2:D:506:HIS:CE1	2:D:530:LEU:HD21	2.47	0.50
2:D:1935:LYS:HE3	2:D:1995:GLN:HE22	1.76	0.50
2:A:1748:LEU:HB3	2:A:1751:ILE:HD13	1.94	0.50
2:A:2080:LEU:O	2:A:2084:MET:HG3	2.11	0.50
2:A:2782:MET:HB2	2:A:2787:TRP:HE3	1.76	0.50
2:A:2830:ASN:HB3	2:B:1435:GLY:HA3	1.94	0.50
2:B:2134:MET:HG2	2:B:2178:VAL:HG22	1.93	0.50
2:B:2250:ASN:HB3	2:B:2253:LEU:HB2	1.93	0.50
2:B:2859:GLU:O	2:B:2862:SER:OG	2.23	0.50
2:B:4055:HIS:CE1	2:B:4057:HIS:CD2	3.00	0.50
2:C:467:ASP:HB3	2:C:470:LEU:HG	1.92	0.50
2:C:3996:GLY:O	2:C:4000:VAL:HG23	2.12	0.50
2:C:4196:THR:HB	2:C:4919:LEU:HD11	1.93	0.50
2:C:4726:MET:HE3	2:C:4726:MET:O	2.11	0.50
2:D:1299:ILE:HD11	2:D:1544:PHE:HB3	1.94	0.50
2:D:3215:MET:O	2:D:3219:VAL:HG13	2.11	0.50
2:D:3246:MET:HG2	2:D:3309:LYS:HZ1	1.75	0.50
2:D:3879:LEU:O	2:D:3882:GLN:HG3	2.11	0.50
2:A:874:LEU:CD1	2:A:940:LEU:HD13	2.42	0.50
1:K:127:ARG:NH1	1:K:135:GLY:C	2.58	0.50
2:B:506:HIS:CE1	2:B:530:LEU:HD21	2.47	0.50
2:B:1014:GLN:O	2:B:1027:ARG:NH2	2.45	0.50
2:B:2587:HIS:HA	2:B:2590:ARG:HG2	1.93	0.50
2:B:2785:TRP:HD1	2:B:2905:ARG:HH22	1.59	0.50
2:C:2831:VAL:HG22	2:D:1435:GLY:HA2	1.94	0.50
2:C:2988:ARG:HB2	2:C:2989:PRO:HD3	1.93	0.50
2:C:3295:TRP:CD1	2:C:3296:MET:SD	3.05	0.50
2:D:874:LEU:CD1	2:D:940:LEU:HD13	2.42	0.50
2:D:2080:LEU:O	2:D:2084:MET:HG3	2.11	0.50
2:D:2765:GLU:HG3	2:D:2769:GLU:OE2	2.11	0.50
2:D:4154:GLU:O	2:D:4158:THR:HG23	2.12	0.50
2:A:318:ASP:O	2:A:322:ALA:HB2	2.12	0.50
2:A:1564:MET:SD	2:A:1565:PRO:HD2	2.52	0.50
2:A:3089:GLY:O	2:A:3093:ILE:HG12	2.12	0.50
2:A:3122:ILE:HA	2:A:3126:VAL:HB	1.94	0.50
2:A:4726:MET:O	2:A:4726:MET:HE3	2.11	0.50
2:B:66:THR:OG1	2:B:124:SER:OG	2.24	0.50
2:B:674:TYR:HE1	2:B:756:SER:HB3	1.77	0.50
2:B:3089:GLY:O	2:B:3093:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3118:GLY:O	2:B:3122:ILE:HG12	2.12	0.50
2:B:4670:LEU:HB2	2:B:4672:MET:HE1	1.94	0.50
2:B:4863:GLN:O	2:B:4867:ILE:HG12	2.12	0.50
2:C:2758:LYS:NZ	2:C:2763:LEU:HA	2.26	0.50
2:C:4055:HIS:CE1	2:C:4057:HIS:CD2	3.00	0.50
2:C:4166:LYS:O	2:C:4170:ARG:HG2	2.11	0.50
2:D:238:HIS:ND1	2:D:243:GLU:OE2	2.45	0.50
2:D:2054:LYS:HE2	2:D:2056:SER:HA	1.94	0.50
2:D:3089:GLY:O	2:D:3093:ILE:HG12	2.12	0.50
2:A:474:ASP:O	2:A:478:ARG:HG2	2.12	0.49
2:A:3295:TRP:CD1	2:A:3296:MET:SD	3.05	0.49
2:B:3046:MET:HG3	2:B:3121:LEU:HA	1.94	0.49
2:B:3295:TRP:CD1	2:B:3296:MET:SD	3.05	0.49
2:C:1564:MET:SD	2:C:1565:PRO:HD2	2.52	0.49
2:C:3118:GLY:O	2:C:3122:ILE:HG12	2.12	0.49
2:C:3805:LEU:HD21	2:C:3888:PHE:HA	1.94	0.49
2:D:1014:GLN:O	2:D:1027:ARG:NH2	2.45	0.49
2:D:1184:ASP:OD2	2:D:1193:LYS:NZ	2.38	0.49
2:D:4726:MET:O	2:D:4726:MET:HE3	2.11	0.49
2:A:506:HIS:CE1	2:A:530:LEU:HD21	2.47	0.49
2:B:62:LEU:O	2:B:66:THR:HG23	2.11	0.49
2:C:317:MET:HE2	2:C:321:LYS:HD2	1.94	0.49
2:C:674:TYR:HE1	2:C:756:SER:HB3	1.76	0.49
2:C:1299:ILE:HD11	2:C:1544:PHE:HB3	1.94	0.49
2:C:3805:LEU:HD11	2:C:3887:ASP:HB3	1.93	0.49
2:D:474:ASP:O	2:D:478:ARG:HG2	2.12	0.49
2:D:2833:LEU:HB2	2:D:2838[A]:HIS:NE2	2.27	0.49
2:D:3122:ILE:HA	2:D:3126:VAL:HB	1.94	0.49
2:A:2905:ARG:HG3	2:A:2907:PHE:H	1.76	0.49
2:A:3996:GLY:O	2:A:4000:VAL:HG23	2.12	0.49
2:A:4507:LEU:HD21	2:A:4746:ILE:HG22	1.94	0.49
2:B:995:MET:HA	2:B:998:LYS:HD3	1.94	0.49
2:B:2833:LEU:HB2	2:B:2838[B]:HIS:NE2	2.28	0.49
2:C:238:HIS:ND1	2:C:243:GLU:OE2	2.45	0.49
2:C:506:HIS:CE1	2:C:530:LEU:HD21	2.47	0.49
2:C:874:LEU:CD1	2:C:940:LEU:HD13	2.42	0.49
2:C:3879:LEU:O	2:C:3882:GLN:HG3	2.11	0.49
2:D:2924:SER:O	2:D:2928:GLN:HG2	2.12	0.49
2:D:3295:TRP:CD1	2:D:3296:MET:SD	3.05	0.49
2:D:3805:LEU:HD21	2:D:3888:PHE:HA	1.94	0.49
1:I:127:ARG:NH1	1:I:135:GLY:C	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:995:MET:HA	2:A:998:LYS:HD3	1.94	0.49
2:A:1014:GLN:O	2:A:1027:ARG:NH2	2.45	0.49
2:A:2768:LYS:HB3	2:A:2772:ARG:HH21	1.77	0.49
2:B:115:TYR:OH	2:B:179:ASP:OD2	2.31	0.49
2:B:3848:GLU:OE1	2:B:3922:GLU:OE1	2.29	0.49
2:B:4021:LEU:HD22	2:B:4128:TYR:CE2	2.48	0.49
2:C:2587:HIS:HA	2:C:2590:ARG:HG2	1.93	0.49
2:C:3089:GLY:O	2:C:3093:ILE:HG12	2.12	0.49
2:D:318:ASP:O	2:D:322:ALA:HB2	2.12	0.49
2:D:2905:ARG:HG3	2:D:2907:PHE:H	1.76	0.49
2:D:3677:THR:HB	2:D:3679:LYS:HZ2	1.76	0.49
2:D:4863:GLN:O	2:D:4867:ILE:HG12	2.12	0.49
2:A:1040:ASP:HA	2:A:1043:LYS:HG2	1.95	0.49
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:NE2	2.27	0.49
2:A:3046:MET:HG3	2:A:3121:LEU:HA	1.94	0.49
2:A:3118:GLY:O	2:A:3122:ILE:HG12	2.12	0.49
2:A:4769:LEU:HB3	2:D:4753:LEU:HD11	1.94	0.49
2:B:318:ASP:O	2:B:322:ALA:HB2	2.12	0.49
2:B:2691:LYS:HA	2:B:2704:GLN:HE22	1.78	0.49
2:B:3805:LEU:HD11	2:B:3887:ASP:HB3	1.93	0.49
2:B:4753:LEU:HG	2:C:4773:LEU:HD22	1.94	0.49
2:C:318:ASP:O	2:C:322:ALA:HB2	2.12	0.49
2:C:1685:LEU:HD22	2:C:1706:LEU:HB2	1.95	0.49
2:C:4055:HIS:CE1	2:C:4057:HIS:HD2	2.31	0.49
2:C:4268:MET:HA	2:C:4271:VAL:HG22	1.94	0.49
2:D:317:MET:HE2	2:D:321:LYS:HD2	1.95	0.49
2:D:3996:GLY:O	2:D:4000:VAL:HG23	2.12	0.49
2:D:4271:VAL:HA	2:D:4274:MET:HG2	1.95	0.49
2:A:1299:ILE:HD11	2:A:1544:PHE:HB3	1.94	0.49
2:A:1935:LYS:HE3	2:A:1995:GLN:HE22	1.76	0.49
2:B:238:HIS:ND1	2:B:243:GLU:OE2	2.45	0.49
2:B:317:MET:HE2	2:B:321:LYS:HD2	1.94	0.49
2:B:4667:SER:HA	2:B:4672:MET:HE3	1.94	0.49
2:C:474:ASP:O	2:C:478:ARG:HG2	2.12	0.49
2:D:1040:ASP:HA	2:D:1043:LYS:HG2	1.95	0.49
2:D:2691:LYS:HA	2:D:2704:GLN:HE22	1.78	0.49
2:A:115:TYR:OH	2:A:179:ASP:OD2	2.31	0.49
2:A:2087:LEU:O	2:A:2091:GLN:HG2	2.13	0.49
2:A:4271:VAL:HA	2:A:4274:MET:HG2	1.95	0.49
2:B:1299:ILE:HD11	2:B:1544:PHE:HB3	1.94	0.49
2:B:3996:GLY:O	2:B:4000:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4507:LEU:HD21	2:B:4746:ILE:HG22	1.94	0.49
2:C:2924:SER:O	2:C:2928:GLN:HG2	2.12	0.49
2:D:1104:GLU:OE1	2:D:1225:LYS:NZ	2.44	0.49
2:D:2961:LYS:HB2	2:D:2965:LYS:HZ3	1.78	0.49
2:D:4507:LEU:HD21	2:D:4746:ILE:HG22	1.94	0.49
2:A:889:ILE:HA	2:A:892:LEU:HD12	1.95	0.49
2:A:2859:GLU:O	2:A:2862:SER:OG	2.23	0.49
2:B:2054:LYS:HE2	2:B:2056:SER:HA	1.94	0.49
2:C:2833:LEU:HB2	2:C:2838[A]:HIS:NE2	2.27	0.49
2:D:2496:LEU:HD23	2:D:2520:LEU:HD13	1.95	0.49
2:D:2768:LYS:HB3	2:D:2772:ARG:HH21	1.77	0.49
2:D:3046:MET:HG3	2:D:3121:LEU:HA	1.94	0.49
2:A:2691:LYS:HA	2:A:2704:GLN:HE22	1.78	0.49
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:NE2	2.28	0.49
1:J:59:ASP:N	1:J:68:GLU:OE2	2.33	0.49
2:B:1564:MET:SD	2:B:1565:PRO:HD2	2.52	0.49
2:B:2768:LYS:HB3	2:B:2772:ARG:HH21	1.77	0.49
2:B:3096:TYR:CE2	2:B:3101:LEU:HD13	2.48	0.49
2:B:4155:SER:O	2:B:4159:GLN:HG2	2.13	0.49
2:B:4573:ARG:NH2	2:B:4736:ASN:OD1	2.46	0.49
2:C:115:TYR:OH	2:C:179:ASP:OD2	2.31	0.49
2:C:1004:HIS:NE2	2:C:1038:LEU:HD21	2.28	0.49
2:C:1040:ASP:HA	2:C:1043:LYS:HG2	1.95	0.49
2:C:1522:ALA:HB3	2:C:1527:LEU:HD21	1.95	0.49
2:C:2156:TYR:HE1	2:C:2202:TYR:HE2	1.60	0.49
2:C:3046:MET:HG3	2:C:3121:LEU:HA	1.94	0.49
2:C:3096:TYR:CE2	2:C:3101:LEU:HD13	2.48	0.49
2:D:1685:LEU:HD22	2:D:1706:LEU:HB2	1.95	0.49
2:D:3096:TYR:CE2	2:D:3101:LEU:HD13	2.48	0.49
2:D:3118:GLY:O	2:D:3122:ILE:HG12	2.12	0.49
2:D:4055:HIS:CE1	2:D:4057:HIS:HD2	2.31	0.49
2:A:606:ARG:NH1	2:A:644:LEU:HD21	2.25	0.49
2:A:1081:THR:HG23	2:A:1083:GLU:H	1.78	0.49
2:A:3036:LEU:O	2:A:3040:LEU:HG	2.12	0.49
2:A:4863:GLN:O	2:A:4867:ILE:HG12	2.12	0.49
2:B:474:ASP:O	2:B:478:ARG:HG2	2.12	0.49
2:B:1004:HIS:NE2	2:B:1038:LEU:HD21	2.28	0.49
2:B:1081:THR:HG23	2:B:1083:GLU:H	1.78	0.49
2:B:1522:ALA:HB3	2:B:1527:LEU:HD21	1.95	0.49
2:B:3042:ALA:HB1	2:B:3121:LEU:HB2	1.95	0.49
2:B:3211:LEU:HD21	2:B:3245:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3238:ILE:O	2:B:3241:MET:HB3	2.13	0.49
2:B:4268:MET:HA	2:B:4271:VAL:HG22	1.94	0.49
2:C:913:ARG:HG3	2:C:913:ARG:O	2.12	0.49
2:C:2496:LEU:HD23	2:C:2520:LEU:HD13	1.95	0.49
2:C:2691:LYS:HA	2:C:2704:GLN:HE22	1.78	0.49
2:C:3238:ILE:O	2:C:3241:MET:HB3	2.13	0.49
2:C:4021:LEU:HD22	2:C:4128:TYR:CE2	2.48	0.49
2:D:1038:LEU:O	2:D:1043:LYS:NZ	2.36	0.49
2:D:1081:THR:HG23	2:D:1083:GLU:H	1.78	0.49
2:D:2782:MET:HB2	2:D:2787:TRP:HE3	1.76	0.49
2:D:4573:ARG:NH2	2:D:4736:ASN:OD1	2.46	0.49
2:A:317:MET:HE2	2:A:321:LYS:HD2	1.94	0.48
2:A:2156:TYR:HE1	2:A:2202:TYR:HE2	1.60	0.48
2:A:2924:SER:O	2:A:2928:GLN:HG2	2.12	0.48
2:A:3096:TYR:CE2	2:A:3101:LEU:HD13	2.48	0.48
2:A:4021:LEU:HD22	2:A:4128:TYR:CE2	2.48	0.48
1:J:127:ARG:NH1	1:J:135:GLY:C	2.58	0.48
2:B:889:ILE:HA	2:B:892:LEU:HD12	1.95	0.48
2:B:3171:LEU:HD13	2:B:3214:LEU:HD12	1.95	0.48
2:C:889:ILE:HA	2:C:892:LEU:HD12	1.95	0.48
2:C:995:MET:HA	2:C:998:LYS:HD3	1.94	0.48
2:C:2831:VAL:HG22	2:D:1435:GLY:O	2.13	0.48
2:C:2857:LYS:O	2:C:2860:LEU:HG	2.13	0.48
2:C:3036:LEU:O	2:C:3040:LEU:HG	2.12	0.48
2:C:4507:LEU:HD21	2:C:4746:ILE:HG22	1.94	0.48
2:D:889:ILE:HA	2:D:892:LEU:HD12	1.95	0.48
2:D:4155:SER:O	2:D:4159:GLN:HG2	2.13	0.48
2:A:2054:LYS:HE2	2:A:2056:SER:HA	1.94	0.48
2:A:3171:LEU:HD13	2:A:3214:LEU:HD12	1.95	0.48
2:A:3211:LEU:HD21	2:A:3245:TYR:CE2	2.48	0.48
1:L:134:ASP:OD1	2:D:3298:ARG:NH1	2.46	0.48
1:L:137:VAL:HG21	2:D:3587:TRP:CH2	2.47	0.48
2:B:874:LEU:CD1	2:B:940:LEU:HD13	2.42	0.48
2:B:913:ARG:HG3	2:B:913:ARG:O	2.13	0.48
2:B:2729:HIS:CE1	2:B:2763:LEU:HD11	2.49	0.48
2:B:3036:LEU:O	2:B:3040:LEU:HG	2.12	0.48
2:B:3122:ILE:HA	2:B:3126:VAL:HB	1.94	0.48
2:B:3805:LEU:HD21	2:B:3888:PHE:HA	1.94	0.48
2:B:4055:HIS:CE1	2:B:4057:HIS:HD2	2.31	0.48
2:B:4271:VAL:HA	2:B:4274:MET:HG2	1.95	0.48
2:C:1748:LEU:HB3	2:C:1751:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3677:THR:HB	2:C:3679:LYS:HZ2	1.77	0.48
2:D:995:MET:HA	2:D:998:LYS:HD3	1.94	0.48
2:D:1004:HIS:NE2	2:D:1038:LEU:HD21	2.28	0.48
2:D:1748:LEU:HB3	2:D:1751:ILE:HD13	1.94	0.48
2:D:2565:GLN:O	2:D:2569:ILE:HG12	2.14	0.48
2:D:2733:SER:HA	2:D:2736:LYS:NZ	2.28	0.48
2:D:4021:LEU:HD22	2:D:4128:TYR:CE2	2.48	0.48
2:A:238:HIS:ND1	2:A:243:GLU:OE2	2.45	0.48
2:B:2456:MET:SD	2:B:2512:MET:HE1	2.53	0.48
2:D:883:GLU:HG2	2:D:884:LYS:N	2.28	0.48
2:D:1522:ALA:HB3	2:D:1527:LEU:HD21	1.95	0.48
2:D:2087:LEU:O	2:D:2091:GLN:HG2	2.13	0.48
2:D:2729:HIS:CE1	2:D:2763:LEU:HD11	2.49	0.48
2:D:3036:LEU:O	2:D:3040:LEU:HG	2.12	0.48
2:D:3238:ILE:O	2:D:3241:MET:HB3	2.13	0.48
2:D:3269:ASN:O	2:D:3273:MET:HG3	2.14	0.48
2:D:4268:MET:HA	2:D:4271:VAL:HG22	1.94	0.48
2:A:2456:MET:SD	2:A:2512:MET:HE1	2.53	0.48
2:A:3238:ILE:O	2:A:3241:MET:HB3	2.13	0.48
2:A:4573:ARG:NH2	2:A:4736:ASN:OD1	2.46	0.48
2:B:606:ARG:NH1	2:B:644:LEU:HD21	2.26	0.48
2:B:1040:ASP:HA	2:B:1043:LYS:HG2	1.95	0.48
2:B:1748:LEU:HB3	2:B:1751:ILE:HD13	1.94	0.48
2:B:1797:GLU:HA	2:B:1800:LYS:HE3	1.96	0.48
2:C:2224:ASN:O	2:C:2227:VAL:HG23	2.14	0.48
2:C:2733:SER:HA	2:C:2736:LYS:NZ	2.28	0.48
2:C:3122:ILE:HA	2:C:3126:VAL:HB	1.94	0.48
2:C:3269:ASN:O	2:C:3273:MET:HG3	2.14	0.48
2:C:4271:VAL:HA	2:C:4274:MET:HG2	1.95	0.48
2:C:4573:ARG:NH2	2:C:4736:ASN:OD1	2.46	0.48
2:D:2857:LYS:O	2:D:2860:LEU:HG	2.13	0.48
2:D:3043:ARG:HA	2:D:3120:ASP:OD2	2.13	0.48
2:A:913:ARG:HG3	2:A:913:ARG:O	2.13	0.48
2:A:1004:HIS:NE2	2:A:1038:LEU:HD21	2.28	0.48
2:A:2701:PHE:CE2	2:A:2703:PRO:HG3	2.49	0.48
2:A:3295:TRP:HB3	2:A:3298:ARG:HH21	1.79	0.48
2:A:3805:LEU:HD21	2:A:3888:PHE:HA	1.94	0.48
2:A:4055:HIS:CE1	2:A:4057:HIS:HD2	2.31	0.48
3:G:88:HIS:HD2	3:G:89:PRO:HD2	1.79	0.48
2:B:2496:LEU:HD23	2:B:2520:LEU:HD13	1.95	0.48
2:B:2733:SER:HA	2:B:2736:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2924:SER:O	2:B:2928:GLN:HG2	2.12	0.48
2:C:2385:GLY:O	2:C:2389:MET:HG3	2.13	0.48
2:C:2833:LEU:HB2	2:C:2838[B]:HIS:NE2	2.28	0.48
2:C:4155:SER:O	2:C:4159:GLN:HG2	2.13	0.48
2:C:4863:GLN:O	2:C:4867:ILE:HG12	2.12	0.48
2:D:115:TYR:OH	2:D:179:ASP:OD2	2.31	0.48
2:D:3246:MET:HG2	2:D:3309:LYS:HZ2	1.78	0.48
2:A:2224:ASN:O	2:A:2227:VAL:HG23	2.14	0.48
2:A:2729:HIS:CE1	2:A:2763:LEU:HD11	2.49	0.48
2:A:3043:ARG:HA	2:A:3120:ASP:OD2	2.13	0.48
1:L:76:LYS:HB2	1:L:78:LYS:HZ2	1.78	0.48
1:L:127:ARG:HD3	1:L:127:ARG:HA	1.41	0.48
2:B:292:GLY:HA3	2:B:340:VAL:HG21	1.96	0.48
2:B:874:LEU:HD12	2:B:875:PRO:HD2	1.95	0.48
2:B:2565:GLN:O	2:B:2569:ILE:HG12	2.14	0.48
2:B:3159:LEU:HB3	2:B:3241:MET:HE2	1.95	0.48
2:C:883:GLU:HG2	2:C:884:LYS:N	2.28	0.48
2:C:1081:THR:HG23	2:C:1083:GLU:H	1.78	0.48
2:D:661:LEU:HD23	2:D:673:TRP:CD1	2.49	0.48
2:D:1034:PRO:HD2	2:D:1037:LEU:HD12	1.96	0.48
2:D:3211:LEU:HD21	2:D:3245:TYR:CE2	2.48	0.48
2:D:3295:TRP:HB3	2:D:3298:ARG:HH21	1.78	0.48
2:A:292:GLY:HA3	2:A:340:VAL:HG21	1.96	0.48
2:A:375:GLN:HB2	2:A:390:LYS:HB3	1.95	0.48
2:A:883:GLU:HG2	2:A:884:LYS:N	2.28	0.48
2:A:1797:GLU:HA	2:A:1800:LYS:HE3	1.96	0.48
2:B:165:ALA:HB3	2:B:180:ASP:HB3	1.96	0.48
2:B:849:ASP:OD1	2:B:1214:ARG:NE	2.37	0.48
2:B:3269:ASN:O	2:B:3273:MET:HG3	2.14	0.48
2:C:375:GLN:HB2	2:C:390:LYS:HB3	1.95	0.48
2:C:441:LYS:HG3	2:C:444:THR:HG23	1.96	0.48
2:C:2087:LEU:O	2:C:2091:GLN:HG2	2.13	0.48
2:C:2701:PHE:CE2	2:C:2703:PRO:HG3	2.49	0.48
2:C:3200:ASN:CB	2:C:3203:ASP:HB2	2.44	0.48
2:C:3211:LEU:HD21	2:C:3245:TYR:CE2	2.49	0.48
2:D:3068:LEU:O	2:D:3071:THR:OG1	2.27	0.48
2:A:2733:SER:HA	2:A:2736:LYS:NZ	2.28	0.48
2:A:2968:LEU:HD13	2:A:3029:ILE:HG12	1.96	0.48
3:H:88:HIS:HD2	3:H:89:PRO:HD2	1.79	0.48
2:B:1685:LEU:HD22	2:B:1706:LEU:HB2	1.95	0.48
2:B:2156:TYR:HE1	2:B:2202:TYR:HE2	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3295:TRP:HB3	2:B:3298:ARG:HH21	1.78	0.48
2:C:2729:HIS:CE1	2:C:2763:LEU:HD11	2.49	0.48
2:C:3131:TYR:O	2:C:3135:THR:HG23	2.14	0.48
2:D:2946:GLY:HA3	2:D:2954:PHE:HZ	1.79	0.48
2:D:2968:LEU:HD13	2:D:3029:ILE:HG12	1.96	0.48
3:E:88:HIS:HD2	3:E:89:PRO:HD2	1.79	0.48
2:B:2385:GLY:O	2:B:2389:MET:HG3	2.13	0.48
2:B:2857:LYS:O	2:B:2860:LEU:HG	2.13	0.48
2:B:3043:ARG:HA	2:B:3120:ASP:OD2	2.13	0.48
2:C:318:ASP:OD1	2:C:319:LYS:N	2.45	0.48
2:C:1435:GLY:N	2:C:1500:ARG:HH22	2.11	0.48
2:C:1967:SER:O	2:C:1972:GLN:NE2	2.41	0.48
2:C:2768:LYS:HB3	2:C:2772:ARG:HH21	1.77	0.48
2:C:3042:ALA:HB1	2:C:3121:LEU:HB2	1.95	0.48
2:D:606:ARG:NH1	2:D:644:LEU:HD21	2.25	0.48
2:D:2385:GLY:O	2:D:2389:MET:HG3	2.13	0.48
2:A:1685:LEU:HD22	2:A:1706:LEU:HB2	1.95	0.48
2:A:2857:LYS:O	2:A:2860:LEU:HG	2.13	0.48
2:A:3106:SER:OG	2:A:3157:GLU:OE1	2.21	0.48
2:A:4155:SER:O	2:A:4159:GLN:HG2	2.13	0.48
2:A:4800:ASP:OD1	2:A:4801:THR:N	2.47	0.48
2:B:2968:LEU:HD13	2:B:3029:ILE:HG12	1.96	0.48
2:B:3131:TYR:O	2:B:3135:THR:HG23	2.14	0.48
2:C:606:ARG:NH1	2:C:644:LEU:HD21	2.26	0.48
2:C:661:LEU:HD23	2:C:673:TRP:CD1	2.49	0.48
2:C:1034:PRO:HD2	2:C:1037:LEU:HD12	1.96	0.48
2:C:2565:GLN:O	2:C:2569:ILE:HG12	2.14	0.48
2:C:3184:TYR:CG	2:C:3201:VAL:HG22	2.49	0.48
2:D:318:ASP:OD1	2:D:319:LYS:N	2.45	0.48
2:D:375:GLN:HB2	2:D:390:LYS:HB3	1.95	0.48
2:D:3200:ASN:CB	2:D:3203:ASP:HB2	2.44	0.48
2:A:165:ALA:HB3	2:A:180:ASP:HB3	1.96	0.47
2:A:874:LEU:HD12	2:A:875:PRO:HD2	1.95	0.47
2:A:3269:ASN:O	2:A:3273:MET:HG3	2.14	0.47
2:B:2087:LEU:O	2:B:2091:GLN:HG2	2.13	0.47
2:B:2701:PHE:CE2	2:B:2703:PRO:HG3	2.49	0.47
2:C:19:GLU:HG2	2:C:66:THR:HB	1.95	0.47
2:C:2968:LEU:HD13	2:C:3029:ILE:HG12	1.96	0.47
2:C:3295:TRP:HB3	2:C:3298:ARG:HH21	1.79	0.47
2:D:19:GLU:HG2	2:D:66:THR:HB	1.96	0.47
2:D:913:ARG:HG3	2:D:913:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1797:GLU:HA	2:D:1800:LYS:HE3	1.96	0.47
2:D:2156:TYR:HE1	2:D:2202:TYR:HE2	1.60	0.47
2:D:3184:TYR:CG	2:D:3201:VAL:HG22	2.49	0.47
2:A:1143:GLN:HG3	2:A:1151:HIS:HA	1.96	0.47
2:A:1522:ALA:HB3	2:A:1527:LEU:HD21	1.95	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HB2	1.95	0.47
2:A:3166:PHE:CD2	2:A:3170:PHE:HB3	2.50	0.47
2:A:4268:MET:HA	2:A:4271:VAL:HG22	1.94	0.47
2:B:441:LYS:HG3	2:B:444:THR:HG23	1.96	0.47
2:B:661:LEU:HD23	2:B:673:TRP:CD1	2.49	0.47
2:B:2431:ASP:O	2:B:2435:VAL:HG23	2.14	0.47
2:C:912:LYS:HE3	2:C:914:GLN:HG3	1.96	0.47
2:C:2431:ASP:O	2:C:2435:VAL:HG23	2.14	0.47
2:C:2912:LEU:HB3	2:C:2914:THR:HG23	1.96	0.47
2:C:3848:GLU:OE1	2:C:3922:GLU:OE1	2.29	0.47
2:D:441:LYS:HG3	2:D:444:THR:HG23	1.96	0.47
2:D:2224:ASN:O	2:D:2227:VAL:HG23	2.14	0.47
2:D:2701:PHE:CE2	2:D:2703:PRO:HG3	2.49	0.47
2:D:2833:LEU:HB2	2:D:2838[B]:HIS:NE2	2.28	0.47
2:A:19:GLU:HG2	2:A:66:THR:HB	1.96	0.47
2:A:661:LEU:HD23	2:A:673:TRP:CD1	2.49	0.47
2:A:769:ARG:NH2	2:A:816:PRO:HG3	2.30	0.47
2:A:912:LYS:HE3	2:A:914:GLN:HG3	1.96	0.47
2:A:2565:GLN:O	2:A:2569:ILE:HG12	2.14	0.47
2:B:2828:MET:O	2:B:2894:LYS:NZ	2.42	0.47
2:B:3200:ASN:CB	2:B:3203:ASP:HB2	2.44	0.47
2:C:874:LEU:HD12	2:C:875:PRO:HD2	1.95	0.47
2:C:1797:GLU:HA	2:C:1800:LYS:HE3	1.96	0.47
2:C:3159:LEU:HB3	2:C:3241:MET:HE2	1.96	0.47
2:C:3166:PHE:CD2	2:C:3170:PHE:HB3	2.50	0.47
2:D:4027:THR:HG21	2:D:4084:VAL:HG11	1.97	0.47
1:I:50:GLN:NE2	1:I:54:ASN:HD21	2.13	0.47
2:A:1104:GLU:OE1	2:A:1225:LYS:NZ	2.44	0.47
2:A:2385:GLY:O	2:A:2389:MET:HG3	2.13	0.47
2:A:2496:LEU:HD23	2:A:2520:LEU:HD13	1.95	0.47
2:A:2713:ILE:HG12	2:A:2776:LYS:HB2	1.97	0.47
1:L:50:GLN:NE2	1:L:54:ASN:HD21	2.13	0.47
2:B:2224:ASN:O	2:B:2227:VAL:HG23	2.14	0.47
2:C:2456:MET:SD	2:C:2512:MET:HE1	2.55	0.47
2:C:2744:GLY:H	2:C:2755:PRO:HA	1.79	0.47
2:C:3131:TYR:OH	2:C:3205:CYS:O	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4735:ASN:HB3	2:C:4738:PHE:HD2	1.79	0.47
2:D:165:ALA:HB3	2:D:180:ASP:HB3	1.96	0.47
2:D:1552:VAL:HG12	2:D:1553:PHE:HD1	1.80	0.47
2:A:1034:PRO:HD2	2:A:1037:LEU:HD12	1.96	0.47
2:A:2350:ALA:HA	2:A:2353:ILE:HG22	1.96	0.47
2:A:2658:GLU:OE1	2:A:2661:LEU:N	2.37	0.47
2:A:3159:LEU:HB3	2:A:3241:MET:HE2	1.97	0.47
2:A:3200:ASN:CB	2:A:3203:ASP:HB2	2.44	0.47
2:A:4567:TYR:O	2:A:4567:TYR:CD1	2.68	0.47
3:F:88:HIS:HD2	3:F:89:PRO:HD2	1.79	0.47
2:B:3068:LEU:O	2:B:3071:THR:OG1	2.27	0.47
2:C:904:TYR:HE1	2:C:916:PRO:HA	1.80	0.47
2:C:2713:ILE:HG12	2:C:2776:LYS:HB2	1.97	0.47
2:C:3043:ARG:HA	2:C:3120:ASP:OD2	2.13	0.47
2:D:769:ARG:NH2	2:D:816:PRO:HG3	2.30	0.47
2:D:912:LYS:HE3	2:D:914:GLN:HG3	1.96	0.47
2:D:2431:ASP:O	2:D:2435:VAL:HG23	2.14	0.47
2:D:2886:ARG:HG2	2:D:2890:GLN:OE1	2.15	0.47
2:D:3042:ALA:HB1	2:D:3121:LEU:HB2	1.95	0.47
2:D:3131:TYR:O	2:D:3135:THR:HG23	2.14	0.47
2:D:4520:TYR:HD1	2:D:4561:LEU:HD13	1.79	0.47
2:D:4735:ASN:HB3	2:D:4738:PHE:HD2	1.79	0.47
2:A:4276:VAL:O	2:A:4280:VAL:HG23	2.15	0.47
2:A:4707:MET:HG2	2:D:4252:ILE:HG21	1.97	0.47
2:B:375:GLN:HB2	2:B:390:LYS:HB3	1.95	0.47
2:B:769:ARG:NH2	2:B:816:PRO:HG3	2.29	0.47
2:B:2794:GLU:HB2	2:B:2798:MET:HE1	1.97	0.47
2:B:2892:ILE:HG13	2:B:2893:LEU:N	2.30	0.47
2:B:4027:THR:HG21	2:B:4084:VAL:HG11	1.97	0.47
2:C:769:ARG:NH2	2:C:816:PRO:HG3	2.30	0.47
2:D:293:GLN:HG3	2:D:343:ARG:NH1	2.29	0.47
2:D:874:LEU:HD12	2:D:875:PRO:HD2	1.95	0.47
2:D:3171:LEU:HD13	2:D:3214:LEU:HD12	1.95	0.47
2:D:4800:ASP:OD1	2:D:4801:THR:N	2.47	0.47
1:I:126:ILE:O	1:I:130:ASP:N	2.48	0.47
2:A:624:ALA:HB2	2:A:1667:LEU:HD12	1.97	0.47
2:A:1286:THR:OG1	2:A:1550:PRO:O	2.22	0.47
2:A:1564:MET:HE1	2:A:1578:PRO:HA	1.97	0.47
2:A:2293:VAL:O	2:A:2296:GLU:HG2	2.15	0.47
2:A:2886:ARG:HG2	2:A:2890:GLN:OE1	2.15	0.47
2:A:2892:ILE:HG13	2:A:2893:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2946:GLY:HA3	2:A:2954:PHE:HZ	1.79	0.47
2:A:3184:TYR:CG	2:A:3201:VAL:HG22	2.49	0.47
2:A:4520:TYR:HD1	2:A:4561:LEU:HD13	1.79	0.47
2:B:883:GLU:HG2	2:B:884:LYS:N	2.28	0.47
2:B:996:VAL:HG13	2:B:1050:LEU:HD22	1.97	0.47
2:B:2001:GLU:OE1	2:B:2001:GLU:N	2.48	0.47
2:B:2886:ARG:HG2	2:B:2890:GLN:OE1	2.15	0.47
2:B:3042:ALA:HB1	2:B:3121:LEU:HD13	1.97	0.47
2:B:3184:TYR:HB3	2:B:3192:ARG:NH2	2.27	0.47
2:B:3184:TYR:CG	2:B:3201:VAL:HG22	2.49	0.47
2:B:4557:VAL:HG21	2:C:4790:ARG:HH22	1.80	0.47
2:B:4567:TYR:O	2:B:4567:TYR:CD1	2.68	0.47
2:C:514:PHE:HD2	2:C:526:TRP:HB2	1.80	0.47
2:C:891:GLU:O	2:C:895:MET:HE1	2.15	0.47
2:C:1552:VAL:HG12	2:C:1553:PHE:HD1	1.80	0.47
2:C:3246:MET:HG2	2:C:3309:LYS:HZ2	1.78	0.47
2:C:3715:GLU:OE2	2:C:4647:LYS:HE2	2.15	0.47
2:C:4800:ASP:OD1	2:C:4801:THR:N	2.47	0.47
2:D:292:GLY:HA3	2:D:340:VAL:HG21	1.96	0.47
2:D:1143:GLN:HG3	2:D:1151:HIS:HA	1.96	0.47
2:D:1564:MET:HE1	2:D:1578:PRO:HA	1.97	0.47
2:D:1729:MET:CE	2:D:1930:ASP:HB2	2.45	0.47
2:D:3131:TYR:OH	2:D:3205:CYS:O	2.23	0.47
2:D:3166:PHE:CD2	2:D:3170:PHE:HB3	2.50	0.47
2:A:441:LYS:HG3	2:A:444:THR:HG23	1.96	0.47
1:K:50:GLN:NE2	1:K:54:ASN:HD21	2.13	0.47
2:B:514:PHE:HD2	2:B:526:TRP:HB2	1.80	0.47
2:B:912:LYS:HE3	2:B:914:GLN:HG3	1.96	0.47
2:B:1718:ARG:HD3	2:B:1831:MET:HA	1.97	0.47
2:B:2153:LYS:HD3	2:B:2156:TYR:HD2	1.80	0.47
2:B:2744:GLY:H	2:B:2755:PRO:HA	1.79	0.47
2:B:2824:ARG:NH2	2:C:1502:ASN:HB3	2.30	0.47
2:B:4026:LEU:HD13	2:B:4058:TYR:HE2	1.80	0.47
2:C:293:GLN:HG3	2:C:343:ARG:NH1	2.30	0.47
2:C:1732:GLU:O	2:C:1736:ILE:HG13	2.15	0.47
2:C:2422:ILE:O	2:C:2426:LEU:HG	2.15	0.47
2:C:2946:GLY:HA3	2:C:2954:PHE:HZ	1.79	0.47
2:C:3171:LEU:HD13	2:C:3214:LEU:HD12	1.95	0.47
2:C:4567:TYR:CD1	2:C:4567:TYR:O	2.68	0.47
2:D:904:TYR:HE1	2:D:916:PRO:HA	1.79	0.47
2:A:293:GLN:HG3	2:A:343:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1552:VAL:HG12	2:A:1553:PHE:HD1	1.80	0.47
2:A:4806:CYS:HA	2:A:4812:CYS:HB2	1.97	0.47
2:B:1034:PRO:HD2	2:B:1037:LEU:HD12	1.96	0.47
2:B:1435:GLY:N	2:B:1500:ARG:HH22	2.11	0.47
2:B:2685:TYR:HD2	2:B:2686:VAL:O	1.98	0.47
2:B:3166:PHE:CD2	2:B:3170:PHE:HB3	2.50	0.47
2:B:3292:GLU:O	2:B:3296:MET:HE2	2.14	0.47
2:B:4800:ASP:OD1	2:B:4801:THR:N	2.47	0.47
2:C:165:ALA:HB3	2:C:180:ASP:HB3	1.96	0.47
2:C:292:GLY:HA3	2:C:340:VAL:HG21	1.96	0.47
2:C:2293:VAL:O	2:C:2296:GLU:HG2	2.15	0.47
2:C:2662:PHE:HE2	2:C:2962:PHE:HD1	1.62	0.47
2:C:3042:ALA:HB1	2:C:3121:LEU:HD13	1.97	0.47
2:D:913:ARG:HA	2:D:913:ARG:HD2	1.74	0.47
2:D:1176:THR:HG22	2:D:1181:ILE:HA	1.97	0.47
2:D:1435:GLY:N	2:D:1500:ARG:HH22	2.11	0.47
2:D:2642:ARG:HH12	2:D:2921:PHE:HA	1.80	0.47
2:D:2658:GLU:OE1	2:D:2661:LEU:N	2.37	0.47
2:D:2662:PHE:HE2	2:D:2962:PHE:HD1	1.62	0.47
2:D:2713:ILE:HG12	2:D:2776:LYS:HB2	1.97	0.47
2:D:3159:LEU:HB3	2:D:3241:MET:HE2	1.97	0.47
2:D:3166:PHE:O	2:D:3248:ARG:NH1	2.48	0.47
2:D:3715:GLU:OE2	2:D:4647:LYS:HE2	2.15	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HD13	1.97	0.47
2:A:3131:TYR:O	2:A:3135:THR:HG23	2.14	0.47
2:A:3166:PHE:O	2:A:3248:ARG:NH1	2.48	0.47
2:A:3316:LYS:O	2:A:3317:THR:OG1	2.33	0.47
2:A:4853:PHE:HA	2:A:4857:ILE:HD12	1.97	0.47
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.97	0.47
2:B:293:GLN:HG3	2:B:343:ARG:NH1	2.29	0.47
2:B:1729:MET:CE	2:B:1930:ASP:HB2	2.45	0.47
2:B:2293:VAL:O	2:B:2296:GLU:HG2	2.15	0.47
2:B:4648:PHE:CD1	2:B:4651:ARG:HG3	2.50	0.47
2:C:911:ASN:OD1	2:C:912:LYS:N	2.48	0.47
2:C:996:VAL:HG13	2:C:1050:LEU:HD22	1.97	0.47
2:C:1417:TYR:O	2:C:1421:MET:HG2	2.15	0.47
2:C:2350:ALA:HA	2:C:2353:ILE:HG22	1.96	0.47
2:C:4026:LEU:HD13	2:C:4058:TYR:HE2	1.80	0.47
2:C:4276:VAL:O	2:C:4280:VAL:HG23	2.15	0.47
2:D:972:LEU:HD23	2:D:973:THR:N	2.30	0.47
2:D:2422:ILE:O	2:D:2426:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4567:TYR:O	2:D:4567:TYR:CD1	2.68	0.47
2:D:4648:PHE:CD1	2:D:4651:ARG:HG3	2.50	0.47
2:A:1718:ARG:HD3	2:A:1831:MET:HA	1.97	0.46
2:A:4648:PHE:CD1	2:A:4651:ARG:HG3	2.50	0.46
2:A:4956:ASP:HA	2:A:4960:LYS:HD3	1.97	0.46
1:J:50:GLN:NE2	1:J:54:ASN:HD21	2.13	0.46
2:B:972:LEU:HD23	2:B:973:THR:N	2.30	0.46
2:B:1732:GLU:O	2:B:1736:ILE:HG13	2.15	0.46
2:B:1981:ASP:OD2	2:B:1983:LYS:NZ	2.48	0.46
2:B:2713:ILE:HG12	2:B:2776:LYS:HB2	1.97	0.46
2:B:3310:VAL:HG13	2:B:3314:LEU:HD12	1.97	0.46
2:B:4276:VAL:O	2:B:4280:VAL:HG23	2.15	0.46
2:C:1184:ASP:OD2	2:C:1193:LYS:NZ	2.38	0.46
2:C:2642:ARG:HH12	2:C:2921:PHE:HA	1.80	0.46
2:D:1417:TYR:O	2:D:1421:MET:HG2	2.15	0.46
2:D:1718:ARG:HD3	2:D:1831:MET:HA	1.97	0.46
2:D:2001:GLU:OE1	2:D:2001:GLU:N	2.48	0.46
2:D:2153:LYS:HD3	2:D:2156:TYR:HD2	1.80	0.46
2:D:2744:GLY:H	2:D:2755:PRO:HA	1.79	0.46
2:D:2892:ILE:HG13	2:D:2893:LEU:N	2.30	0.46
2:D:3042:ALA:HB1	2:D:3121:LEU:HD13	1.97	0.46
2:D:3106:SER:OG	2:D:3157:GLU:OE1	2.21	0.46
2:D:4079:ASP:O	2:D:4082:GLU:HG3	2.15	0.46
2:D:4276:VAL:O	2:D:4280:VAL:HG23	2.15	0.46
2:A:1732:GLU:O	2:A:1736:ILE:HG13	2.15	0.46
2:A:1981:ASP:OD2	2:A:1983:LYS:NZ	2.48	0.46
2:A:2001:GLU:OE1	2:A:2001:GLU:N	2.48	0.46
2:A:2422:ILE:O	2:A:2426:LEU:HG	2.15	0.46
2:A:2431:ASP:O	2:A:2435:VAL:HG23	2.14	0.46
2:A:3043:ARG:HB3	2:A:3117:PHE:CD1	2.51	0.46
2:A:3310:VAL:HG13	2:A:3314:LEU:HD12	1.97	0.46
2:B:1143:GLN:HG3	2:B:1151:HIS:HA	1.96	0.46
2:B:2891:ASP:OD1	2:B:2892:ILE:N	2.48	0.46
2:B:4079:ASP:O	2:B:4082:GLU:HG3	2.16	0.46
2:B:4853:PHE:HA	2:B:4857:ILE:HD12	1.97	0.46
2:C:1610:ARG:HA	2:C:1617:TRP:HA	1.98	0.46
2:C:2001:GLU:N	2:C:2001:GLU:OE1	2.48	0.46
2:C:2153:LYS:HD3	2:C:2156:TYR:HD2	1.80	0.46
2:C:2891:ASP:OD1	2:C:2892:ILE:N	2.48	0.46
2:C:3043:ARG:HB3	2:C:3117:PHE:CD1	2.50	0.46
2:C:3166:PHE:O	2:C:3248:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4079:ASP:O	2:C:4082:GLU:HG3	2.16	0.46
2:C:4853:PHE:HA	2:C:4857:ILE:HD12	1.97	0.46
2:D:4806:CYS:HA	2:D:4812:CYS:HB2	1.97	0.46
1:I:10:ILE:HA	1:I:13:PHE:HB2	1.97	0.46
2:A:2733:SER:HA	2:A:2736:LYS:HZ3	1.80	0.46
2:A:4079:ASP:O	2:A:4082:GLU:HG3	2.15	0.46
2:B:904:TYR:HE1	2:B:916:PRO:HA	1.80	0.46
2:B:2912:LEU:HB3	2:B:2914:THR:HG23	1.96	0.46
2:B:3166:PHE:O	2:B:3248:ARG:NH1	2.48	0.46
2:B:3715:GLU:OE2	2:B:4647:LYS:HE2	2.15	0.46
2:C:419:ILE:HD13	2:C:492:GLU:HG3	1.97	0.46
2:C:436:LEU:HD23	2:C:436:LEU:HA	1.81	0.46
2:C:2892:ILE:HG13	2:C:2893:LEU:N	2.30	0.46
2:C:4520:TYR:HD1	2:C:4561:LEU:HD13	1.80	0.46
2:C:4774:LEU:O	2:C:4778:VAL:HG23	2.16	0.46
2:D:173:GLU:OE2	2:D:176:ARG:NH2	2.36	0.46
2:A:2891:ASP:OD1	2:A:2892:ILE:N	2.48	0.46
2:A:4026:LEU:HD13	2:A:4058:TYR:HE2	1.80	0.46
3:E:19:LYS:HB2	3:E:19:LYS:HE3	1.84	0.46
1:L:10:ILE:HA	1:L:13:PHE:HB2	1.98	0.46
1:K:137:VAL:HG21	2:C:3587:TRP:CH2	2.49	0.46
2:B:19:GLU:HG2	2:B:66:THR:HB	1.96	0.46
2:B:3925:GLN:HE22	2:B:4934:THR:HA	1.80	0.46
2:B:4806:CYS:HA	2:B:4812:CYS:HB2	1.97	0.46
2:C:2172:MET:HE3	2:C:2172:MET:HA	1.98	0.46
2:C:2685:TYR:HD2	2:C:2686:VAL:O	1.98	0.46
2:C:4648:PHE:CD1	2:C:4651:ARG:HG3	2.50	0.46
2:D:1610:ARG:HA	2:D:1617:TRP:HA	1.97	0.46
2:D:2912:LEU:HB3	2:D:2914:THR:HG23	1.96	0.46
2:D:4008:ASN:OD1	2:D:4009:ASN:N	2.49	0.46
2:D:4026:LEU:HD13	2:D:4058:TYR:HE2	1.80	0.46
2:D:4853:PHE:HA	2:D:4857:ILE:HD12	1.97	0.46
2:A:2646:TRP:CH2	2:A:2928:GLN:HG3	2.51	0.46
2:A:2685:TYR:HD2	2:A:2686:VAL:O	1.98	0.46
2:A:2912:LEU:HB3	2:A:2914:THR:HG23	1.96	0.46
2:A:3604:ARG:O	2:A:3604:ARG:HD3	2.16	0.46
2:A:4008:ASN:OD1	2:A:4009:ASN:N	2.49	0.46
2:B:1176:THR:HG22	2:B:1181:ILE:HA	1.97	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:HZ	1.79	0.46
2:B:4774:LEU:O	2:B:4778:VAL:HG23	2.16	0.46
2:C:1038:LEU:O	2:C:1043:LYS:NZ	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1143:GLN:HG3	2:C:1151:HIS:HA	1.96	0.46
2:C:1718:ARG:HD3	2:C:1831:MET:HA	1.97	0.46
2:C:4027:THR:HG21	2:C:4084:VAL:HG11	1.97	0.46
2:D:624:ALA:HB2	2:D:1667:LEU:HD12	1.97	0.46
2:D:2293:VAL:O	2:D:2296:GLU:HG2	2.15	0.46
2:D:2350:ALA:HA	2:D:2353:ILE:HG22	1.96	0.46
2:D:3925:GLN:HE22	2:D:4934:THR:HA	1.80	0.46
2:A:2744:GLY:H	2:A:2755:PRO:HA	1.79	0.46
2:B:334:SER:OG	2:B:336:GLU:OE1	2.22	0.46
2:B:1552:VAL:HG12	2:B:1553:PHE:HD1	1.80	0.46
2:B:2422:ILE:O	2:B:2426:LEU:HG	2.15	0.46
2:B:3604:ARG:O	2:B:3604:ARG:HD3	2.16	0.46
2:B:4956:ASP:HA	2:B:4960:LYS:HD3	1.97	0.46
2:C:972:LEU:HD23	2:C:973:THR:N	2.30	0.46
2:C:1014:GLN:HB3	2:C:1027:ARG:HH21	1.81	0.46
2:C:1729:MET:CE	2:C:1930:ASP:HB2	2.45	0.46
2:C:2886:ARG:HG2	2:C:2890:GLN:OE1	2.15	0.46
2:C:3184:TYR:HB3	2:C:3192:ARG:NH2	2.27	0.46
2:C:3925:GLN:HE22	2:C:4934:THR:HA	1.80	0.46
2:C:4008:ASN:OD1	2:C:4009:ASN:N	2.49	0.46
2:C:4116:GLN:HA	2:C:4119:LEU:HD12	1.98	0.46
2:D:419:ILE:HD13	2:D:492:GLU:HG3	1.97	0.46
2:D:514:PHE:HD2	2:D:526:TRP:HB2	1.80	0.46
2:D:2891:ASP:OD1	2:D:2892:ILE:N	2.48	0.46
2:D:3156:GLY:O	2:D:3240:PRO:HB2	2.16	0.46
2:D:3292:GLU:O	2:D:3296:MET:HE2	2.16	0.46
2:A:902:TRP:CD1	2:A:913:ARG:NH2	2.84	0.46
2:A:972:LEU:HD23	2:A:973:THR:N	2.30	0.46
2:A:2525:LEU:HG	2:A:2569:ILE:HD13	1.98	0.46
2:A:2779:LEU:O	2:A:2782:MET:HG3	2.16	0.46
2:A:2828:MET:O	2:A:2894:LYS:NZ	2.42	0.46
2:A:2946:GLY:HA3	2:A:2954:PHE:CZ	2.51	0.46
2:A:3022:PHE:HB3	2:A:3025:ASP:OD1	2.16	0.46
2:A:3715:GLU:OE2	2:A:4647:LYS:HE2	2.15	0.46
2:A:4027:THR:HG21	2:A:4084:VAL:HG11	1.97	0.46
2:A:4735:ASN:HB3	2:A:4738:PHE:HD2	1.79	0.46
2:A:4921:PHE:HE2	2:A:4940:VAL:HG11	1.81	0.46
2:B:1417:TYR:O	2:B:1421:MET:HG2	2.15	0.46
2:B:3022:PHE:HB3	2:B:3025:ASP:OD1	2.16	0.46
2:C:1564:MET:HE1	2:C:1578:PRO:HA	1.98	0.46
2:C:3156:GLY:O	2:C:3240:PRO:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3293:GLY:HA3	2:C:3295:TRP:CZ3	2.51	0.46
2:C:4806:CYS:HA	2:C:4812:CYS:HB2	1.97	0.46
2:C:4956:ASP:HA	2:C:4960:LYS:HD3	1.97	0.46
2:D:902:TRP:CD1	2:D:913:ARG:NH2	2.84	0.46
2:D:2685:TYR:HD2	2:D:2686:VAL:O	1.98	0.46
1:I:110:MET:HA	2:A:3590:LEU:HD21	1.97	0.46
2:A:218:SER:HB3	2:A:286:GLY:HA3	1.98	0.46
2:A:1008:ALA:O	2:A:1012:ILE:HG12	2.16	0.46
2:A:2642:ARG:HH12	2:A:2921:PHE:HA	1.80	0.46
1:J:127:ARG:HD3	1:J:127:ARG:HA	1.41	0.46
2:B:1014:GLN:HB3	2:B:1027:ARG:HH21	1.81	0.46
2:B:2350:ALA:HA	2:B:2353:ILE:HG22	1.96	0.46
2:B:2629:ASN:OD1	2:B:2630:PHE:N	2.49	0.46
2:B:2779:LEU:O	2:B:2782:MET:HG3	2.16	0.46
2:B:3127:GLN:HG3	2:B:3183:ILE:HB	1.98	0.46
2:B:4008:ASN:OD1	2:B:4009:ASN:N	2.49	0.46
2:D:2525:LEU:HG	2:D:2569:ILE:HD13	1.98	0.46
2:D:2629:ASN:OD1	2:D:2630:PHE:N	2.49	0.46
2:D:3604:ARG:O	2:D:3604:ARG:HD3	2.16	0.46
2:D:4116:GLN:HA	2:D:4119:LEU:HD12	1.98	0.46
2:A:514:PHE:HD2	2:A:526:TRP:HB2	1.80	0.46
2:A:1014:GLN:HB3	2:A:1027:ARG:HH21	1.81	0.46
2:B:658:ASN:HD21	2:B:833:LYS:HG2	1.81	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:CZ	2.51	0.46
2:B:2956:TYR:HA	2:B:2959:GLU:OE1	2.16	0.46
2:B:3293:GLY:HA3	2:B:3295:TRP:CZ3	2.51	0.46
2:B:4520:TYR:HD1	2:B:4561:LEU:HD13	1.79	0.46
2:B:4921:PHE:HE2	2:B:4940:VAL:HG11	1.81	0.46
2:C:678:MET:HB2	2:C:754:VAL:HG22	1.98	0.46
2:C:2946:GLY:HA3	2:C:2954:PHE:CZ	2.51	0.46
2:D:1008:ALA:O	2:D:1012:ILE:HG12	2.16	0.46
2:D:1967:SER:O	2:D:1972:GLN:NE2	2.41	0.46
2:D:2779:LEU:O	2:D:2782:MET:HG3	2.16	0.46
2:D:3293:GLY:HA3	2:D:3295:TRP:CZ3	2.51	0.46
2:A:166:SER:OG	2:A:168:GLN:OE1	2.34	0.46
2:A:1176:THR:HG22	2:A:1181:ILE:HA	1.97	0.46
2:A:2629:ASN:OD1	2:A:2630:PHE:N	2.49	0.46
2:A:2662:PHE:HE2	2:A:2962:PHE:HD1	1.62	0.46
2:A:3848:GLU:OE1	2:A:3922:GLU:OE1	2.29	0.46
2:B:908:ARG:NH2	2:B:928:GLU:OE2	2.49	0.46
2:B:3316:LYS:O	2:B:3317:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:785:ASP:OD1	2:C:786:GLY:N	2.49	0.46
2:C:2447:LYS:HE2	2:C:2864:GLY:HA3	1.98	0.46
2:C:2629:ASN:OD1	2:C:2630:PHE:N	2.49	0.46
2:D:194:LEU:HD11	2:D:201:LEU:HB3	1.98	0.46
2:D:658:ASN:HD21	2:D:833:LYS:HG2	1.81	0.46
2:D:785:ASP:OD1	2:D:786:GLY:N	2.49	0.46
2:D:3043:ARG:HB3	2:D:3117:PHE:CD1	2.51	0.46
2:A:1729:MET:CE	2:A:1930:ASP:HB2	2.45	0.45
1:L:48:GLU:O	1:L:52:MET:HG2	2.17	0.45
1:K:126:ILE:O	1:K:130:ASP:N	2.48	0.45
2:B:2642:ARG:HH12	2:B:2921:PHE:HA	1.80	0.45
2:B:4735:ASN:HB3	2:B:4738:PHE:HD2	1.79	0.45
2:C:1981:ASP:OD2	2:C:1983:LYS:NZ	2.48	0.45
2:C:3127:GLN:HG3	2:C:3183:ILE:HB	1.98	0.45
2:D:911:ASN:OD1	2:D:912:LYS:N	2.48	0.45
2:D:996:VAL:HG13	2:D:1050:LEU:HD22	1.97	0.45
2:D:1732:GLU:O	2:D:1736:ILE:HG13	2.15	0.45
2:D:2646:TRP:CH2	2:D:2928:GLN:HG3	2.51	0.45
2:D:4269:LYS:HA	2:D:4272:LYS:HE2	1.98	0.45
2:D:4774:LEU:O	2:D:4778:VAL:HG23	2.16	0.45
1:I:48:GLU:O	1:I:52:MET:HG2	2.17	0.45
1:I:61:ASN:ND2	1:I:63:THR:O	2.50	0.45
1:I:106:LEU:HD22	2:A:3587:TRP:HE1	1.82	0.45
2:A:66:THR:OG1	2:A:124:SER:OG	2.24	0.45
2:A:1151:HIS:ND1	2:A:1185:ASP:OD1	2.32	0.45
2:A:1417:TYR:O	2:A:1421:MET:HG2	2.15	0.45
2:A:1435:GLY:N	2:A:1500:ARG:HH22	2.12	0.45
1:J:61:ASN:ND2	1:J:63:THR:O	2.50	0.45
1:K:80:THR:OG1	1:K:83:GLU:OE2	2.32	0.45
2:B:624:ALA:HB2	2:B:1667:LEU:HD12	1.97	0.45
2:B:1610:ARG:HA	2:B:1617:TRP:HA	1.98	0.45
2:B:2703:PRO:HB2	2:B:2854:LYS:HE2	1.99	0.45
2:B:2821:TYR:CE2	2:B:2823:PRO:HG3	2.51	0.45
2:B:3043:ARG:HB3	2:B:3117:PHE:CD1	2.50	0.45
2:B:3253:GLY:O	2:B:3257:ASN:HB3	2.16	0.45
2:C:658:ASN:HD21	2:C:833:LYS:HG2	1.82	0.45
2:C:1176:THR:HG22	2:C:1181:ILE:HA	1.97	0.45
2:C:2791:ARG:NH1	2:C:2796:ASP:OD2	2.50	0.45
2:C:4921:PHE:HE2	2:C:4940:VAL:HG11	1.81	0.45
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.97	0.45
2:D:891:GLU:O	2:D:895:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:989:THR:HG22	2:D:992:GLN:HG2	1.98	0.45
2:D:3022:PHE:HB3	2:D:3025:ASP:OD1	2.16	0.45
2:D:3310:VAL:HG13	2:D:3314:LEU:HD12	1.97	0.45
2:D:4956:ASP:HA	2:D:4960:LYS:HD3	1.97	0.45
2:A:887:GLU:O	2:A:891:GLU:HG2	2.17	0.45
2:A:911:ASN:OD1	2:A:912:LYS:N	2.48	0.45
2:A:3292:GLU:O	2:A:3296:MET:HE2	2.16	0.45
2:A:3963:SER:OG	2:A:3964:GLN:OE1	2.30	0.45
2:A:4774:LEU:O	2:A:4778:VAL:HG23	2.16	0.45
3:E:78:THR:O	3:E:81:VAL:HG12	2.17	0.45
1:J:10:ILE:HA	1:J:13:PHE:HB2	1.98	0.45
2:B:1008:ALA:O	2:B:1012:ILE:HG12	2.16	0.45
2:B:2972:ASP:OD1	2:B:2976:LYS:NZ	2.49	0.45
2:B:3156:GLY:O	2:B:3240:PRO:HB2	2.16	0.45
2:C:908:ARG:NH2	2:C:928:GLU:OE2	2.49	0.45
2:C:2592:LEU:HD22	2:C:2606:PRO:HB3	1.98	0.45
2:C:2956:TYR:HA	2:C:2959:GLU:OE1	2.16	0.45
2:C:2961:LYS:HB2	2:C:2965:LYS:HZ3	1.81	0.45
2:D:66:THR:OG1	2:D:124:SER:OG	2.24	0.45
2:D:166:SER:OG	2:D:168:GLN:OE1	2.34	0.45
2:D:2591:ARG:HH22	2:D:2875:ASP:CG	2.20	0.45
2:D:2956:TYR:HA	2:D:2959:GLU:OE1	2.16	0.45
2:D:4921:PHE:HE2	2:D:4940:VAL:HG11	1.81	0.45
2:A:785:ASP:OD1	2:A:786:GLY:N	2.49	0.45
2:A:1118:SER:HB2	2:A:1204:VAL:HG11	1.98	0.45
2:A:1979:PHE:HE1	2:A:1988:CYS:HB3	1.82	0.45
2:A:2791:ARG:NH1	2:A:2796:ASP:OD2	2.50	0.45
2:A:3156:GLY:O	2:A:3240:PRO:HB2	2.16	0.45
2:A:3293:GLY:HA3	2:A:3295:TRP:CZ3	2.51	0.45
3:H:78:THR:O	3:H:81:VAL:HG12	2.17	0.45
1:L:59:ASP:N	1:L:68:GLU:OE2	2.33	0.45
2:B:2106:TYR:HH	2:B:3615:ARG:HH12	1.64	0.45
2:B:2857:LYS:O	2:B:2861:GLU:OE1	2.34	0.45
2:B:4269:LYS:HA	2:B:4272:LYS:HE2	1.99	0.45
2:B:4609:LYS:HE3	2:B:4615:LEU:HD13	1.99	0.45
2:C:902:TRP:CD1	2:C:913:ARG:NH2	2.84	0.45
2:C:2646:TRP:CH2	2:C:2928:GLN:HG3	2.51	0.45
2:C:2779:LEU:O	2:C:2782:MET:HG3	2.16	0.45
2:C:2821:TYR:CE2	2:C:2823:PRO:HG3	2.51	0.45
2:C:2857:LYS:O	2:C:2861:GLU:OE1	2.34	0.45
2:C:3022:PHE:HB3	2:C:3025:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4242:ARG:HH22	2:C:4249:ARG:NH1	2.15	0.45
2:D:50:GLU:OE2	2:D:61:ASP:N	2.48	0.45
2:D:1981:ASP:OD2	2:D:1983:LYS:NZ	2.48	0.45
2:D:4242:ARG:HH22	2:D:4249:ARG:NH1	2.15	0.45
2:D:4858:LEU:HD23	2:D:4861:ILE:HD12	1.98	0.45
2:A:989:THR:HG22	2:A:992:GLN:HG2	1.98	0.45
2:A:1610:ARG:HA	2:A:1617:TRP:HA	1.98	0.45
2:A:2153:LYS:HD3	2:A:2156:TYR:HD2	1.80	0.45
2:A:2425:SER:O	2:B:142:LYS:NZ	2.49	0.45
2:A:2426:LEU:HB2	2:A:2427:ILE:HD12	1.99	0.45
2:A:2591:ARG:HH22	2:A:2875:ASP:CG	2.20	0.45
2:A:3276:LEU:O	2:A:3280:ILE:HG12	2.17	0.45
2:A:3664:LEU:O	2:A:3668:ILE:HG13	2.17	0.45
1:L:10:ILE:O	1:L:14:LYS:N	2.38	0.45
2:B:887:GLU:O	2:B:891:GLU:HG2	2.17	0.45
2:B:902:TRP:CD1	2:B:913:ARG:NH2	2.84	0.45
2:B:1979:PHE:HE1	2:B:1988:CYS:HB3	1.82	0.45
2:C:227:TYR:CG	2:C:352:SER:HB2	2.52	0.45
2:C:1008:ALA:O	2:C:1012:ILE:HG12	2.16	0.45
2:C:2640:LEU:HD23	2:C:2643:LYS:HZ1	1.82	0.45
2:C:3310:VAL:HG13	2:C:3314:LEU:HD12	1.97	0.45
2:D:908:ARG:NH2	2:D:928:GLU:OE2	2.49	0.45
2:D:2592:LEU:HD22	2:D:2606:PRO:HB3	1.98	0.45
2:D:3253:GLY:O	2:D:3257:ASN:HB3	2.16	0.45
2:A:658:ASN:HD21	2:A:833:LYS:HG2	1.82	0.45
2:A:678:MET:HB2	2:A:754:VAL:HG22	1.98	0.45
2:A:891:GLU:O	2:A:895:MET:HE1	2.17	0.45
2:A:904:TYR:HE1	2:A:916:PRO:HA	1.80	0.45
2:A:2821:TYR:CE2	2:A:2823:PRO:HG3	2.51	0.45
2:A:3107:SER:O	2:A:3111:HIS:HD2	2.00	0.45
2:A:4117:THR:O	2:A:4120:GLU:HG3	2.16	0.45
2:A:4269:LYS:HA	2:A:4272:LYS:HE2	1.99	0.45
2:A:4719:PHE:HE2	2:D:4294:LEU:HD22	1.79	0.45
1:K:10:ILE:HA	1:K:13:PHE:HB2	1.97	0.45
1:K:48:GLU:O	1:K:52:MET:HG2	2.17	0.45
1:K:127:ARG:HD3	1:K:127:ARG:HA	1.41	0.45
2:B:194:LEU:HD11	2:B:201:LEU:HB3	1.98	0.45
2:B:785:ASP:OD1	2:B:786:GLY:N	2.49	0.45
2:B:911:ASN:OD1	2:B:912:LYS:N	2.48	0.45
2:B:2646:TRP:CH2	2:B:2928:GLN:HG3	2.51	0.45
2:B:3107:SER:O	2:B:3111:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3276:LEU:O	2:B:3280:ILE:HG12	2.17	0.45
2:B:4117:THR:O	2:B:4120:GLU:HG3	2.17	0.45
2:C:2849:HIS:NE2	2:C:2877:LEU:HD11	2.32	0.45
2:C:3604:ARG:O	2:C:3604:ARG:HD3	2.16	0.45
2:C:4257:ARG:O	2:C:4261:LEU:HG	2.17	0.45
2:A:314:LEU:HD11	2:A:372:LEU:HD13	1.99	0.45
2:A:908:ARG:NH2	2:A:928:GLU:OE2	2.49	0.45
2:A:2849:HIS:NE2	2:A:2877:LEU:HD11	2.32	0.45
2:A:3187:LYS:O	2:A:3191:GLU:HB2	2.17	0.45
2:A:3925:GLN:HE22	2:A:4934:THR:HA	1.80	0.45
2:A:4714:PHE:CG	2:D:4294:LEU:HD13	2.51	0.45
3:F:78:THR:O	3:F:81:VAL:HG12	2.17	0.45
2:B:419:ILE:HD13	2:B:492:GLU:HG3	1.97	0.45
2:B:2591:ARG:HH22	2:B:2875:ASP:CG	2.20	0.45
2:B:2791:ARG:NH1	2:B:2796:ASP:OD2	2.50	0.45
2:C:624:ALA:HB2	2:C:1667:LEU:HD12	1.97	0.45
2:C:2591:ARG:HH22	2:C:2875:ASP:CG	2.20	0.45
2:C:2658:GLU:OE1	2:C:2661:LEU:N	2.37	0.45
2:C:4287:TYR:HA	2:C:4290:ILE:HD12	1.99	0.45
2:C:4609:LYS:HE3	2:C:4615:LEU:HD13	1.99	0.45
2:D:887:GLU:O	2:D:891:GLU:HG2	2.17	0.45
2:D:1151:HIS:ND1	2:D:1185:ASP:OD1	2.32	0.45
2:D:2426:LEU:HB2	2:D:2427:ILE:HD12	1.99	0.45
2:D:2640:LEU:HD23	2:D:2643:LYS:HZ1	1.81	0.45
2:D:2791:ARG:NH1	2:D:2796:ASP:OD2	2.50	0.45
2:D:2849:HIS:NE2	2:D:2877:LEU:HD11	2.32	0.45
2:D:3276:LEU:O	2:D:3280:ILE:HG12	2.17	0.45
2:D:3963:SER:OG	2:D:3964:GLN:OE1	2.30	0.45
2:D:4257:ARG:O	2:D:4261:LEU:HG	2.17	0.45
2:D:4667:SER:HA	2:D:4672:MET:HE3	1.97	0.45
2:A:436:LEU:HD23	2:A:436:LEU:HA	1.81	0.45
2:A:2347:MET:O	2:A:2351:ILE:HG12	2.17	0.45
2:A:2956:TYR:HA	2:A:2959:GLU:OE1	2.16	0.45
2:A:4257:ARG:O	2:A:4261:LEU:HG	2.17	0.45
2:B:2662:PHE:HE2	2:B:2962:PHE:HD1	1.62	0.45
2:B:2849:HIS:NE2	2:B:2877:LEU:HD11	2.32	0.45
2:B:3184:TYR:CE2	2:B:3197:LEU:HB3	2.52	0.45
2:B:4287:TYR:HA	2:B:4290:ILE:HD12	1.99	0.45
2:C:2447:LYS:HD3	2:C:2447:LYS:HA	1.80	0.45
2:D:1014:GLN:HB3	2:D:1027:ARG:HH21	1.81	0.45
2:D:3067:ASP:O	2:D:3071:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3184:TYR:HB3	2:D:3192:ARG:NH2	2.27	0.45
1:I:133:GLY:O	2:A:3298:ARG:HG2	2.17	0.45
2:A:419:ILE:HD13	2:A:492:GLU:HG3	1.97	0.45
2:A:4277:LYS:HD3	2:A:4277:LYS:HA	1.75	0.45
2:A:4609:LYS:HE3	2:A:4615:LEU:HD13	1.99	0.45
3:F:3:VAL:HG21	3:F:59:GLY:HA2	1.98	0.45
1:J:76:LYS:HB2	1:J:78:LYS:HZ2	1.81	0.45
2:B:314:LEU:HD11	2:B:372:LEU:HD13	1.99	0.45
2:B:318:ASP:OD1	2:B:319:LYS:N	2.45	0.45
2:B:527:LYS:HE2	2:B:527:LYS:HB2	1.82	0.45
2:B:989:THR:HG22	2:B:992:GLN:HG2	1.98	0.45
2:B:2447:LYS:HE2	2:B:2864:GLY:HA3	1.99	0.45
2:B:2525:LEU:HG	2:B:2569:ILE:HD13	1.98	0.45
2:B:2620:TYR:HB2	2:B:2627:TRP:HD1	1.82	0.45
2:B:4242:ARG:HH22	2:B:4249:ARG:NH1	2.15	0.45
2:C:910:ASP:OD1	2:C:911:ASN:N	2.50	0.45
2:C:3171:LEU:O	2:C:3210:SER:HA	2.17	0.45
2:C:3276:LEU:O	2:C:3280:ILE:HG12	2.17	0.45
2:D:227:TYR:CG	2:D:352:SER:HB2	2.52	0.45
2:D:2794:GLU:HB2	2:D:2798:MET:CE	2.47	0.45
2:D:2857:LYS:O	2:D:2861:GLU:OE1	2.35	0.45
2:D:2946:GLY:HA3	2:D:2954:PHE:CZ	2.51	0.45
2:D:3107:SER:O	2:D:3111:HIS:HD2	2.00	0.45
2:D:3184:TYR:CE2	2:D:3197:LEU:HB3	2.52	0.45
2:A:2703:PRO:HB2	2:A:2854:LYS:HE2	1.99	0.45
3:G:3:VAL:HG21	3:G:59:GLY:HA2	1.98	0.45
2:B:2640:LEU:HD23	2:B:2643:LYS:HZ1	1.82	0.45
2:B:3067:ASP:O	2:B:3071:THR:HG23	2.17	0.45
2:B:3664:LEU:O	2:B:3668:ILE:HG13	2.17	0.45
2:B:4116:GLN:HA	2:B:4119:LEU:HD12	1.98	0.45
2:C:218:SER:HB3	2:C:286:GLY:HA3	1.97	0.45
2:C:314:LEU:HD11	2:C:372:LEU:HD13	1.99	0.45
2:C:989:THR:HG22	2:C:992:GLN:HG2	1.98	0.45
2:C:3107:SER:O	2:C:3111:HIS:HD2	2.00	0.45
2:C:3148:VAL:HA	2:C:3151:GLN:HG3	1.99	0.45
2:C:3253:GLY:O	2:C:3257:ASN:HB3	2.16	0.45
2:C:4117:THR:O	2:C:4120:GLU:HG3	2.16	0.45
2:D:2447:LYS:HE2	2:D:2864:GLY:HA3	1.99	0.45
2:D:2821:TYR:CE2	2:D:2823:PRO:HG3	2.51	0.45
2:D:3830:LEU:HB3	2:D:3833:ASP:OD1	2.17	0.45
1:I:40:LEU:HD11	2:A:3596:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1967:SER:O	2:A:1972:GLN:NE2	2.41	0.44
2:A:2715:GLU:OE1	2:A:2715:GLU:N	2.44	0.44
2:A:3171:LEU:O	2:A:3210:SER:HA	2.17	0.44
2:A:3184:TYR:CE2	2:A:3197:LEU:HB3	2.52	0.44
2:A:4116:GLN:HA	2:A:4119:LEU:HD12	1.98	0.44
2:A:4649:VAL:O	2:A:4653:VAL:HG23	2.17	0.44
3:E:3:VAL:HG21	3:E:59:GLY:HA2	1.98	0.44
1:K:19:LEU:HD11	2:C:3595:ARG:HH21	1.82	0.44
2:B:227:TYR:CG	2:B:352:SER:HB2	2.52	0.44
2:B:3187:LYS:O	2:B:3191:GLU:HB2	2.17	0.44
2:C:3200:ASN:HB3	2:C:3203:ASP:HB2	2.00	0.44
2:D:2176:VAL:HG22	2:D:2220:TYR:CZ	2.53	0.44
2:D:4287:TYR:HA	2:D:4290:ILE:HD12	1.99	0.44
2:D:4609:LYS:HE3	2:D:4615:LEU:HD13	1.99	0.44
1:I:45:THR:HG22	2:A:3817:LEU:HD23	1.99	0.44
2:A:836:HIS:ND1	2:A:841:LYS:HE3	2.32	0.44
2:A:910:ASP:OD1	2:A:911:ASN:N	2.50	0.44
2:A:2757:MET:N	2:A:2757:MET:SD	2.91	0.44
2:A:3067:ASP:O	2:A:3071:THR:HG23	2.17	0.44
2:A:3184:TYR:HB3	2:A:3192:ARG:NH2	2.27	0.44
2:A:4949:TRP:HB3	2:A:4952:PHE:HD2	1.82	0.44
2:B:678:MET:HB2	2:B:754:VAL:HG22	1.98	0.44
2:B:2961:LYS:HB2	2:B:2965:LYS:HZ3	1.82	0.44
2:B:4858:LEU:HD23	2:B:4861:ILE:HD12	1.98	0.44
2:C:1979:PHE:HE1	2:C:1988:CYS:HB3	1.82	0.44
2:C:2715:GLU:OE1	2:C:2715:GLU:N	2.44	0.44
2:C:3184:TYR:CE2	2:C:3197:LEU:HB3	2.52	0.44
2:C:4858:LEU:HD23	2:C:4861:ILE:HD12	1.98	0.44
2:D:314:LEU:HD11	2:D:372:LEU:HD13	1.99	0.44
2:D:890:HIS:O	2:D:894:VAL:HG13	2.18	0.44
2:D:3067:ASP:HA	2:D:3070:LYS:NZ	2.29	0.44
2:D:3187:LYS:O	2:D:3191:GLU:HB2	2.17	0.44
2:D:3664:LEU:O	2:D:3668:ILE:HG13	2.17	0.44
2:D:4949:TRP:HB3	2:D:4952:PHE:HD2	1.82	0.44
2:A:194:LEU:HD11	2:A:201:LEU:HB3	1.98	0.44
2:A:2377:GLU:O	2:A:2381:THR:N	2.50	0.44
2:A:2620:TYR:HB2	2:A:2627:TRP:HD1	1.82	0.44
2:A:2794:GLU:HB2	2:A:2798:MET:CE	2.47	0.44
2:A:3127:GLN:HG3	2:A:3183:ILE:HB	1.98	0.44
2:A:3253:GLY:O	2:A:3257:ASN:HB3	2.16	0.44
2:B:1948:MET:HE2	2:B:1948:MET:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2222:LEU:HD11	2:B:2301:PHE:CZ	2.52	0.44
2:B:3122:ILE:O	2:B:3127:GLN:HG2	2.18	0.44
2:B:3240:PRO:HG3	2:B:3299:LEU:HG	2.00	0.44
2:B:3830:LEU:HB3	2:B:3833:ASP:OD1	2.18	0.44
2:B:4753:LEU:HD23	2:C:4773:LEU:HD13	1.99	0.44
2:C:877:HIS:O	2:C:880:ARG:HG3	2.18	0.44
2:C:1118:SER:HB2	2:C:1204:VAL:HG11	1.98	0.44
2:C:2176:VAL:HG22	2:C:2220:TYR:CZ	2.53	0.44
2:C:2525:LEU:HG	2:C:2569:ILE:HD13	1.98	0.44
2:D:483:LYS:HE2	2:D:483:LYS:HB2	1.68	0.44
2:A:996:VAL:HG13	2:A:1050:LEU:HD22	1.97	0.44
2:A:1852:LYS:NZ	2:A:2054:LYS:HD2	2.32	0.44
2:A:2204:CYS:SG	2:A:2214:MET:HG3	2.58	0.44
2:A:3068:LEU:O	2:A:3071:THR:OG1	2.27	0.44
2:A:4287:TYR:HA	2:A:4290:ILE:HD12	1.99	0.44
2:A:4798:ASP:N	2:A:4798:ASP:OD1	2.51	0.44
3:H:3:VAL:HG21	3:H:59:GLY:HA2	1.98	0.44
2:B:1118:SER:HB2	2:B:1204:VAL:HG11	1.98	0.44
2:B:2772:ARG:HG3	2:B:2776:LYS:HZ2	1.83	0.44
2:B:3106:SER:OG	2:B:3157:GLU:OE1	2.21	0.44
2:B:3200:ASN:HB3	2:B:3203:ASP:HB2	2.00	0.44
2:C:2794:GLU:HB2	2:C:2798:MET:CE	2.47	0.44
2:C:4269:LYS:HA	2:C:4272:LYS:HE2	1.99	0.44
2:C:4649:VAL:O	2:C:4653:VAL:HG23	2.17	0.44
2:D:2831:VAL:HB	2:D:2894:LYS:CE	2.47	0.44
2:D:3001:LYS:NZ	2:D:3041:ASP:OD2	2.33	0.44
2:D:3171:LEU:O	2:D:3210:SER:HA	2.17	0.44
2:D:3200:ASN:HB3	2:D:3203:ASP:HB2	2.00	0.44
2:D:4117:THR:O	2:D:4120:GLU:HG3	2.17	0.44
2:D:4649:VAL:O	2:D:4653:VAL:HG23	2.17	0.44
2:A:227:TYR:CG	2:A:352:SER:HB2	2.52	0.44
2:A:874:LEU:HB3	2:A:879:GLU:OE2	2.18	0.44
2:A:877:HIS:O	2:A:880:ARG:HG3	2.18	0.44
2:A:1100:ARG:HB3	2:A:1236:TYR:CD2	2.53	0.44
2:A:2640:LEU:HA	2:A:2643:LYS:HZ1	1.82	0.44
2:A:3830:LEU:HB3	2:A:3833:ASP:OD1	2.17	0.44
2:C:836:HIS:ND1	2:C:841:LYS:HE3	2.32	0.44
2:C:2757:MET:N	2:C:2757:MET:SD	2.91	0.44
2:C:4511:PHE:HZ	2:C:4746:ILE:HG21	1.83	0.44
2:D:1564:MET:CE	2:D:1565:PRO:HD2	2.48	0.44
2:D:3122:ILE:O	2:D:3127:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3744:ILE:O	2:D:3747:SER:OG	2.31	0.44
2:D:4093:ASP:OD1	2:D:4094:ILE:HD12	2.18	0.44
2:A:2176:VAL:HG22	2:A:2220:TYR:CZ	2.53	0.44
3:G:78:THR:O	3:G:81:VAL:HG12	2.17	0.44
1:J:42:GLN:HE21	2:B:1957:LEU:HD21	1.82	0.44
1:L:126:ILE:O	1:L:130:ASP:N	2.48	0.44
1:K:121:GLU:O	1:K:124:GLU:HB2	2.18	0.44
2:B:335:LYS:HZ1	2:B:397:GLY:HA3	1.81	0.44
2:B:1852:LYS:NZ	2:B:2054:LYS:HD2	2.32	0.44
2:B:2176:VAL:HG22	2:B:2220:TYR:CZ	2.53	0.44
2:B:2377:GLU:O	2:B:2381:THR:N	2.50	0.44
2:B:2592:LEU:HD22	2:B:2606:PRO:HB3	1.98	0.44
2:B:4649:VAL:O	2:B:4653:VAL:HG23	2.17	0.44
2:B:4798:ASP:OD1	2:B:4798:ASP:N	2.51	0.44
2:C:194:LEU:HD11	2:C:201:LEU:HB3	1.98	0.44
2:C:1852:LYS:NZ	2:C:2054:LYS:HD2	2.32	0.44
2:C:2377:GLU:O	2:C:2381:THR:N	2.50	0.44
2:C:3067:ASP:O	2:C:3071:THR:HG23	2.17	0.44
2:D:910:ASP:OD1	2:D:911:ASN:N	2.50	0.44
2:D:949:HIS:O	2:D:1065:GLU:N	2.51	0.44
2:D:2347:MET:O	2:D:2351:ILE:HG12	2.17	0.44
2:D:3127:GLN:HG3	2:D:3183:ILE:HB	1.98	0.44
2:D:4511:PHE:HZ	2:D:4746:ILE:HG21	1.83	0.44
2:D:4798:ASP:OD1	2:D:4798:ASP:N	2.51	0.44
2:A:3200:ASN:HB3	2:A:3203:ASP:HB2	2.00	0.44
2:A:3955:GLN:HE21	2:A:3972:MET:HG2	1.83	0.44
1:L:61:ASN:ND2	1:L:63:THR:O	2.50	0.44
2:B:891:GLU:O	2:B:895:MET:HE1	2.18	0.44
2:B:1564:MET:CE	2:B:1565:PRO:HD2	2.48	0.44
2:B:2383:HIS:CG	2:B:2458:ALA:HB2	2.53	0.44
2:B:2426:LEU:HB2	2:B:2427:ILE:HD12	1.99	0.44
2:B:4093:ASP:OD1	2:B:4094:ILE:HD12	2.18	0.44
2:B:4511:PHE:HZ	2:B:4746:ILE:HG21	1.83	0.44
2:C:21:VAL:HB	2:C:36:CYS:SG	2.58	0.44
2:C:2426:LEU:HB2	2:C:2427:ILE:HD12	1.99	0.44
2:D:1100:ARG:HB3	2:D:1236:TYR:CD2	2.53	0.44
2:D:1979:PHE:HE1	2:D:1988:CYS:HB3	1.82	0.44
2:D:2222:LEU:HD11	2:D:2301:PHE:CZ	2.52	0.44
2:D:2733:SER:HA	2:D:2736:LYS:HZ3	1.82	0.44
1:I:122:VAL:HA	1:I:125:MET:HE3	2.00	0.44
2:A:515:ALA:HB2	2:A:523:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2222:LEU:HD23	2:A:2222:LEU:HA	1.88	0.44
2:A:2447:LYS:HE2	2:A:2864:GLY:HA3	1.99	0.44
2:A:2857:LYS:O	2:A:2861:GLU:OE1	2.34	0.44
2:A:3122:ILE:O	2:A:3127:GLN:HG2	2.18	0.44
2:A:3246:MET:HG2	2:A:3309:LYS:HZ2	1.81	0.44
2:A:4242:ARG:HH22	2:A:4249:ARG:NH1	2.15	0.44
2:A:4707:MET:HA	2:D:4252:ILE:HG21	2.00	0.44
1:L:121:GLU:O	1:L:124:GLU:HB2	2.18	0.44
2:B:903:GLN:H	2:B:913:ARG:NE	2.16	0.44
2:B:3955:GLN:HE21	2:B:3972:MET:HG2	1.83	0.44
2:B:4257:ARG:O	2:B:4261:LEU:HG	2.17	0.44
2:C:887:GLU:O	2:C:891:GLU:HG2	2.17	0.44
2:C:2844:MET:SD	2:C:2888:LYS:NZ	2.91	0.44
2:C:3163:ALA:HB1	2:C:3245:TYR:CD1	2.52	0.44
2:C:3955:GLN:HE21	2:C:3972:MET:HG2	1.83	0.44
2:D:836:HIS:ND1	2:D:841:LYS:HE3	2.32	0.44
2:D:1286:THR:OG1	2:D:1550:PRO:O	2.22	0.44
2:D:2620:TYR:HB2	2:D:2627:TRP:HD1	1.82	0.44
1:I:121:GLU:O	1:I:124:GLU:HB2	2.18	0.44
2:A:2772:ARG:HG3	2:A:2776:LYS:HZ2	1.83	0.44
2:A:2926:LEU:HD23	2:A:2929:LEU:HD12	2.00	0.44
2:A:3240:PRO:HG3	2:A:3299:LEU:HG	2.00	0.44
2:A:4591:TYR:CD2	2:D:4287:TYR:HE1	2.36	0.44
3:G:50:ARG:HH21	3:G:53:LYS:NZ	2.16	0.44
2:B:836:HIS:ND1	2:B:841:LYS:HE3	2.33	0.44
2:B:874:LEU:HB3	2:B:879:GLU:OE2	2.18	0.44
2:B:1100:ARG:HB3	2:B:1236:TYR:CD2	2.53	0.44
2:B:2347:MET:O	2:B:2351:ILE:HG12	2.17	0.44
2:B:2794:GLU:HB2	2:B:2798:MET:CE	2.47	0.44
2:B:3171:LEU:O	2:B:3210:SER:HA	2.18	0.44
2:C:335:LYS:HZ1	2:C:397:GLY:HA3	1.83	0.44
2:C:637:LEU:HD22	2:C:1679:HIS:CD2	2.53	0.44
2:C:948:CYS:HA	2:C:1067:PRO:HD3	2.00	0.44
2:C:1100:ARG:HB3	2:C:1236:TYR:CD2	2.53	0.44
2:C:1283:LEU:HB2	2:C:1555:PHE:HB2	2.00	0.44
2:C:2620:TYR:HB2	2:C:2627:TRP:HD1	1.82	0.44
2:C:4731:LEU:HD23	2:C:4734:TYR:HD2	1.83	0.44
2:D:675:TYR:HB3	2:D:822:CYS:SG	2.58	0.44
2:D:874:LEU:HB3	2:D:879:GLU:OE2	2.18	0.44
2:D:948:CYS:HA	2:D:1067:PRO:HD3	2.00	0.44
2:D:1433:PHE:O	2:D:1500:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1852:LYS:NZ	2:D:2054:LYS:HD2	2.32	0.44
2:D:2926:LEU:HD23	2:D:2929:LEU:HD12	2.00	0.44
2:D:3955:GLN:HE21	2:D:3972:MET:HG2	1.83	0.44
2:D:4731:LEU:HD23	2:D:4734:TYR:HD2	1.83	0.44
2:A:890:HIS:O	2:A:894:VAL:HG13	2.18	0.43
2:A:949:HIS:O	2:A:1065:GLU:N	2.51	0.43
2:A:2222:LEU:HD11	2:A:2301:PHE:CZ	2.52	0.43
2:A:2383:HIS:CG	2:A:2458:ALA:HB2	2.53	0.43
2:A:3292:GLU:O	2:A:3292:GLU:HG2	2.18	0.43
2:A:3589:LYS:HE2	2:A:3589:LYS:HB2	1.74	0.43
2:A:4858:LEU:HD23	2:A:4861:ILE:HD12	1.98	0.43
1:J:121:GLU:O	1:J:124:GLU:HB2	2.18	0.43
2:B:890:HIS:O	2:B:894:VAL:HG13	2.18	0.43
2:B:910:ASP:OD1	2:B:911:ASN:N	2.50	0.43
2:B:1132:GLU:HA	2:B:1146:HIS:CE1	2.53	0.43
2:B:2943:PHE:O	2:B:2947:SER:OG	2.25	0.43
2:B:3697:LYS:HA	2:B:3700:HIS:CD2	2.53	0.43
2:C:874:LEU:HB3	2:C:879:GLU:OE2	2.18	0.43
2:C:1433:PHE:O	2:C:1500:ARG:NH1	2.51	0.43
2:C:2204:CYS:SG	2:C:2214:MET:HG3	2.58	0.43
2:C:2824:ARG:O	2:C:2824:ARG:HD2	2.18	0.43
2:C:3664:LEU:O	2:C:3668:ILE:HG13	2.17	0.43
2:C:3830:LEU:HB3	2:C:3833:ASP:OD1	2.17	0.43
2:C:4949:TRP:HB3	2:C:4952:PHE:HD2	1.83	0.43
2:D:637:LEU:HD22	2:D:1679:HIS:CD2	2.53	0.43
2:D:678:MET:HB2	2:D:754:VAL:HG22	1.98	0.43
2:D:2377:GLU:O	2:D:2381:THR:N	2.50	0.43
2:D:2757:MET:SD	2:D:2757:MET:N	2.91	0.43
2:D:3188:SER:O	2:D:3192:ARG:HB2	2.18	0.43
2:A:21:VAL:HB	2:A:36:CYS:SG	2.58	0.43
2:A:675:TYR:HB3	2:A:822:CYS:SG	2.58	0.43
2:A:3148:VAL:HA	2:A:3151:GLN:HG3	2.00	0.43
2:A:4093:ASP:OD1	2:A:4094:ILE:HD12	2.18	0.43
2:A:4630:TRP:HE3	2:D:4245:LEU:HD23	1.81	0.43
3:G:83:TYR:OH	2:C:1768:PHE:O	2.24	0.43
2:B:877:HIS:O	2:B:880:ARG:HG3	2.18	0.43
2:B:2204:CYS:SG	2:B:2214:MET:HG3	2.58	0.43
2:B:3148:VAL:HA	2:B:3151:GLN:HG3	1.99	0.43
2:C:1564:MET:CE	2:C:1565:PRO:HD2	2.48	0.43
2:C:2062:ILE:HG21	2:C:2087:LEU:HG	1.99	0.43
2:C:3122:ILE:O	2:C:3127:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3187:LYS:O	2:C:3191:GLU:HB2	2.17	0.43
2:C:4093:ASP:OD1	2:C:4094:ILE:HD12	2.18	0.43
2:D:853:PRO:HG2	2:D:1084:ARG:O	2.18	0.43
2:D:874:LEU:HD23	2:D:879:GLU:HG3	2.00	0.43
2:D:1118:SER:HB2	2:D:1204:VAL:HG11	1.98	0.43
2:D:2204:CYS:SG	2:D:2214:MET:HG3	2.58	0.43
2:D:2646:TRP:CZ3	2:D:2928:GLN:HG3	2.54	0.43
2:D:2703:PRO:HB2	2:D:2854:LYS:HE2	1.99	0.43
2:D:2828:MET:O	2:D:2894:LYS:NZ	2.42	0.43
1:I:59:ASP:N	1:I:68:GLU:OE2	2.33	0.43
1:I:137:VAL:HG21	2:A:3587:TRP:CH2	2.53	0.43
2:A:2592:LEU:HD22	2:A:2606:PRO:HB3	1.98	0.43
2:A:2646:TRP:CZ3	2:A:2928:GLN:HG3	2.53	0.43
2:A:3946:GLY:O	2:A:3950:VAL:HG23	2.18	0.43
1:J:126:ILE:O	1:J:130:ASP:N	2.48	0.43
1:L:80:THR:OG1	1:L:83:GLU:OE2	2.32	0.43
2:B:21:VAL:HB	2:B:36:CYS:SG	2.58	0.43
2:B:913:ARG:HA	2:B:913:ARG:HD2	1.74	0.43
2:B:1564:MET:HE1	2:B:1578:PRO:HA	2.00	0.43
2:B:2705:PRO:HG3	2:B:2854:LYS:HZ2	1.83	0.43
2:B:2757:MET:N	2:B:2757:MET:SD	2.91	0.43
2:B:4731:LEU:HD23	2:B:4734:TYR:HD2	1.83	0.43
2:B:4949:TRP:HB3	2:B:4952:PHE:HD2	1.83	0.43
2:C:902:TRP:CD2	2:C:913:ARG:CZ	3.01	0.43
2:C:1132:GLU:HA	2:C:1146:HIS:CE1	2.54	0.43
2:C:2222:LEU:HD11	2:C:2301:PHE:CZ	2.52	0.43
2:C:2943:PHE:O	2:C:2947:SER:OG	2.25	0.43
2:C:4277:LYS:HD3	2:C:4277:LYS:HA	1.75	0.43
2:D:877:HIS:O	2:D:880:ARG:HG3	2.18	0.43
2:D:1446:ILE:HG12	2:D:1542:ALA:HB2	2.00	0.43
2:A:1446:ILE:HG12	2:A:1542:ALA:HB2	2.00	0.43
2:A:2000:HIS:O	2:A:2004:MET:HG2	2.18	0.43
2:A:3067:ASP:HA	2:A:3070:LYS:NZ	2.29	0.43
2:A:3131:TYR:HE1	2:A:3208:ILE:HB	1.84	0.43
1:L:122:VAL:HA	1:L:125:MET:HE3	2.01	0.43
1:K:15:GLU:O	1:K:19:LEU:HG	2.19	0.43
2:B:675:TYR:HB3	2:B:822:CYS:SG	2.58	0.43
2:B:1452:GLN:HE22	2:B:1484:ASN:ND2	2.16	0.43
2:B:2150:MET:O	2:B:2156:TYR:OH	2.26	0.43
2:B:2824:ARG:HD2	2:B:2824:ARG:O	2.18	0.43
2:B:3589:LYS:HB2	2:B:3589:LYS:HE2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2347:MET:O	2:C:2351:ILE:HG12	2.17	0.43
2:C:2383:HIS:CG	2:C:2458:ALA:HB2	2.53	0.43
2:C:2926:LEU:HD23	2:C:2929:LEU:HD12	2.00	0.43
2:D:2157:GLN:O	2:D:3615:ARG:NH2	2.52	0.43
2:D:3148:VAL:HA	2:D:3151:GLN:HG3	1.99	0.43
2:A:14:LEU:HG	2:A:177:VAL:HA	2.00	0.43
2:A:1132:GLU:HA	2:A:1146:HIS:CE1	2.54	0.43
2:A:4057:HIS:CE1	2:B:4660:PHE:CZ	3.04	0.43
2:A:4630:TRP:CH2	2:D:4248:LEU:HB3	2.54	0.43
3:H:50:ARG:HH21	3:H:53:LYS:NZ	2.16	0.43
3:H:79:PRO:O	3:H:84:GLY:HA2	2.19	0.43
2:B:897:LYS:HA	2:B:900:LEU:HB2	2.01	0.43
2:B:948:CYS:HA	2:B:1067:PRO:HD3	2.00	0.43
2:B:1039:ASP:OD1	2:B:1042:THR:HB	2.18	0.43
2:B:2844:MET:SD	2:B:2888:LYS:NZ	2.91	0.43
2:C:648:LEU:HD23	2:C:648:LEU:HA	1.89	0.43
2:C:890:HIS:O	2:C:894:VAL:HG13	2.18	0.43
2:C:1988:CYS:HA	2:C:1989:PRO:HD3	1.87	0.43
2:D:2000:HIS:O	2:D:2004:MET:HG2	2.18	0.43
2:D:3253:GLY:C	2:D:3255:GLU:N	2.72	0.43
1:I:76:LYS:HB2	1:I:78:LYS:HZ2	1.84	0.43
2:A:2926:LEU:HD23	2:A:2926:LEU:HA	1.87	0.43
2:A:3253:GLY:C	2:A:3255:GLU:N	2.72	0.43
2:A:3650:GLU:HB2	2:A:3651:PRO:HD3	2.01	0.43
1:J:48:GLU:O	1:J:52:MET:HG2	2.17	0.43
1:J:122:VAL:HA	1:J:125:MET:HE3	2.01	0.43
2:B:637:LEU:HD22	2:B:1679:HIS:CD2	2.53	0.43
2:B:2427:ILE:HD13	2:B:2471:PHE:CZ	2.54	0.43
2:B:2926:LEU:HD23	2:B:2929:LEU:HD12	2.00	0.43
2:C:483:LYS:HB2	2:C:483:LYS:HE2	1.68	0.43
2:C:897:LYS:HA	2:C:900:LEU:HB2	2.01	0.43
2:C:949:HIS:O	2:C:1065:GLU:N	2.51	0.43
2:C:2646:TRP:CZ3	2:C:2928:GLN:HG3	2.54	0.43
2:D:515:ALA:HB2	2:D:523:GLY:HA3	2.00	0.43
2:D:2785:TRP:HE1	2:D:2905:ARG:HH12	1.67	0.43
2:D:2824:ARG:HD2	2:D:2824:ARG:O	2.18	0.43
2:D:3102:LEU:HD12	2:D:3102:LEU:HA	1.86	0.43
2:D:3240:PRO:HG3	2:D:3299:LEU:HG	2.00	0.43
2:A:897:LYS:HA	2:A:900:LEU:HB2	2.01	0.43
2:A:3016:ARG:O	2:A:3018:ARG:NE	2.32	0.43
3:F:50:ARG:HH21	3:F:53:LYS:NZ	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67:MET:HE2	3:F:104:LEU:HB2	2.01	0.43
1:K:10:ILE:O	1:K:14:LYS:N	2.38	0.43
2:B:949:HIS:O	2:B:1065:GLU:N	2.51	0.43
2:B:1433:PHE:O	2:B:1500:ARG:NH1	2.51	0.43
2:B:2658:GLU:OE1	2:B:2661:LEU:N	2.37	0.43
2:B:2945:GLY:HA2	2:B:2948:ARG:CZ	2.49	0.43
2:C:675:TYR:HB3	2:C:822:CYS:SG	2.58	0.43
2:C:694:ARG:NH1	2:C:718:VAL:O	2.49	0.43
2:C:968:LYS:HA	2:C:968:LYS:HD2	1.91	0.43
2:C:1183:LEU:HB3	2:C:1189:GLU:OE1	2.19	0.43
2:C:1260:GLN:OE1	2:C:1261:VAL:N	2.52	0.43
2:C:1538:LYS:HD2	2:C:1636:ASN:ND2	2.34	0.43
2:C:1724:GLU:HG2	2:C:2165:LEU:HD23	2.00	0.43
2:C:2000:HIS:O	2:C:2004:MET:HG2	2.18	0.43
2:C:2907:PHE:CE2	2:C:2909:ASP:HA	2.54	0.43
2:C:4107:GLU:OE2	2:C:4149:TYR:OH	2.15	0.43
2:D:902:TRP:CD2	2:D:913:ARG:CZ	3.01	0.43
2:D:1436:GLN:H	2:D:1500:ARG:HH12	1.67	0.43
2:D:2222:LEU:HD23	2:D:2222:LEU:HA	1.89	0.43
2:D:3198:PRO:O	2:D:3199:THR:OG1	2.33	0.43
2:D:3697:LYS:HA	2:D:3700:HIS:CD2	2.54	0.43
2:A:483:LYS:HE2	2:A:483:LYS:HB2	1.68	0.43
2:A:637:LEU:HD22	2:A:1679:HIS:CD2	2.53	0.43
2:A:913:ARG:HA	2:A:913:ARG:HD2	1.74	0.43
2:A:1433:PHE:O	2:A:1500:ARG:NH1	2.51	0.43
2:A:1724:GLU:HG2	2:A:2165:LEU:HD23	2.00	0.43
2:A:2436:ILE:HA	2:A:2465:LYS:HE3	2.01	0.43
2:A:3188:SER:O	2:A:3192:ARG:HB2	2.18	0.43
2:A:3697:LYS:HA	2:A:3700:HIS:CD2	2.54	0.43
2:A:4689:LYS:HD2	2:A:4689:LYS:HA	1.82	0.43
3:E:79:PRO:O	3:E:84:GLY:HA2	2.19	0.43
3:F:79:PRO:O	3:F:84:GLY:HA2	2.19	0.43
3:G:67:MET:HE2	3:G:104:LEU:HB2	2.01	0.43
3:G:79:PRO:O	3:G:84:GLY:HA2	2.19	0.43
1:J:117:LEU:HD23	1:J:118:THR:N	2.34	0.43
1:K:117:LEU:HD23	1:K:118:THR:N	2.34	0.43
2:B:902:TRP:CD2	2:B:913:ARG:CZ	3.01	0.43
2:B:1081:THR:OG1	2:B:1082:GLY:N	2.51	0.43
2:B:1283:LEU:HB2	2:B:1555:PHE:HB2	2.00	0.43
2:B:1538:LYS:HD2	2:B:1636:ASN:ND2	2.34	0.43
2:B:1714:TYR:CE2	2:B:1718:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:515:ALA:HB2	2:C:523:GLY:HA3	2.00	0.43
2:C:874:LEU:HD23	2:C:879:GLU:HG3	2.01	0.43
2:C:2972:ASP:OD1	2:C:2976:LYS:NZ	2.49	0.43
2:C:3188:SER:O	2:C:3192:ARG:HB2	2.18	0.43
2:D:1107:THR:OG1	2:D:1160:ASP:O	2.26	0.43
2:D:1183:LEU:HB3	2:D:1189:GLU:OE1	2.19	0.43
2:D:1260:GLN:OE1	2:D:1261:VAL:N	2.52	0.43
2:D:2106:TYR:HH	2:D:3615:ARG:HH12	1.67	0.43
2:A:902:TRP:CD2	2:A:913:ARG:CZ	3.01	0.43
2:A:1649:GLU:HG2	2:A:1650:LEU:N	2.34	0.43
2:A:2824:ARG:HD2	2:A:2824:ARG:O	2.18	0.43
2:A:2831:VAL:HB	2:A:2894:LYS:CE	2.47	0.43
2:A:2945:GLY:HA2	2:A:2948:ARG:CZ	2.49	0.43
2:A:3743:THR:HB	2:A:3758:THR:HG21	2.01	0.43
2:A:4237:SER:O	2:A:4240:THR:OG1	2.37	0.43
2:A:4511:PHE:HZ	2:A:4746:ILE:HG21	1.83	0.43
1:K:114:GLY:O	1:K:116:LYS:NZ	2.31	0.43
2:B:166:SER:OG	2:B:168:GLN:OE1	2.34	0.43
2:B:1151:HIS:ND1	2:B:1185:ASP:OD1	2.32	0.43
2:B:1183:LEU:HB3	2:B:1189:GLU:OE1	2.19	0.43
2:B:2157:GLN:O	2:B:3615:ARG:NH2	2.52	0.43
2:B:2733:SER:HA	2:B:2736:LYS:HZ3	1.83	0.43
2:B:3188:SER:O	2:B:3192:ARG:HB2	2.18	0.43
2:B:4735:ASN:HB3	2:B:4738:PHE:CD2	2.54	0.43
2:C:940:LEU:HD12	2:C:941:LYS:N	2.34	0.43
2:C:1452:GLN:HE22	2:C:1484:ASN:ND2	2.16	0.43
2:C:2427:ILE:HD13	2:C:2471:PHE:CZ	2.54	0.43
2:C:2945:GLY:HA2	2:C:2948:ARG:CZ	2.49	0.43
2:C:4663:ARG:HA	2:C:4663:ARG:HD2	1.88	0.43
2:D:21:VAL:HB	2:D:36:CYS:SG	2.58	0.43
2:D:940:LEU:HD12	2:D:941:LYS:N	2.34	0.43
2:D:1948:MET:HA	2:D:1948:MET:HE2	2.00	0.43
2:D:3655:ASP:HB2	2:D:3660:ARG:HE	1.84	0.43
1:I:80:THR:OG1	1:I:83:GLU:OE2	2.32	0.43
1:I:127:ARG:HD3	1:I:127:ARG:HA	1.41	0.43
2:A:1304:LEU:HD23	2:A:1304:LEU:HA	1.90	0.43
2:A:1512:ASP:OD2	2:A:1515:SER:OG	2.26	0.43
2:A:1931:ASP:OD1	2:A:1932:PHE:N	2.52	0.43
2:B:2062:ILE:HG21	2:B:2087:LEU:HG	2.00	0.43
2:B:3149:GLU:OE2	2:B:3232:PRO:HG2	2.19	0.43
2:B:3292:GLU:O	2:B:3292:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3946:GLY:O	2:B:3950:VAL:HG23	2.18	0.43
2:C:853:PRO:HG2	2:C:1084:ARG:O	2.18	0.43
2:C:2259:GLU:HB2	2:C:2260:PRO:HD3	2.01	0.43
2:C:2703:PRO:HB2	2:C:2854:LYS:HE2	1.99	0.43
2:C:2733:SER:HA	2:C:2736:LYS:HZ3	1.82	0.43
2:D:1714:TYR:CE2	2:D:1718:ARG:HD2	2.54	0.43
2:D:2907:PHE:CE2	2:D:2909:ASP:HA	2.54	0.43
1:I:6:THR:O	1:I:10:ILE:HD12	2.19	0.42
2:A:4731:LEU:HD23	2:A:4734:TYR:HD2	1.83	0.42
1:K:61:ASN:ND2	1:K:63:THR:O	2.50	0.42
1:K:76:LYS:HB2	1:K:78:LYS:HZ2	1.84	0.42
1:K:122:VAL:HA	1:K:125:MET:HE3	2.01	0.42
2:B:940:LEU:HD12	2:B:941:LYS:N	2.34	0.42
2:B:1166:VAL:HG23	2:B:1173:MET:HG2	2.01	0.42
2:B:2259:GLU:HB2	2:B:2260:PRO:HD3	2.01	0.42
2:B:2646:TRP:CZ3	2:B:2928:GLN:HG3	2.53	0.42
2:C:14:LEU:HG	2:C:177:VAL:HA	2.00	0.42
2:C:765:SER:HA	2:C:779:PHE:O	2.19	0.42
2:C:1039:ASP:OD1	2:C:1042:THR:HB	2.18	0.42
2:C:1649:GLU:HG2	2:C:1650:LEU:N	2.34	0.42
2:C:2157:GLN:O	2:C:3615:ARG:NH2	2.51	0.42
2:C:3149:GLU:OE2	2:C:3232:PRO:HG2	2.19	0.42
2:C:3689:MET:CE	2:C:3753:PRO:HB2	2.49	0.42
2:C:3697:LYS:HA	2:C:3700:HIS:CD2	2.54	0.42
2:D:737:ILE:HD13	2:D:1482:ARG:HD3	2.00	0.42
2:D:1132:GLU:HA	2:D:1146:HIS:CE1	2.54	0.42
2:D:2259:GLU:HB2	2:D:2260:PRO:HD3	2.01	0.42
2:D:2436:ILE:HA	2:D:2465:LYS:HE3	2.01	0.42
2:D:2844:MET:SD	2:D:2888:LYS:NZ	2.91	0.42
2:D:2945:GLY:HA2	2:D:2948:ARG:CZ	2.49	0.42
2:D:3292:GLU:O	2:D:3292:GLU:HG2	2.18	0.42
2:D:3946:GLY:O	2:D:3950:VAL:HG23	2.18	0.42
2:D:4735:ASN:HB3	2:D:4738:PHE:CD2	2.54	0.42
2:D:4964:ASP:OD1	2:D:4965:GLN:N	2.52	0.42
2:A:318:ASP:OD1	2:A:319:LYS:N	2.45	0.42
2:A:1039:ASP:OD1	2:A:1042:THR:HB	2.18	0.42
2:A:1166:VAL:HG23	2:A:1173:MET:HG2	2.01	0.42
2:A:1538:LYS:HD2	2:A:1636:ASN:ND2	2.34	0.42
2:A:2259:GLU:HB2	2:A:2260:PRO:HD3	2.01	0.42
2:A:3088:LYS:HG3	2:A:3090:VAL:HG22	2.01	0.42
2:A:3180:ILE:HG23	2:A:3181:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:GLU:O	1:J:19:LEU:HG	2.19	0.42
1:L:19:LEU:HD11	2:D:3595:ARG:HH21	1.84	0.42
1:K:6:THR:O	1:K:10:ILE:HD12	2.19	0.42
1:K:36:VAL:O	1:K:39:SER:OG	2.27	0.42
2:B:3180:ILE:HG23	2:B:3181:TYR:CD1	2.54	0.42
2:B:3192:ARG:O	2:B:3197:LEU:HB2	2.20	0.42
2:C:274:LEU:HD23	2:C:274:LEU:HA	1.81	0.42
2:C:1962:THR:HG22	2:C:1966:ARG:HG3	2.02	0.42
2:C:3131:TYR:HE1	2:C:3208:ILE:HB	1.84	0.42
2:C:3134:LEU:HD22	2:C:3162:PHE:CE2	2.54	0.42
2:C:3188:SER:O	2:C:3192:ARG:CB	2.67	0.42
2:C:3946:GLY:O	2:C:3950:VAL:HG23	2.18	0.42
2:D:765:SER:HA	2:D:779:PHE:O	2.19	0.42
2:D:1724:GLU:HG2	2:D:2165:LEU:HD23	2.00	0.42
2:D:2383:HIS:CG	2:D:2458:ALA:HB2	2.53	0.42
2:D:3693:ASP:O	2:D:3697:LYS:HG2	2.19	0.42
1:I:15:GLU:O	1:I:19:LEU:HG	2.19	0.42
2:A:261:HIS:CE1	2:A:388:GLN:HE22	2.37	0.42
2:A:1183:LEU:HB3	2:A:1189:GLU:OE1	2.19	0.42
2:A:1220:ASP:O	2:A:1223:THR:OG1	2.37	0.42
2:A:1452:GLN:HE22	2:A:1484:ASN:ND2	2.16	0.42
2:A:1564:MET:CE	2:A:1565:PRO:HD2	2.48	0.42
2:A:1825:PHE:CE1	2:A:1842:ILE:HG12	2.54	0.42
2:A:2062:ILE:HG21	2:A:2087:LEU:HG	2.00	0.42
2:A:2427:ILE:HD13	2:A:2471:PHE:CZ	2.54	0.42
2:A:3655:ASP:HB2	2:A:3660:ARG:HE	1.84	0.42
2:A:4735:ASN:HB3	2:A:4738:PHE:CD2	2.54	0.42
2:A:4809:MET:HB2	2:D:4520:TYR:O	2.19	0.42
1:L:89:ALA:HA	1:L:92:VAL:HG22	2.01	0.42
2:B:561:ARG:HG3	2:B:561:ARG:NH1	2.34	0.42
2:B:1446:ILE:HG12	2:B:1542:ALA:HB2	2.00	0.42
2:B:1931:ASP:OD1	2:B:1932:PHE:N	2.52	0.42
2:B:3125:ASP:H	2:B:3183:ILE:CD1	2.32	0.42
2:B:3131:TYR:HE1	2:B:3208:ILE:HB	1.84	0.42
2:B:3655:ASP:HB2	2:B:3660:ARG:HE	1.84	0.42
2:B:4237:SER:O	2:B:4240:THR:OG1	2.37	0.42
2:C:166:SER:OG	2:C:168:GLN:OE1	2.34	0.42
2:C:603:LYS:HB3	2:C:603:LYS:HE2	1.88	0.42
2:C:712:GLU:HG3	2:C:838:ARG:HB3	2.02	0.42
2:C:1825:PHE:CE1	2:C:1842:ILE:HG12	2.54	0.42
2:C:2086:VAL:HG22	2:C:3687:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3240:PRO:HG3	2:C:3299:LEU:HG	2.00	0.42
2:C:3655:ASP:HB2	2:C:3660:ARG:HE	1.84	0.42
2:C:4798:ASP:OD1	2:C:4798:ASP:N	2.51	0.42
2:D:332:ARG:NH1	2:D:364:GLN:OE1	2.52	0.42
2:D:2062:ILE:HG21	2:D:2087:LEU:HG	2.00	0.42
2:D:2741:TRP:HH2	2:D:2752:LYS:HD3	1.84	0.42
2:D:3180:ILE:HG23	2:D:3181:TYR:CD1	2.55	0.42
2:D:3650:GLU:HB2	2:D:3651:PRO:HD3	2.00	0.42
2:D:3689:MET:CE	2:D:3753:PRO:HB2	2.49	0.42
2:D:3743:THR:HB	2:D:3758:THR:HG21	2.01	0.42
2:D:4268:MET:O	2:D:4271:VAL:HG22	2.20	0.42
2:A:1948:MET:HA	2:A:1948:MET:CE	2.50	0.42
2:A:2157:GLN:O	2:A:3615:ARG:NH2	2.52	0.42
2:A:2907:PHE:CE2	2:A:2909:ASP:HA	2.54	0.42
2:A:3125:ASP:H	2:A:3183:ILE:CD1	2.32	0.42
1:L:6:THR:O	1:L:10:ILE:HD12	2.19	0.42
1:L:15:GLU:O	1:L:19:LEU:HG	2.19	0.42
1:L:76:LYS:HB2	1:L:78:LYS:NZ	2.34	0.42
1:K:76:LYS:HB2	1:K:78:LYS:NZ	2.35	0.42
2:B:332:ARG:NH1	2:B:364:GLN:OE1	2.53	0.42
2:B:902:TRP:CE2	2:B:913:ARG:CZ	3.02	0.42
2:B:2907:PHE:CE2	2:B:2909:ASP:HA	2.54	0.42
2:B:3067:ASP:HA	2:B:3070:LYS:NZ	2.29	0.42
2:B:3693:ASP:O	2:B:3697:LYS:HG2	2.19	0.42
2:B:3743:THR:HB	2:B:3758:THR:HG21	2.01	0.42
2:B:3955:GLN:NE2	2:B:3972:MET:HG2	2.35	0.42
2:C:902:TRP:CE2	2:C:913:ARG:CZ	3.03	0.42
2:C:2785:TRP:HE1	2:C:2905:ARG:HH12	1.67	0.42
2:C:3292:GLU:O	2:C:3292:GLU:HG2	2.18	0.42
2:D:1039:ASP:OD1	2:D:1042:THR:HB	2.18	0.42
2:D:1825:PHE:CE1	2:D:1842:ILE:HG12	2.54	0.42
2:D:2086:VAL:HG22	2:D:3687:LEU:HD13	2.01	0.42
2:D:4277:LYS:HA	2:D:4277:LYS:HD3	1.75	0.42
2:A:940:LEU:HD12	2:A:941:LYS:N	2.34	0.42
2:A:948:CYS:HA	2:A:1067:PRO:HD3	2.00	0.42
2:A:1714:TYR:CE2	2:A:1718:ARG:HD2	2.54	0.42
2:A:2704:GLN:HA	2:A:2705:PRO:HD3	1.91	0.42
2:A:3192:ARG:O	2:A:3197:LEU:HB2	2.20	0.42
2:B:261:HIS:CE1	2:B:388:GLN:HE22	2.37	0.42
2:B:712:GLU:HG3	2:B:838:ARG:HB3	2.02	0.42
2:B:874:LEU:HD23	2:B:879:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:ARG:NH1	2:C:364:GLN:OE1	2.52	0.42
2:C:737:ILE:HD13	2:C:1482:ARG:HD3	2.00	0.42
2:C:903:GLN:H	2:C:913:ARG:NE	2.16	0.42
2:C:913:ARG:HA	2:C:913:ARG:HD2	1.74	0.42
2:C:2828:MET:O	2:C:2894:LYS:NZ	2.42	0.42
2:C:3693:ASP:O	2:C:3697:LYS:HG2	2.19	0.42
2:C:4689:LYS:HA	2:C:4689:LYS:HD2	1.82	0.42
2:C:4735:ASN:HB3	2:C:4738:PHE:CD2	2.54	0.42
2:C:4964:ASP:OD1	2:C:4965:GLN:N	2.52	0.42
2:D:261:HIS:CE1	2:D:388:GLN:HE22	2.37	0.42
2:D:712:GLU:HG3	2:D:838:ARG:HB3	2.02	0.42
2:D:897:LYS:HA	2:D:900:LEU:HB2	2.00	0.42
2:D:1538:LYS:HD2	2:D:1636:ASN:ND2	2.34	0.42
2:D:1810:VAL:HB	2:D:1817:LEU:HD13	2.01	0.42
2:D:3955:GLN:NE2	2:D:3972:MET:HG2	2.35	0.42
2:A:853:PRO:HG2	2:A:1084:ARG:O	2.18	0.42
2:A:2086:VAL:HG22	2:A:3687:LEU:HD13	2.01	0.42
2:A:3188:SER:O	2:A:3192:ARG:CB	2.67	0.42
2:A:3693:ASP:O	2:A:3697:LYS:HG2	2.19	0.42
2:A:3955:GLN:NE2	2:A:3972:MET:HG2	2.35	0.42
2:A:4183:LYS:HG3	2:A:4184:GLU:HG3	2.01	0.42
2:B:1260:GLN:OE1	2:B:1261:VAL:N	2.52	0.42
2:B:1649:GLU:HG2	2:B:1650:LEU:N	2.34	0.42
2:B:2000:HIS:O	2:B:2004:MET:HG2	2.18	0.42
2:B:3006:SER:C	2:B:3010:LYS:HZ2	2.22	0.42
2:B:3650:GLU:HB2	2:B:3651:PRO:HD3	2.00	0.42
2:B:4036:ASP:HB2	2:B:4043:ILE:HD13	2.02	0.42
2:B:4964:ASP:OD1	2:B:4965:GLN:N	2.52	0.42
2:C:1220:ASP:O	2:C:1223:THR:OG1	2.37	0.42
2:C:1714:TYR:CE2	2:C:1718:ARG:HD2	2.54	0.42
2:C:1973:ILE:HG13	2:C:3608:LEU:HD11	2.02	0.42
2:C:2831:VAL:HB	2:C:2894:LYS:CE	2.47	0.42
2:C:3009:CYS:O	2:C:3013:VAL:HG23	2.19	0.42
2:C:3253:GLY:C	2:C:3255:GLU:N	2.72	0.42
2:C:3743:THR:HB	2:C:3758:THR:HG21	2.01	0.42
2:C:4237:SER:O	2:C:4240:THR:OG1	2.37	0.42
2:D:1452:GLN:HE22	2:D:1484:ASN:ND2	2.16	0.42
2:D:1914:CYS:HB3	2:D:2090:ARG:NH2	2.35	0.42
2:A:902:TRP:CE2	2:A:913:ARG:CZ	3.03	0.42
2:A:1283:LEU:HB2	2:A:1555:PHE:HB2	2.00	0.42
2:A:1436:GLN:H	2:A:1500:ARG:HH12	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1810:VAL:HB	2:A:1817:LEU:HD13	2.01	0.42
2:A:1914:CYS:HB3	2:A:2090:ARG:NH2	2.35	0.42
2:A:1979:PHE:CD2	2:A:1996:LEU:HD23	2.55	0.42
2:A:3763:ILE:HD11	2:A:3838:ASP:O	2.20	0.42
2:A:4660:PHE:HZ	2:D:4057:HIS:CE1	2.37	0.42
2:B:1979:PHE:CD2	2:B:1996:LEU:HD23	2.55	0.42
2:B:2086:VAL:HG22	2:B:3687:LEU:HD13	2.01	0.42
2:B:2831:VAL:HB	2:B:2894:LYS:CE	2.47	0.42
2:B:3095:ASN:O	2:B:3099:VAL:HG22	2.20	0.42
2:B:3188:SER:O	2:B:3192:ARG:CB	2.67	0.42
2:B:3253:GLY:C	2:B:3255:GLU:N	2.72	0.42
2:B:3806:ASN:O	2:B:3810:ARG:HG3	2.20	0.42
2:C:261:HIS:CE1	2:C:388:GLN:HE22	2.37	0.42
2:C:1104:GLU:OE1	2:C:1225:LYS:NZ	2.44	0.42
2:C:3125:ASP:H	2:C:3183:ILE:CD1	2.32	0.42
2:C:3192:ARG:O	2:C:3197:LEU:HB2	2.20	0.42
2:C:3806:ASN:O	2:C:3810:ARG:HG3	2.20	0.42
2:D:4183:LYS:HG3	2:D:4184:GLU:HG3	2.01	0.42
2:A:50:GLU:OE2	2:A:61:ASP:N	2.48	0.42
2:A:737:ILE:HD13	2:A:1482:ARG:HD3	2.00	0.42
2:A:877:HIS:CE1	2:A:878:LEU:HG	2.55	0.42
2:A:3806:ASN:O	2:A:3810:ARG:HG3	2.20	0.42
1:J:89:ALA:HA	1:J:92:VAL:HG22	2.01	0.42
1:K:127:ARG:NH1	1:K:135:GLY:N	2.55	0.42
2:B:50:GLU:OE2	2:B:61:ASP:N	2.48	0.42
2:B:515:ALA:HB2	2:B:523:GLY:HA3	2.00	0.42
2:B:853:PRO:HG2	2:B:1084:ARG:O	2.18	0.42
2:B:877:HIS:CE1	2:B:878:LEU:HG	2.55	0.42
2:B:1810:VAL:HB	2:B:1817:LEU:HD13	2.01	0.42
2:B:3689:MET:CE	2:B:3753:PRO:HB2	2.49	0.42
2:C:756:SER:HB2	2:C:769:ARG:HB3	2.02	0.42
2:C:1166:VAL:HG23	2:C:1173:MET:HG2	2.01	0.42
2:C:1446:ILE:HG12	2:C:1542:ALA:HB2	2.00	0.42
2:C:1914:CYS:HB3	2:C:2090:ARG:NH2	2.35	0.42
2:C:2436:ILE:HA	2:C:2465:LYS:HE3	2.01	0.42
2:C:3088:LYS:HG3	2:C:3090:VAL:HG22	2.01	0.42
2:C:3095:ASN:O	2:C:3099:VAL:HG22	2.20	0.42
2:C:3164:GLY:C	2:C:3248:ARG:HH12	2.23	0.42
2:D:436:LEU:HD23	2:D:436:LEU:HA	1.81	0.42
2:D:1729:MET:HE1	2:D:1930:ASP:HB2	2.01	0.42
2:D:1979:PHE:CD2	2:D:1996:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3134:LEU:HD22	2:D:3162:PHE:CE2	2.54	0.42
2:D:4743:LEU:O	2:D:4746:ILE:HG12	2.20	0.42
2:A:163:HIS:HB2	2:A:182:ILE:HG13	2.02	0.42
2:A:527:LYS:HE2	2:A:527:LYS:HB2	1.82	0.42
2:A:756:SER:HB2	2:A:769:ARG:HB3	2.02	0.42
2:A:1040:ASP:HA	2:A:1043:LYS:HZ2	1.85	0.42
2:A:1260:GLN:OE1	2:A:1261:VAL:N	2.52	0.42
2:A:1962:THR:HG22	2:A:1966:ARG:HG3	2.02	0.42
2:A:1973:ILE:HG13	2:A:3608:LEU:HD11	2.02	0.42
2:A:2447:LYS:HA	2:A:2447:LYS:HD3	1.80	0.42
2:A:2508:SER:HB3	2:A:2560:SER:HB3	2.02	0.42
2:A:3149:GLU:OE2	2:A:3232:PRO:HG2	2.19	0.42
1:L:117:LEU:HD23	1:L:118:THR:N	2.34	0.42
2:B:491:GLU:OE2	2:B:546:LYS:NZ	2.47	0.42
2:B:1724:GLU:HG2	2:B:2165:LEU:HD23	2.00	0.42
2:B:3017:HIS:O	2:B:3092:GLN:NE2	2.53	0.42
2:B:3164:GLY:C	2:B:3248:ARG:HH12	2.23	0.42
2:B:3763:ILE:HD11	2:B:3838:ASP:O	2.20	0.42
2:B:3975:GLN:O	2:B:3979:VAL:HG23	2.20	0.42
2:C:680:ASP:O	2:C:751:THR:HG23	2.20	0.42
2:C:1931:ASP:OD1	2:C:1932:PHE:N	2.52	0.42
2:C:1948:MET:HA	2:C:1948:MET:CE	2.50	0.42
2:C:2379:ASP:OD2	2:C:2380:ASP:N	2.53	0.42
2:C:2741:TRP:HH2	2:C:2752:LYS:HD3	1.84	0.42
2:C:3145:SER:H	2:C:3148:VAL:HB	1.85	0.42
2:C:3955:GLN:NE2	2:C:3972:MET:HG2	2.35	0.42
2:C:3975:GLN:O	2:C:3979:VAL:HG23	2.20	0.42
2:C:4240:THR:HG22	2:C:4308:ILE:HD13	2.02	0.42
2:D:680:ASP:O	2:D:751:THR:HG23	2.20	0.42
2:D:877:HIS:CE1	2:D:878:LEU:HG	2.55	0.42
2:D:1081:THR:OG1	2:D:1082:GLY:N	2.51	0.42
2:D:1649:GLU:HG2	2:D:1650:LEU:N	2.34	0.42
2:D:3125:ASP:H	2:D:3183:ILE:CD1	2.32	0.42
2:D:3149:GLU:OE2	2:D:3232:PRO:HG2	2.19	0.42
1:I:89:ALA:HA	1:I:92:VAL:HG22	2.01	0.42
2:A:1914:CYS:O	2:A:1918:VAL:HG23	2.20	0.42
2:A:3017:HIS:O	2:A:3092:GLN:NE2	2.53	0.42
2:A:4240:THR:HG22	2:A:4308:ILE:HD13	2.02	0.42
3:E:50:ARG:HH21	3:E:53:LYS:NZ	2.16	0.42
1:J:6:THR:O	1:J:10:ILE:HD12	2.19	0.42
2:B:14:LEU:HG	2:B:177:VAL:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:ASN:O	2:B:899:GLU:HG3	2.20	0.42
2:B:1973:ILE:HG13	2:B:3608:LEU:HD11	2.02	0.42
2:C:1046:ASN:OD1	2:C:1047:LYS:N	2.53	0.42
2:C:1948:MET:HA	2:C:1948:MET:HE2	2.01	0.42
2:C:3006:SER:C	2:C:3010:LYS:HZ2	2.23	0.42
2:C:3017:HIS:O	2:C:3092:GLN:NE2	2.53	0.42
2:C:3106:SER:OG	2:C:3157:GLU:OE1	2.21	0.42
2:C:3763:ILE:HD11	2:C:3838:ASP:O	2.20	0.42
2:C:4268:MET:O	2:C:4271:VAL:HG22	2.20	0.42
2:D:14:LEU:HG	2:D:177:VAL:HA	2.00	0.42
2:D:896:ASN:O	2:D:899:GLU:HG3	2.20	0.42
2:D:903:GLN:H	2:D:913:ARG:NE	2.16	0.42
2:D:2736:LYS:HD2	2:D:2754:GLN:OE1	2.20	0.42
2:D:2826:ILE:H	2:D:2826:ILE:HD12	1.85	0.42
2:D:2930:ILE:HG23	2:D:3010:LYS:HE2	2.02	0.42
2:D:3009:CYS:O	2:D:3013:VAL:HG23	2.19	0.42
2:D:3095:ASN:O	2:D:3099:VAL:HG22	2.20	0.42
1:I:116:LYS:HB2	1:I:116:LYS:HE2	1.85	0.41
2:A:399:MET:SD	2:A:399:MET:N	2.92	0.41
2:A:2844:MET:SD	2:A:2888:LYS:NZ	2.91	0.41
2:A:3145:SER:H	2:A:3148:VAL:HB	1.85	0.41
2:A:3592:SER:O	2:A:3596:LYS:HD3	2.20	0.41
2:A:4237:SER:N	2:A:4240:THR:OG1	2.51	0.41
3:E:67:MET:HE2	3:E:104:LEU:HB2	2.02	0.41
1:K:42:GLN:HE21	2:C:1957:LEU:CD2	2.33	0.41
1:K:64:ILE:HG23	1:K:68:GLU:HB3	2.02	0.41
2:B:50:GLU:CD	2:B:61:ASP:H	2.22	0.41
2:B:680:ASP:O	2:B:751:THR:HG23	2.20	0.41
2:B:737:ILE:HD13	2:B:1482:ARG:HD3	2.00	0.41
2:B:808:HIS:O	2:B:1616:GLY:HA2	2.20	0.41
2:B:1914:CYS:HB3	2:B:2090:ARG:NH2	2.35	0.41
2:B:1962:THR:HG22	2:B:1966:ARG:HG3	2.02	0.41
2:B:2508:SER:HB3	2:B:2560:SER:HB3	2.02	0.41
2:B:2586:GLN:HE22	2:B:2590:ARG:NH2	2.19	0.41
2:B:3009:CYS:O	2:B:3013:VAL:HG23	2.19	0.41
2:B:3088:LYS:HG3	2:B:3090:VAL:HG22	2.02	0.41
2:B:3163:ALA:HB1	2:B:3245:TYR:CD1	2.52	0.41
2:B:4670:LEU:HB2	2:B:4672:MET:CE	2.49	0.41
2:C:808:HIS:O	2:C:1616:GLY:HA2	2.20	0.41
2:C:943:LEU:HD11	2:C:1064:LEU:HD12	2.02	0.41
2:C:1436:GLN:H	2:C:1500:ARG:HH12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1810:VAL:HB	2:C:1817:LEU:HD13	2.01	0.41
2:C:2153:LYS:HD3	2:C:2153:LYS:HA	1.82	0.41
2:C:2736:LYS:HD2	2:C:2754:GLN:OE1	2.20	0.41
2:C:4183:LYS:HG3	2:C:4184:GLU:HG3	2.01	0.41
2:D:561:ARG:HG3	2:D:561:ARG:NH1	2.34	0.41
2:D:643:LEU:O	2:D:645:GLN:NE2	2.53	0.41
2:D:902:TRP:CE2	2:D:913:ARG:CZ	3.03	0.41
2:D:1046:ASN:OD1	2:D:1047:LYS:N	2.53	0.41
2:D:1283:LEU:HB2	2:D:1555:PHE:HB2	2.00	0.41
2:D:1948:MET:HA	2:D:1948:MET:CE	2.50	0.41
2:D:2427:ILE:HD13	2:D:2471:PHE:CZ	2.54	0.41
2:D:2508:SER:HB3	2:D:2560:SER:HB3	2.02	0.41
2:D:3188:SER:O	2:D:3192:ARG:CB	2.67	0.41
2:D:3806:ASN:O	2:D:3810:ARG:HG3	2.20	0.41
2:D:4670:LEU:HB2	2:D:4672:MET:CE	2.49	0.41
1:I:76:LYS:HB2	1:I:78:LYS:NZ	2.35	0.41
1:I:123:ASP:HA	1:I:126:ILE:HG23	2.02	0.41
2:A:2785:TRP:HE1	2:A:2905:ARG:HH12	1.67	0.41
2:A:3006:SER:C	2:A:3010:LYS:HZ2	2.23	0.41
2:A:3689:MET:CE	2:A:3753:PRO:HB2	2.49	0.41
2:A:4036:ASP:HB2	2:A:4043:ILE:HD13	2.02	0.41
2:A:4268:MET:O	2:A:4271:VAL:HG22	2.20	0.41
2:A:4743:LEU:O	2:A:4746:ILE:HG12	2.20	0.41
2:A:4964:ASP:OD1	2:A:4965:GLN:N	2.52	0.41
2:B:765:SER:HA	2:B:779:PHE:O	2.19	0.41
2:B:1962:THR:O	2:B:1966:ARG:HG3	2.20	0.41
2:B:2379:ASP:OD2	2:B:2380:ASP:N	2.53	0.41
2:B:2436:ILE:HA	2:B:2465:LYS:HE3	2.01	0.41
2:B:2908:LYS:HE2	2:B:2908:LYS:HB2	1.95	0.41
2:B:3211:LEU:HD21	2:B:3245:TYR:HE2	1.85	0.41
2:B:3906:PHE:HB3	2:B:3967:LEU:HD11	2.02	0.41
2:B:4183:LYS:HG3	2:B:4184:GLU:HG3	2.01	0.41
2:C:399:MET:SD	2:C:399:MET:N	2.92	0.41
2:C:1979:PHE:CD2	2:C:1996:LEU:HD23	2.55	0.41
2:C:2508:SER:HB3	2:C:2560:SER:HB3	2.02	0.41
2:C:3180:ILE:HG23	2:C:3181:TYR:CD1	2.54	0.41
2:C:3650:GLU:HB2	2:C:3651:PRO:HD3	2.00	0.41
2:C:4057:HIS:CE1	2:D:4660:PHE:HZ	2.38	0.41
2:D:808:HIS:O	2:D:1616:GLY:HA2	2.20	0.41
2:D:1220:ASP:O	2:D:1223:THR:OG1	2.37	0.41
2:D:1962:THR:O	2:D:1966:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2447:LYS:HD3	2:D:2447:LYS:HA	1.80	0.41
2:D:3145:SER:H	2:D:3148:VAL:HB	1.85	0.41
2:D:3164:GLY:C	2:D:3248:ARG:HH12	2.23	0.41
2:D:3192:ARG:O	2:D:3197:LEU:HB2	2.20	0.41
2:D:3592:SER:O	2:D:3596:LYS:HD3	2.20	0.41
2:D:4237:SER:O	2:D:4240:THR:OG1	2.37	0.41
2:A:712:GLU:HG3	2:A:838:ARG:HB3	2.02	0.41
2:A:2106:TYR:HH	2:A:3615:ARG:HH12	1.69	0.41
2:A:2640:LEU:HD23	2:A:2643:LYS:HZ1	1.85	0.41
2:A:2736:LYS:HD2	2:A:2754:GLN:OE1	2.20	0.41
2:A:2833:LEU:HB3	2:A:2837:LEU:CD1	2.49	0.41
2:A:3848:GLU:OE1	2:A:3922:GLU:HG3	2.20	0.41
2:B:163:HIS:HB2	2:B:182:ILE:HG13	2.02	0.41
2:B:1797:GLU:HA	2:B:1800:LYS:HG2	2.02	0.41
2:B:2741:TRP:HH2	2:B:2752:LYS:HD3	1.84	0.41
2:B:2785:TRP:HE1	2:B:2905:ARG:HH12	1.67	0.41
2:B:3134:LEU:HD22	2:B:3162:PHE:CE2	2.54	0.41
2:B:3246:MET:HG2	2:B:3309:LYS:HZ1	1.85	0.41
2:B:3679:LYS:HE2	2:B:3679:LYS:HB2	1.92	0.41
2:B:4268:MET:O	2:B:4271:VAL:HG22	2.20	0.41
2:C:487:ASN:O	2:C:491:GLU:HG2	2.21	0.41
2:C:896:ASN:O	2:C:899:GLU:HG3	2.20	0.41
2:C:1697:LEU:HD23	2:C:1697:LEU:HA	1.95	0.41
2:C:4130:GLN:HB3	2:C:4131:PRO:HD3	2.02	0.41
2:D:943:LEU:HD11	2:D:1064:LEU:HD12	2.02	0.41
2:D:3017:HIS:O	2:D:3092:GLN:NE2	2.53	0.41
2:D:3651:PRO:HB2	2:D:3652:PRO:HD3	2.03	0.41
2:D:3763:ILE:HD11	2:D:3838:ASP:O	2.20	0.41
1:I:117:LEU:HD23	1:I:118:THR:N	2.34	0.41
2:A:274:LEU:HD23	2:A:274:LEU:HA	1.81	0.41
2:A:874:LEU:HD23	2:A:879:GLU:HG3	2.01	0.41
2:A:943:LEU:HD11	2:A:1064:LEU:HD12	2.02	0.41
2:A:3163:ALA:HB1	2:A:3245:TYR:CD1	2.52	0.41
2:A:4746:ILE:HD11	2:B:4776:VAL:HG21	2.03	0.41
2:A:4753:LEU:HG	2:B:4773:LEU:HD22	2.02	0.41
1:K:89:ALA:HA	1:K:92:VAL:HG22	2.01	0.41
2:B:1046:ASN:OD1	2:B:1047:LYS:N	2.53	0.41
2:B:1967:SER:O	2:B:1972:GLN:NE2	2.41	0.41
2:B:2344:LEU:HD22	2:B:2434:GLY:HA3	2.02	0.41
2:B:2736:LYS:HD2	2:B:2754:GLN:OE1	2.20	0.41
2:B:2833:LEU:HB3	2:B:2837:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3145:SER:H	2:B:3148:VAL:HB	1.85	0.41
2:B:3592:SER:O	2:B:3596:LYS:HD3	2.20	0.41
2:B:4743:LEU:O	2:B:4746:ILE:HG12	2.20	0.41
2:C:1592:SER:OG	2:C:1594:VAL:HG12	2.21	0.41
2:C:1797:GLU:HA	2:C:1800:LYS:HG2	2.03	0.41
2:D:487:ASN:O	2:D:491:GLU:HG2	2.21	0.41
2:D:1166:VAL:HG23	2:D:1173:MET:HG2	2.01	0.41
2:D:1914:CYS:O	2:D:1918:VAL:HG23	2.20	0.41
2:D:1931:ASP:OD1	2:D:1932:PHE:N	2.52	0.41
2:D:1973:ILE:HG13	2:D:3608:LEU:HD11	2.02	0.41
2:D:4107:GLU:OE2	2:D:4149:TYR:OH	2.15	0.41
1:I:122:VAL:O	1:I:126:ILE:N	2.43	0.41
2:A:487:ASN:O	2:A:491:GLU:HG2	2.21	0.41
2:A:3211:LEU:HD21	2:A:3245:TYR:HE2	1.85	0.41
2:A:3679:LYS:HE2	2:A:3679:LYS:HB2	1.92	0.41
2:A:4858:LEU:HD23	2:A:4858:LEU:HA	1.94	0.41
3:F:58:LYS:O	3:F:62:GLU:OE1	2.39	0.41
1:J:123:ASP:HA	1:J:126:ILE:HG23	2.02	0.41
2:B:586:LEU:HD11	2:B:620:CYS:HB2	2.02	0.41
2:B:889:ILE:O	2:B:893:TRP:CE3	2.74	0.41
2:B:1436:GLN:H	2:B:1500:ARG:HH12	1.67	0.41
2:B:2715:GLU:OE1	2:B:2715:GLU:N	2.44	0.41
2:B:2930:ILE:HG23	2:B:3010:LYS:HE2	2.02	0.41
2:B:3744:ILE:O	2:B:3747:SER:OG	2.31	0.41
2:B:4130:GLN:HB3	2:B:4131:PRO:HD3	2.02	0.41
2:C:194:LEU:HD23	2:C:196:TYR:HE1	1.85	0.41
2:C:875:PRO:HA	2:C:876:PRO:HD3	1.94	0.41
2:C:2344:LEU:HD22	2:C:2434:GLY:HA3	2.02	0.41
2:C:3906:PHE:HB3	2:C:3967:LEU:HD11	2.03	0.41
2:D:335:LYS:HZ1	2:D:397:GLY:HA3	1.85	0.41
2:D:1758:ARG:HA	2:D:1758:ARG:HD2	1.83	0.41
2:D:2379:ASP:OD2	2:D:2380:ASP:N	2.53	0.41
2:D:2923:TYR:CD2	2:D:3003:MET:HE2	2.55	0.41
2:D:2945:GLY:HA2	2:D:2948:ARG:NH2	2.36	0.41
2:A:332:ARG:NH1	2:A:364:GLN:OE1	2.52	0.41
2:A:643:LEU:O	2:A:645:GLN:NE2	2.53	0.41
2:A:1727:VAL:HG11	2:A:1926:VAL:HG21	2.02	0.41
2:A:1962:THR:O	2:A:1966:ARG:HG3	2.20	0.41
2:A:2826:ILE:H	2:A:2826:ILE:HD12	1.85	0.41
2:A:2945:GLY:HA2	2:A:2948:ARG:NH2	2.36	0.41
2:A:3164:GLY:C	2:A:3248:ARG:HH12	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4948:CYS:SG	2:A:4950:GLU:HG2	2.61	0.41
3:H:58:LYS:O	3:H:62:GLU:OE1	2.39	0.41
1:L:16:ALA:HA	1:L:19:LEU:HD12	2.03	0.41
1:K:116:LYS:HB2	1:K:116:LYS:HE2	1.85	0.41
2:B:603:LYS:HB3	2:B:603:LYS:HE2	1.88	0.41
2:B:1748:LEU:HD23	2:B:1748:LEU:HA	1.88	0.41
2:B:4649:VAL:HA	2:B:4652:LYS:HE2	2.03	0.41
2:C:877:HIS:CE1	2:C:878:LEU:HG	2.55	0.41
2:C:1585:ARG:O	2:C:1587:HIS:ND1	2.54	0.41
2:C:2824:ARG:CZ	2:D:1502:ASN:HB3	2.50	0.41
2:C:2826:ILE:H	2:C:2826:ILE:HD12	1.85	0.41
2:C:2930:ILE:HG23	2:C:3010:LYS:HE2	2.02	0.41
2:C:3068:LEU:O	2:C:3071:THR:OG1	2.27	0.41
2:C:3592:SER:O	2:C:3596:LYS:HD3	2.20	0.41
2:D:1592:SER:OG	2:D:1594:VAL:HG12	2.21	0.41
2:D:2868:HIS:HB3	2:D:2871:LEU:HD23	2.03	0.41
2:D:3131:TYR:HE1	2:D:3208:ILE:HB	1.84	0.41
2:D:3211:LEU:HD21	2:D:3245:TYR:HE2	1.85	0.41
2:D:4481:TRP:O	2:D:4485:ILE:HG12	2.21	0.41
2:D:4649:VAL:HA	2:D:4652:LYS:HE2	2.03	0.41
2:D:4948:CYS:SG	2:D:4950:GLU:HG2	2.61	0.41
2:A:390:LYS:HD2	2:A:390:LYS:HA	1.86	0.41
2:A:1729:MET:HE1	2:A:1930:ASP:HB2	2.02	0.41
2:A:2379:ASP:OD2	2:A:2380:ASP:N	2.53	0.41
2:A:2868:HIS:HB3	2:A:2871:LEU:HD23	2.03	0.41
2:A:3009:CYS:O	2:A:3013:VAL:HG23	2.19	0.41
3:E:58:LYS:O	3:E:62:GLU:OE1	2.39	0.41
3:H:43:ARG:HD3	2:D:1766:PRO:HG2	2.02	0.41
2:B:487:ASN:O	2:B:491:GLU:HG2	2.21	0.41
2:B:756:SER:HB2	2:B:769:ARG:HB3	2.02	0.41
2:B:2926:LEU:HD23	2:B:2926:LEU:HA	1.87	0.41
2:B:3212:GLU:O	2:B:3216:GLU:OE1	2.39	0.41
2:C:659:ILE:HD12	2:C:661:LEU:HD11	2.03	0.41
2:C:972:LEU:HD23	2:C:973:THR:H	1.86	0.41
2:C:1727:VAL:HG11	2:C:1926:VAL:HG21	2.02	0.41
2:C:1911:GLN:OE1	2:C:2090:ARG:NH1	2.54	0.41
2:C:3965:ILE:HG13	2:C:4086:ARG:HH11	1.86	0.41
2:D:491:GLU:OE2	2:D:546:LYS:NZ	2.47	0.41
2:D:1911:GLN:OE1	2:D:2090:ARG:NH1	2.54	0.41
2:D:2106:TYR:OH	2:D:3615:ARG:NH1	2.53	0.41
2:D:2972:ASP:OD1	2:D:2976:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3906:PHE:HB3	2:D:3967:LEU:HD11	2.02	0.41
2:D:4130:GLN:HB3	2:D:4131:PRO:HD3	2.02	0.41
1:I:64:ILE:HG23	1:I:68:GLU:HB3	2.02	0.41
2:A:50:GLU:CD	2:A:61:ASP:H	2.22	0.41
2:A:694:ARG:NH1	2:A:718:VAL:O	2.49	0.41
2:A:896:ASN:O	2:A:899:GLU:HG3	2.20	0.41
2:A:1046:ASN:OD1	2:A:1047:LYS:N	2.53	0.41
2:A:2408:LEU:HD22	2:A:2413:LYS:HD3	2.03	0.41
2:A:2741:TRP:HH2	2:A:2752:LYS:HD3	1.84	0.41
2:A:2930:ILE:HG23	2:A:3010:LYS:HE2	2.02	0.41
2:A:3651:PRO:HB2	2:A:3652:PRO:HD3	2.03	0.41
2:A:4481:TRP:O	2:A:4485:ILE:HG12	2.21	0.41
2:A:4649:VAL:HA	2:A:4652:LYS:HE2	2.03	0.41
3:G:58:LYS:O	3:G:62:GLU:OE1	2.39	0.41
3:H:67:MET:HE2	3:H:104:LEU:HB2	2.02	0.41
1:J:76:LYS:HB2	1:J:78:LYS:NZ	2.35	0.41
2:B:643:LEU:O	2:B:645:GLN:NE2	2.53	0.41
2:B:904:TYR:CE1	2:B:916:PRO:HA	2.56	0.41
2:B:972:LEU:HD23	2:B:973:THR:H	1.86	0.41
2:B:1585:ARG:O	2:B:1587:HIS:ND1	2.53	0.41
2:B:2593:VAL:HA	2:B:2644:LEU:HD13	2.03	0.41
2:B:3304:GLN:HB3	2:B:3305:PRO:HD3	2.03	0.41
2:C:1758:ARG:HA	2:C:1758:ARG:HD2	1.83	0.41
2:C:1962:THR:O	2:C:1966:ARG:HG3	2.20	0.41
2:C:2928:GLN:HA	2:C:2931:ARG:CZ	2.51	0.41
2:C:4649:VAL:HA	2:C:4652:LYS:HE2	2.03	0.41
2:C:4743:LEU:O	2:C:4746:ILE:HG12	2.20	0.41
2:C:4948:CYS:SG	2:C:4950:GLU:HG2	2.61	0.41
2:D:182:ILE:HG13	2:D:182:ILE:O	2.21	0.41
2:D:586:LEU:HD11	2:D:620:CYS:HB2	2.02	0.41
2:D:904:TYR:CE1	2:D:916:PRO:HA	2.56	0.41
2:D:1304:LEU:HD23	2:D:1304:LEU:HA	1.90	0.41
2:D:1421:MET:SD	2:D:1576:LYS:HD2	2.61	0.41
2:D:2833:LEU:HB3	2:D:2837:LEU:CD1	2.48	0.41
2:D:3924:ILE:HG21	2:D:3935:LEU:HD12	2.03	0.41
2:D:3975:GLN:O	2:D:3979:VAL:HG23	2.20	0.41
2:A:49:LEU:CD1	2:A:194:LEU:HD13	2.51	0.41
2:A:194:LEU:HD23	2:A:196:TYR:HE1	1.85	0.41
2:A:680:ASP:O	2:A:751:THR:HG23	2.20	0.41
2:A:808:HIS:O	2:A:1616:GLY:HA2	2.20	0.41
2:A:889:ILE:O	2:A:893:TRP:CE3	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:972:LEU:HD23	2:A:973:THR:H	1.86	0.41
2:A:1421:MET:SD	2:A:1576:LYS:HD2	2.61	0.41
2:A:1797:GLU:HA	2:A:1800:LYS:HG2	2.03	0.41
2:A:1893:LEU:HD23	2:A:1896:MET:SD	2.60	0.41
2:A:1948:MET:HA	2:A:1948:MET:HE2	2.03	0.41
2:A:2487:LEU:HA	2:A:2490:VAL:HG22	2.03	0.41
2:A:2586:GLN:HE22	2:A:2590:ARG:NH2	2.19	0.41
2:A:3095:ASN:O	2:A:3099:VAL:HG22	2.20	0.41
2:A:3134:LEU:HD22	2:A:3162:PHE:CE2	2.54	0.41
2:A:3143:SER:O	2:A:3148:VAL:HG11	2.21	0.41
2:A:3965:ILE:HG13	2:A:4086:ARG:HH11	1.86	0.41
2:A:3975:GLN:O	2:A:3979:VAL:HG23	2.20	0.41
2:A:4196:THR:O	2:A:4200:MET:HG3	2.21	0.41
2:A:4914:ASN:HB3	2:A:4917:ASN:ND2	2.36	0.41
3:G:19:LYS:HB2	3:G:19:LYS:HE3	1.84	0.41
1:J:16:ALA:HA	1:J:19:LEU:HD12	2.03	0.41
1:J:116:LYS:HE2	1:J:116:LYS:HB2	1.85	0.41
1:L:36:VAL:O	1:L:39:SER:OG	2.27	0.41
1:L:64:ILE:HG23	1:L:68:GLU:HB3	2.02	0.41
1:L:122:VAL:O	1:L:126:ILE:N	2.43	0.41
2:B:943:LEU:HD11	2:B:1064:LEU:HD12	2.02	0.41
2:B:1592:SER:OG	2:B:1594:VAL:HG12	2.20	0.41
2:B:1825:PHE:CE1	2:B:1842:ILE:HG12	2.54	0.41
2:B:1948:MET:HA	2:B:1948:MET:CE	2.50	0.41
2:B:2253:LEU:HD23	2:B:2253:LEU:HA	1.85	0.41
2:B:2928:GLN:HA	2:B:2931:ARG:CZ	2.51	0.41
2:B:3310:VAL:HG11	2:B:3319:PHE:CE2	2.56	0.41
2:B:3965:ILE:HG13	2:B:4086:ARG:HH11	1.86	0.41
2:B:4481:TRP:O	2:B:4485:ILE:HG12	2.21	0.41
2:B:4663:ARG:HD2	2:B:4663:ARG:HA	1.89	0.41
2:B:4948:CYS:SG	2:B:4950:GLU:HG2	2.61	0.41
2:C:643:LEU:O	2:C:645:GLN:NE2	2.53	0.41
2:C:2945:GLY:HA2	2:C:2948:ARG:NH2	2.36	0.41
2:C:3101:LEU:O	2:C:3104:MET:HB3	2.21	0.41
2:C:3212:GLU:O	2:C:3216:GLU:OE1	2.39	0.41
2:C:4036:ASP:HB2	2:C:4043:ILE:HD13	2.02	0.41
2:C:4670:LEU:HB2	2:C:4672:MET:CE	2.49	0.41
2:C:4914:ASN:HB3	2:C:4917:ASN:ND2	2.36	0.41
2:C:4943:MET:HE3	2:C:4948:CYS:O	2.21	0.41
2:D:194:LEU:HD23	2:D:196:TYR:HE1	1.85	0.41
2:D:659:ILE:HD12	2:D:661:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:889:ILE:O	2:D:893:TRP:CE3	2.74	0.41
2:D:1727:VAL:HG11	2:D:1926:VAL:HG21	2.02	0.41
2:D:1893:LEU:HD23	2:D:1896:MET:SD	2.60	0.41
2:D:1988:CYS:HA	2:D:1989:PRO:HD3	1.87	0.41
2:D:2276:SER:OG	2:D:2277:CYS:N	2.54	0.41
2:D:2408:LEU:HD22	2:D:2413:LYS:HD3	2.03	0.41
2:D:2734:MET:HE2	2:D:2737:LEU:HD11	2.03	0.41
2:D:2928:GLN:HA	2:D:2931:ARG:CZ	2.51	0.41
2:D:3163:ALA:HB1	2:D:3245:TYR:CD1	2.52	0.41
2:D:4036:ASP:HB2	2:D:4043:ILE:HD13	2.02	0.41
2:D:4041:GLY:HA2	2:D:4080:TYR:HE1	1.86	0.41
2:D:4240:THR:HG22	2:D:4308:ILE:HD13	2.02	0.41
2:A:561:ARG:HG3	2:A:561:ARG:NH1	2.34	0.41
2:A:659:ILE:HD12	2:A:661:LEU:HD11	2.03	0.41
2:A:765:SER:HA	2:A:779:PHE:O	2.20	0.41
2:A:844:ARG:HH11	2:A:845:THR:H	1.69	0.41
2:A:1585:ARG:O	2:A:1587:HIS:ND1	2.54	0.41
2:A:1592:SER:OG	2:A:1594:VAL:HG12	2.21	0.41
2:A:1911:GLN:OE1	2:A:2090:ARG:NH1	2.54	0.41
2:A:2497:ARG:NH1	2:A:2881:GLU:OE2	2.53	0.41
2:A:3088:LYS:HA	2:A:3088:LYS:HD3	1.90	0.41
2:A:3191:GLU:HA	2:A:3194:ALA:HB3	2.03	0.41
2:A:4265:LYS:O	2:A:4269:LYS:HG2	2.21	0.41
3:F:19:LYS:HB2	3:F:19:LYS:HE3	1.84	0.41
1:K:16:ALA:HA	1:K:19:LEU:HD12	2.03	0.41
2:B:2734:MET:HE2	2:B:2737:LEU:HD11	2.03	0.41
2:B:4073:ASP:OD2	2:B:4075:ASN:ND2	2.54	0.41
2:C:735:GLY:O	2:C:737:ILE:HD12	2.21	0.41
2:C:889:ILE:O	2:C:893:TRP:CE3	2.74	0.41
2:C:1893:LEU:HD23	2:C:1896:MET:SD	2.60	0.41
2:C:1914:CYS:O	2:C:1918:VAL:HG23	2.20	0.41
2:C:2487:LEU:HA	2:C:2490:VAL:HG22	2.03	0.41
2:C:2586:GLN:HE22	2:C:2590:ARG:NH2	2.19	0.41
2:C:2659:GLN:HG2	2:C:2660:GLU:N	2.36	0.41
2:C:3102:LEU:HD12	2:C:3102:LEU:HA	1.86	0.41
2:C:3651:PRO:HB2	2:C:3652:PRO:HD3	2.03	0.41
2:D:756:SER:HB2	2:D:769:ARG:HB3	2.02	0.41
2:D:2487:LEU:HA	2:D:2490:VAL:HG22	2.03	0.41
2:D:3006:SER:C	2:D:3010:LYS:HZ2	2.23	0.41
2:D:3143:SER:O	2:D:3148:VAL:HG11	2.21	0.41
1:I:16:ALA:HA	1:I:19:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:MET:HG2	1:I:42:GLN:HB2	2.03	0.40
2:A:2928:GLN:HA	2:A:2931:ARG:CZ	2.51	0.40
2:A:3924:ILE:HG21	2:A:3935:LEU:HD12	2.03	0.40
1:J:64:ILE:HG23	1:J:68:GLU:HB3	2.02	0.40
1:L:37:MET:HG2	1:L:42:GLN:HB2	2.03	0.40
2:B:194:LEU:HD23	2:B:196:TYR:HE1	1.85	0.40
2:B:399:MET:SD	2:B:399:MET:N	2.92	0.40
2:B:810:GLU:N	2:B:810:GLU:OE2	2.54	0.40
2:B:2463:ASP:OD1	2:B:2464:HIS:N	2.55	0.40
2:B:2945:GLY:HA2	2:B:2948:ARG:NH2	2.36	0.40
2:B:3191:GLU:HA	2:B:3194:ALA:HB3	2.03	0.40
2:B:4196:THR:O	2:B:4200:MET:HG3	2.21	0.40
2:B:4265:LYS:O	2:B:4269:LYS:HG2	2.21	0.40
2:C:50:GLU:CD	2:C:61:ASP:H	2.22	0.40
2:C:527:LYS:HE2	2:C:527:LYS:HB2	1.82	0.40
2:C:2833:LEU:HB3	2:C:2837:LEU:CD1	2.49	0.40
2:C:4502:MET:SD	2:C:4585:PHE:HB3	2.61	0.40
2:D:49:LEU:CD1	2:D:194:LEU:HD13	2.51	0.40
2:D:1968:PRO:O	2:D:1972:GLN:HG3	2.21	0.40
2:D:2463:ASP:OD1	2:D:2464:HIS:N	2.54	0.40
2:D:2592:LEU:HD23	2:D:2592:LEU:HA	1.90	0.40
2:D:2593:VAL:HA	2:D:2644:LEU:HD13	2.03	0.40
2:D:3848:GLU:OE1	2:D:3922:GLU:HG3	2.21	0.40
2:D:4502:MET:SD	2:D:4585:PHE:HB3	2.61	0.40
2:A:648:LEU:HD23	2:A:648:LEU:HA	1.89	0.40
2:A:1176:THR:HG22	2:A:1181:ILE:HG13	2.03	0.40
2:A:1968:PRO:O	2:A:1972:GLN:HG3	2.21	0.40
2:A:2106:TYR:OH	2:A:3615:ARG:NH1	2.53	0.40
2:A:3906:PHE:HB3	2:A:3967:LEU:HD11	2.02	0.40
1:J:125:MET:HG3	2:B:3584:LYS:HE2	2.02	0.40
1:K:123:ASP:HA	1:K:126:ILE:HG23	2.03	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.81	0.40
2:B:364:GLN:NE2	2:B:369:GLY:O	2.53	0.40
2:B:1421:MET:SD	2:B:1576:LYS:HD2	2.61	0.40
2:B:2447:LYS:HD3	2:B:2447:LYS:HA	1.80	0.40
2:B:2826:ILE:H	2:B:2826:ILE:HD12	1.85	0.40
2:C:49:LEU:CD1	2:C:194:LEU:HD13	2.51	0.40
2:C:1421:MET:SD	2:C:1576:LYS:HD2	2.61	0.40
2:C:1968:PRO:O	2:C:1972:GLN:HG3	2.21	0.40
2:C:2106:TYR:OH	2:C:3615:ARG:NH1	2.53	0.40
2:C:2170:THR:O	2:C:2174:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3778:LEU:HD13	2:C:3854:PHE:HD1	1.87	0.40
2:C:4167:GLU:O	2:C:4171:GLN:HG2	2.22	0.40
2:D:884:LYS:HA	2:D:887:GLU:CG	2.51	0.40
2:D:920:GLU:O	2:D:924:LEU:N	2.55	0.40
2:D:1797:GLU:HA	2:D:1800:LYS:HG2	2.03	0.40
2:D:2229:LEU:HD11	2:D:2240:LEU:HD22	2.03	0.40
2:D:2344:LEU:HD22	2:D:2434:GLY:HA3	2.02	0.40
2:D:2488:LEU:HD11	2:D:2548:LEU:HD13	2.03	0.40
2:D:3088:LYS:HG3	2:D:3090:VAL:HG22	2.01	0.40
2:D:3101:LEU:O	2:D:3104:MET:HB3	2.21	0.40
2:A:182:ILE:HG13	2:A:182:ILE:O	2.21	0.40
2:A:997:ASP:O	2:A:1001:GLU:OE1	2.40	0.40
2:A:1748:LEU:HD23	2:A:1748:LEU:HA	1.88	0.40
2:A:3101:LEU:O	2:A:3104:MET:HB3	2.21	0.40
2:A:3661:VAL:HG23	2:A:3666:GLN:HG2	2.03	0.40
2:A:4130:GLN:HB3	2:A:4131:PRO:HD3	2.02	0.40
2:A:4670:LEU:HB2	2:A:4672:MET:CE	2.49	0.40
2:B:49:LEU:CD1	2:B:194:LEU:HD13	2.51	0.40
2:B:968:LYS:HA	2:B:968:LYS:HD2	1.91	0.40
2:B:1727:VAL:HG11	2:B:1926:VAL:HG21	2.02	0.40
2:B:1785:ASP:OD1	2:B:1786:ILE:N	2.55	0.40
2:B:1914:CYS:O	2:B:1918:VAL:HG23	2.20	0.40
2:B:2276:SER:OG	2:B:2277:CYS:N	2.54	0.40
2:B:2487:LEU:HA	2:B:2490:VAL:HG22	2.03	0.40
2:B:2874:TYR:O	2:B:2882:LYS:HE2	2.22	0.40
2:B:3651:PRO:HB2	2:B:3652:PRO:HD3	2.03	0.40
2:B:4240:THR:HG22	2:B:4308:ILE:HD13	2.02	0.40
2:C:884:LYS:HA	2:C:887:GLU:CG	2.51	0.40
2:C:2705:PRO:HG3	2:C:2854:LYS:HZ2	1.86	0.40
2:C:3304:GLN:HB3	2:C:3305:PRO:HD3	2.03	0.40
2:D:972:LEU:HD23	2:D:973:THR:H	1.86	0.40
2:D:1585:ARG:O	2:D:1587:HIS:ND1	2.54	0.40
2:D:2170:THR:O	2:D:2174:VAL:HG13	2.21	0.40
2:D:2586:GLN:HE22	2:D:2590:ARG:NH2	2.19	0.40
2:D:2659:GLN:HG2	2:D:2660:GLU:N	2.36	0.40
2:D:2913:ASP:HB3	2:D:2919:LYS:HE3	2.03	0.40
2:D:3281:LEU:HD22	2:D:3322:LEU:HD22	2.03	0.40
2:D:4914:ASN:HB3	2:D:4917:ASN:ND2	2.36	0.40
1:I:57:ASP:OD2	1:I:62:GLY:N	2.46	0.40
2:A:2344:LEU:HD22	2:A:2434:GLY:HA3	2.02	0.40
2:A:2488:LEU:HD11	2:A:2548:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2691:LYS:HD3	2:A:2704:GLN:NE2	2.37	0.40
2:A:2824:ARG:NH2	2:B:1502:ASN:HB3	2.37	0.40
2:A:3310:VAL:HG11	2:A:3319:PHE:CE2	2.57	0.40
2:A:3812:ASN:HA	2:A:3815:GLU:CD	2.42	0.40
1:L:123:ASP:HA	1:L:126:ILE:HG23	2.03	0.40
2:B:735:GLY:O	2:B:737:ILE:HD12	2.22	0.40
2:B:1226:TYR:HD1	2:B:1229:ILE:HD11	1.87	0.40
2:B:1829:LEU:HD12	2:B:1829:LEU:HA	1.96	0.40
2:B:1893:LEU:HD23	2:B:1896:MET:SD	2.60	0.40
2:B:1968:PRO:O	2:B:1972:GLN:HG3	2.21	0.40
2:B:2570:GLU:HG2	2:B:2605:MET:HG3	2.03	0.40
2:B:2913:ASP:HB3	2:B:2919:LYS:HE3	2.03	0.40
2:B:3183:ILE:HD12	2:B:3187:LYS:CE	2.52	0.40
2:B:3778:LEU:HD13	2:B:3854:PHE:HD1	1.87	0.40
2:B:3924:ILE:HG21	2:B:3935:LEU:HD12	2.03	0.40
2:B:3958:LEU:HB2	2:B:3968:LEU:HD13	2.03	0.40
2:B:4057:HIS:CE1	2:C:4660:PHE:HZ	2.40	0.40
2:C:810:GLU:N	2:C:810:GLU:OE2	2.55	0.40
2:C:997:ASP:OD1	2:C:1047:LYS:NZ	2.32	0.40
2:C:2874:TYR:O	2:C:2882:LYS:HE2	2.22	0.40
2:C:3184:TYR:CD1	2:C:3201:VAL:HG22	2.56	0.40
2:C:3211:LEU:HD21	2:C:3245:TYR:HE2	1.86	0.40
2:C:4041:GLY:HA2	2:C:4080:TYR:HE1	1.86	0.40
2:D:59:PRO:HA	2:D:60:PRO:HD3	1.98	0.40
2:D:287:SER:HA	2:D:349:MET:HE3	2.03	0.40
2:D:875:PRO:HA	2:D:876:PRO:HD3	1.94	0.40
2:D:1962:THR:HG22	2:D:1966:ARG:HG3	2.02	0.40
2:D:2327:ARG:HB3	2:D:2329:GLU:OE2	2.21	0.40
2:D:2874:TYR:O	2:D:2882:LYS:HE2	2.22	0.40
2:D:3649:ALA:C	2:D:3652:PRO:HD2	2.42	0.40
2:D:4167:GLU:O	2:D:4171:GLN:HG2	2.22	0.40
2:A:139:SER:O	2:A:141:ASP:N	2.54	0.40
2:A:1848:PRO:HG3	2:A:1890:LYS:NZ	2.37	0.40
2:A:2463:ASP:OD1	2:A:2464:HIS:N	2.55	0.40
2:A:2931:ARG:NH1	2:A:2932:TYR:CE1	2.90	0.40
2:A:2967:VAL:O	2:A:2971:ILE:HG13	2.22	0.40
2:A:3168:VAL:HG12	2:A:3179:ASN:ND2	2.37	0.40
2:A:4898:PHE:O	2:A:4904:GLY:HA3	2.22	0.40
1:K:10:ILE:HG22	1:K:14:LYS:NZ	2.37	0.40
2:B:884:LYS:HA	2:B:887:GLU:CG	2.51	0.40
2:B:997:ASP:O	2:B:1001:GLU:OE1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:LEU:O	2:B:1180:GLU:HG3	2.22	0.40
2:B:1911:GLN:OE1	2:B:2090:ARG:NH1	2.54	0.40
2:B:2153:LYS:HD3	2:B:2153:LYS:HA	1.83	0.40
2:B:2408:LEU:HD22	2:B:2413:LYS:HD3	2.03	0.40
2:B:3649:ALA:HB1	2:B:3652:PRO:HB2	2.04	0.40
2:B:4502:MET:SD	2:B:4585:PHE:HB3	2.61	0.40
2:B:4607:ALA:HB1	2:B:4649:VAL:HG21	2.04	0.40
2:C:2463:ASP:OD1	2:C:2464:HIS:N	2.55	0.40
2:C:3191:GLU:HA	2:C:3194:ALA:HB3	2.03	0.40
2:D:1177:LEU:O	2:D:1180:GLU:HG3	2.22	0.40
2:D:1711:LEU:HB3	2:D:1831:MET:SD	2.62	0.40
2:D:3062:ASP:O	2:D:3065:ALA:HB3	2.22	0.40
2:D:3191:GLU:HA	2:D:3194:ALA:HB3	2.03	0.40
2:D:3832:ASP:HB2	2:D:3835:PHE:HB3	2.04	0.40
2:D:4265:LYS:O	2:D:4269:LYS:HG2	2.21	0.40
2:D:4607:ALA:HB1	2:D:4649:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	L	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	A	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	51	84
2	B	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	51	84
2	C	4205/4967 (85%)	4082 (97%)	118 (3%)	5 (0%)	51	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	4205/4967 (85%)	4080 (97%)	120 (3%)	5 (0%)	51	84
3	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17804/20896 (85%)	17292 (97%)	492 (3%)	20 (0%)	54	84

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	3927	PRO
2	C	4641	PRO
2	D	3927	PRO
2	D	4641	PRO
2	A	1081	THR
2	A	3851	ASN
2	B	1081	THR
2	B	3851	ASN
2	C	1081	THR
2	C	3851	ASN
2	D	1081	THR
2	D	3851	ASN
2	A	1959	ALA
2	B	1959	ALA
2	C	1959	ALA
2	D	1959	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	123/127 (97%)	112 (91%)	11 (9%)	9	39
1	J	123/127 (97%)	112 (91%)	11 (9%)	9	39
1	K	123/127 (97%)	112 (91%)	11 (9%)	9	39
1	L	123/127 (97%)	112 (91%)	11 (9%)	9	39
2	A	3715/4358 (85%)	3678 (99%)	37 (1%)	76	89
2	B	3715/4358 (85%)	3678 (99%)	37 (1%)	76	89
2	C	3715/4358 (85%)	3678 (99%)	37 (1%)	76	89
2	D	3715/4358 (85%)	3678 (99%)	37 (1%)	76	89
3	E	88/89 (99%)	87 (99%)	1 (1%)	73	88
3	F	88/89 (99%)	87 (99%)	1 (1%)	73	88
3	G	88/89 (99%)	87 (99%)	1 (1%)	73	88
3	H	88/89 (99%)	87 (99%)	1 (1%)	73	88
All	All	15704/18296 (86%)	15508 (99%)	196 (1%)	72	87

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	77	MET
1	I	124	GLU
1	I	125	MET
1	I	126	ILE
1	I	127	ARG
1	I	128	GLU
1	I	130	ASP
1	I	142	PHE
1	I	143	VAL
1	I	145	MET
1	I	146	MET
2	A	290	ARG
2	A	321	LYS
2	A	349	MET
2	A	393	MET
2	A	441	LYS
2	A	884	LYS
2	A	929	ARG
2	A	944	LEU
2	A	1564	MET
2	A	1939	ASN
2	A	1948	MET

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Mol	Chain	Res	Type
2	A	2134	MET
2	A	2303	ARG
2	A	2512	MET
2	A	2685	TYR
2	A	2689	MET
2	A	2737	LEU
2	A	2757	MET
2	A	2766	LYS
2	A	2772	ARG
2	A	2782	MET
2	A	2783	LEU
2	A	2801	TYR
2	A	2931	ARG
2	A	3018	ARG
2	A	3190	ARG
2	A	3323	MET
2	A	3584	LYS
2	A	3591	LEU
2	A	3605	MET
2	A	3847	CYS
2	A	4279	MET
2	A	4307	ARG
2	A	4504	MET
2	A	4748	MET
2	A	4884	MET
2	A	4932	GLU
3	E	19	LYS
3	F	19	LYS
3	G	19	LYS
3	H	19	LYS
1	J	77	MET
1	J	124	GLU
1	J	125	MET
1	J	126	ILE
1	J	127	ARG
1	J	128	GLU
1	J	130	ASP
1	J	142	PHE
1	J	143	VAL
1	J	145	MET
1	J	146	MET
1	L	77	MET

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Mol	Chain	Res	Type
1	L	124	GLU
1	L	125	MET
1	L	126	ILE
1	L	127	ARG
1	L	128	GLU
1	L	130	ASP
1	L	142	PHE
1	L	143	VAL
1	L	145	MET
1	L	146	MET
1	K	77	MET
1	K	124	GLU
1	K	125	MET
1	K	126	ILE
1	K	127	ARG
1	K	128	GLU
1	K	130	ASP
1	K	142	PHE
1	K	143	VAL
1	K	145	MET
1	K	146	MET
2	B	290	ARG
2	B	321	LYS
2	B	349	MET
2	B	393	MET
2	B	441	LYS
2	B	884	LYS
2	B	929	ARG
2	B	944	LEU
2	B	1564	MET
2	B	1939	ASN
2	B	1948	MET
2	B	2134	MET
2	B	2303	ARG
2	B	2512	MET
2	B	2685	TYR
2	B	2689	MET
2	B	2737	LEU
2	B	2757	MET
2	B	2766	LYS
2	B	2772	ARG
2	B	2782	MET

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Mol	Chain	Res	Type
2	B	2783	LEU
2	B	2801	TYR
2	B	2931	ARG
2	B	3018	ARG
2	B	3190	ARG
2	B	3323	MET
2	B	3584	LYS
2	B	3591	LEU
2	B	3605	MET
2	B	3847	CYS
2	B	4279	MET
2	B	4307	ARG
2	B	4504	MET
2	B	4748	MET
2	B	4884	MET
2	B	4932	GLU
2	C	290	ARG
2	C	321	LYS
2	C	349	MET
2	C	393	MET
2	C	441	LYS
2	C	884	LYS
2	C	929	ARG
2	C	944	LEU
2	C	1564	MET
2	C	1939	ASN
2	C	1948	MET
2	C	2134	MET
2	C	2303	ARG
2	C	2512	MET
2	C	2685	TYR
2	C	2689	MET
2	C	2737	LEU
2	C	2757	MET
2	C	2766	LYS
2	C	2772	ARG
2	C	2782	MET
2	C	2783	LEU
2	C	2801	TYR
2	C	2931	ARG
2	C	3018	ARG
2	C	3190	ARG

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Mol	Chain	Res	Type
2	C	3323	MET
2	C	3584	LYS
2	C	3591	LEU
2	C	3605	MET
2	C	3847	CYS
2	C	4279	MET
2	C	4307	ARG
2	C	4504	MET
2	C	4748	MET
2	C	4884	MET
2	C	4932	GLU
2	D	290	ARG
2	D	321	LYS
2	D	349	MET
2	D	393	MET
2	D	441	LYS
2	D	884	LYS
2	D	929	ARG
2	D	944	LEU
2	D	1564	MET
2	D	1939	ASN
2	D	1948	MET
2	D	2134	MET
2	D	2303	ARG
2	D	2512	MET
2	D	2685	TYR
2	D	2689	MET
2	D	2737	LEU
2	D	2757	MET
2	D	2766	LYS
2	D	2772	ARG
2	D	2782	MET
2	D	2783	LEU
2	D	2801	TYR
2	D	2931	ARG
2	D	3018	ARG
2	D	3190	ARG
2	D	3323	MET
2	D	3584	LYS
2	D	3591	LEU
2	D	3605	MET
2	D	3847	CYS

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Mol	Chain	Res	Type
2	D	4279	MET
2	D	4307	ARG
2	D	4504	MET
2	D	4748	MET
2	D	4884	MET
2	D	4932	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	50	GLN
2	A	29	HIS
2	A	388	GLN
2	A	658	ASN
2	A	669	GLN
2	A	888	ASN
2	A	1146	HIS
2	A	1452	GLN
2	A	2217	HIS
2	A	2540	HIS
2	A	2850	ASN
2	A	2927	GLN
2	A	2998	ASN
2	A	3017	HIS
2	A	3151	GLN
2	A	3287	ASN
2	A	4049	HIS
2	A	4057	HIS
2	A	4933	HIS
1	J	54	ASN
1	L	54	ASN
1	K	50	GLN
2	B	388	GLN
2	B	658	ASN
2	B	669	GLN
2	B	888	ASN
2	B	1146	HIS
2	B	1452	GLN
2	B	2217	HIS
2	B	2540	HIS
2	B	2850	ASN
2	B	2927	GLN

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Mol	Chain	Res	Type
2	B	2998	ASN
2	B	3017	HIS
2	B	3034	HIS
2	B	3151	GLN
2	B	3287	ASN
2	B	4049	HIS
2	B	4057	HIS
2	B	4933	HIS
2	C	29	HIS
2	C	388	GLN
2	C	658	ASN
2	C	669	GLN
2	C	888	ASN
2	C	1146	HIS
2	C	1452	GLN
2	C	2217	HIS
2	C	2540	HIS
2	C	2850	ASN
2	C	2927	GLN
2	C	2998	ASN
2	C	3017	HIS
2	C	3151	GLN
2	C	3287	ASN
2	C	4049	HIS
2	C	4057	HIS
2	C	4933	HIS
2	D	388	GLN
2	D	658	ASN
2	D	669	GLN
2	D	888	ASN
2	D	1146	HIS
2	D	1452	GLN
2	D	2217	HIS
2	D	2540	HIS
2	D	2850	ASN
2	D	2927	GLN
2	D	2998	ASN
2	D	3017	HIS
2	D	3034	HIS
2	D	3151	GLN
2	D	3287	ASN
2	D	4049	HIS

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Mol	Chain	Res	Type
2	D	4057	HIS
2	D	4933	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 24 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ATP	D	5002	-	26,33,33	0.67	0	31,52,52	0.72	1 (3%)
6	ATP	A	5002	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
6	ATP	C	5002	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
6	ATP	D	5004	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
6	ATP	C	5004	-	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
6	ATP	A	5004	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
6	ATP	B	5002	-	26,33,33	0.67	0	31,52,52	0.72	1 (3%)
6	ATP	B	5004	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	5002	-	-	7/18/38/38	0/3/3/3
6	ATP	A	5002	-	-	7/18/38/38	0/3/3/3
6	ATP	C	5002	-	-	7/18/38/38	0/3/3/3
6	ATP	D	5004	-	-	9/18/38/38	0/3/3/3
6	ATP	C	5004	-	-	9/18/38/38	0/3/3/3
6	ATP	A	5004	-	-	9/18/38/38	0/3/3/3
6	ATP	B	5002	-	-	7/18/38/38	0/3/3/3
6	ATP	B	5004	-	-	9/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5002	ATP	C5-C6-N6	2.32	123.88	120.35
6	B	5002	ATP	C5-C6-N6	2.31	123.86	120.35
6	C	5002	ATP	C5-C6-N6	2.31	123.86	120.35
6	A	5004	ATP	C5-C6-N6	2.30	123.84	120.35
6	C	5004	ATP	C5-C6-N6	2.29	123.84	120.35
6	D	5002	ATP	C5-C6-N6	2.29	123.84	120.35
6	B	5004	ATP	C5-C6-N6	2.29	123.83	120.35
6	D	5004	ATP	C5-C6-N6	2.27	123.81	120.35
6	C	5004	ATP	PB-O3B-PG	2.06	139.90	132.83
6	A	5004	ATP	PB-O3B-PG	2.05	139.85	132.83
6	B	5004	ATP	PB-O3B-PG	2.05	139.85	132.83
6	D	5004	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5002	ATP	C5'-O5'-PA-O1A
6	A	5002	ATP	C5'-O5'-PA-O2A
6	A	5004	ATP	PB-O3A-PA-O5'
6	A	5004	ATP	C5'-O5'-PA-O1A
6	A	5004	ATP	C5'-O5'-PA-O2A
6	A	5004	ATP	O4'-C4'-C5'-O5'
6	B	5002	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	B	5002	ATP	C5'-O5'-PA-O2A
6	B	5004	ATP	PB-O3A-PA-O5'
6	B	5004	ATP	C5'-O5'-PA-O1A
6	B	5004	ATP	C5'-O5'-PA-O2A
6	B	5004	ATP	O4'-C4'-C5'-O5'
6	C	5002	ATP	C5'-O5'-PA-O1A
6	C	5002	ATP	C5'-O5'-PA-O2A
6	C	5004	ATP	PB-O3A-PA-O5'
6	C	5004	ATP	C5'-O5'-PA-O1A
6	C	5004	ATP	C5'-O5'-PA-O2A
6	C	5004	ATP	O4'-C4'-C5'-O5'
6	D	5002	ATP	C5'-O5'-PA-O1A
6	D	5002	ATP	C5'-O5'-PA-O2A
6	D	5004	ATP	PB-O3A-PA-O5'
6	D	5004	ATP	C5'-O5'-PA-O1A
6	D	5004	ATP	C5'-O5'-PA-O2A
6	D	5004	ATP	O4'-C4'-C5'-O5'
6	A	5002	ATP	O4'-C4'-C5'-O5'
6	A	5004	ATP	C3'-C4'-C5'-O5'
6	B	5002	ATP	O4'-C4'-C5'-O5'
6	B	5004	ATP	C3'-C4'-C5'-O5'
6	C	5002	ATP	O4'-C4'-C5'-O5'
6	C	5004	ATP	C3'-C4'-C5'-O5'
6	D	5002	ATP	O4'-C4'-C5'-O5'
6	D	5004	ATP	C3'-C4'-C5'-O5'
6	A	5002	ATP	C4'-C5'-O5'-PA
6	B	5002	ATP	C4'-C5'-O5'-PA
6	C	5002	ATP	C4'-C5'-O5'-PA
6	D	5002	ATP	C4'-C5'-O5'-PA
6	A	5004	ATP	C5'-O5'-PA-O3A
6	B	5004	ATP	C5'-O5'-PA-O3A
6	C	5004	ATP	C5'-O5'-PA-O3A
6	D	5004	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PA-O3A-PB-O1B
6	B	5004	ATP	PA-O3A-PB-O1B
6	C	5004	ATP	PA-O3A-PB-O1B
6	D	5004	ATP	PA-O3A-PB-O1B
6	A	5002	ATP	PB-O3B-PG-O3G
6	A	5004	ATP	PB-O3B-PG-O3G
6	B	5002	ATP	PB-O3B-PG-O3G
6	B	5004	ATP	PB-O3B-PG-O3G
6	C	5002	ATP	PB-O3B-PG-O3G

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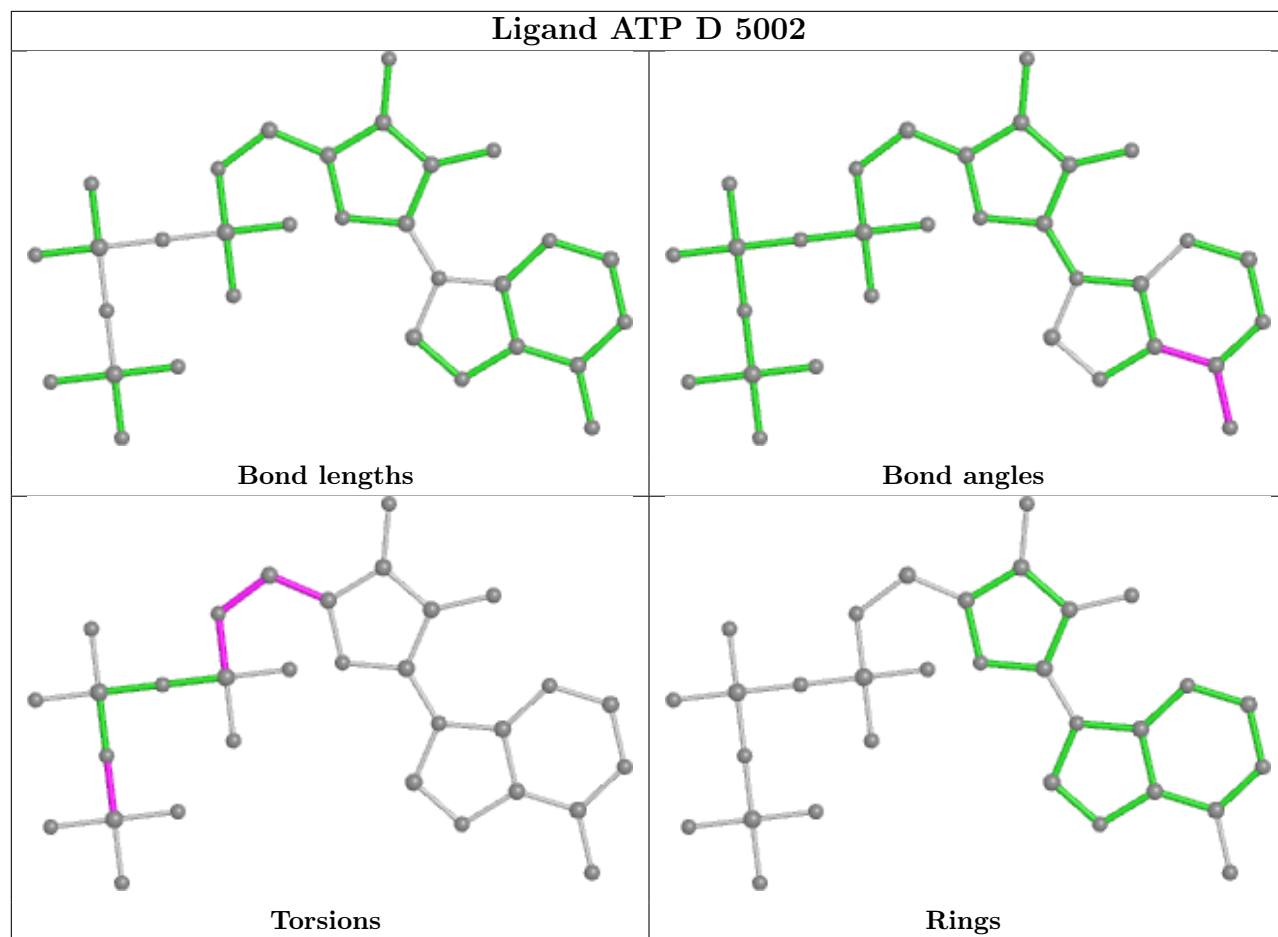
Mol	Chain	Res	Type	Atoms
6	C	5004	ATP	PB-O3B-PG-O3G
6	D	5002	ATP	PB-O3B-PG-O3G
6	D	5004	ATP	PB-O3B-PG-O3G
6	A	5002	ATP	C5'-O5'-PA-O3A
6	B	5002	ATP	C5'-O5'-PA-O3A
6	C	5002	ATP	C5'-O5'-PA-O3A
6	D	5002	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PA-O3A-PB-O2B
6	B	5004	ATP	PA-O3A-PB-O2B
6	C	5004	ATP	PA-O3A-PB-O2B
6	D	5004	ATP	PA-O3A-PB-O2B
6	A	5002	ATP	PB-O3B-PG-O1G
6	B	5002	ATP	PB-O3B-PG-O1G
6	C	5002	ATP	PB-O3B-PG-O1G
6	D	5002	ATP	PB-O3B-PG-O1G

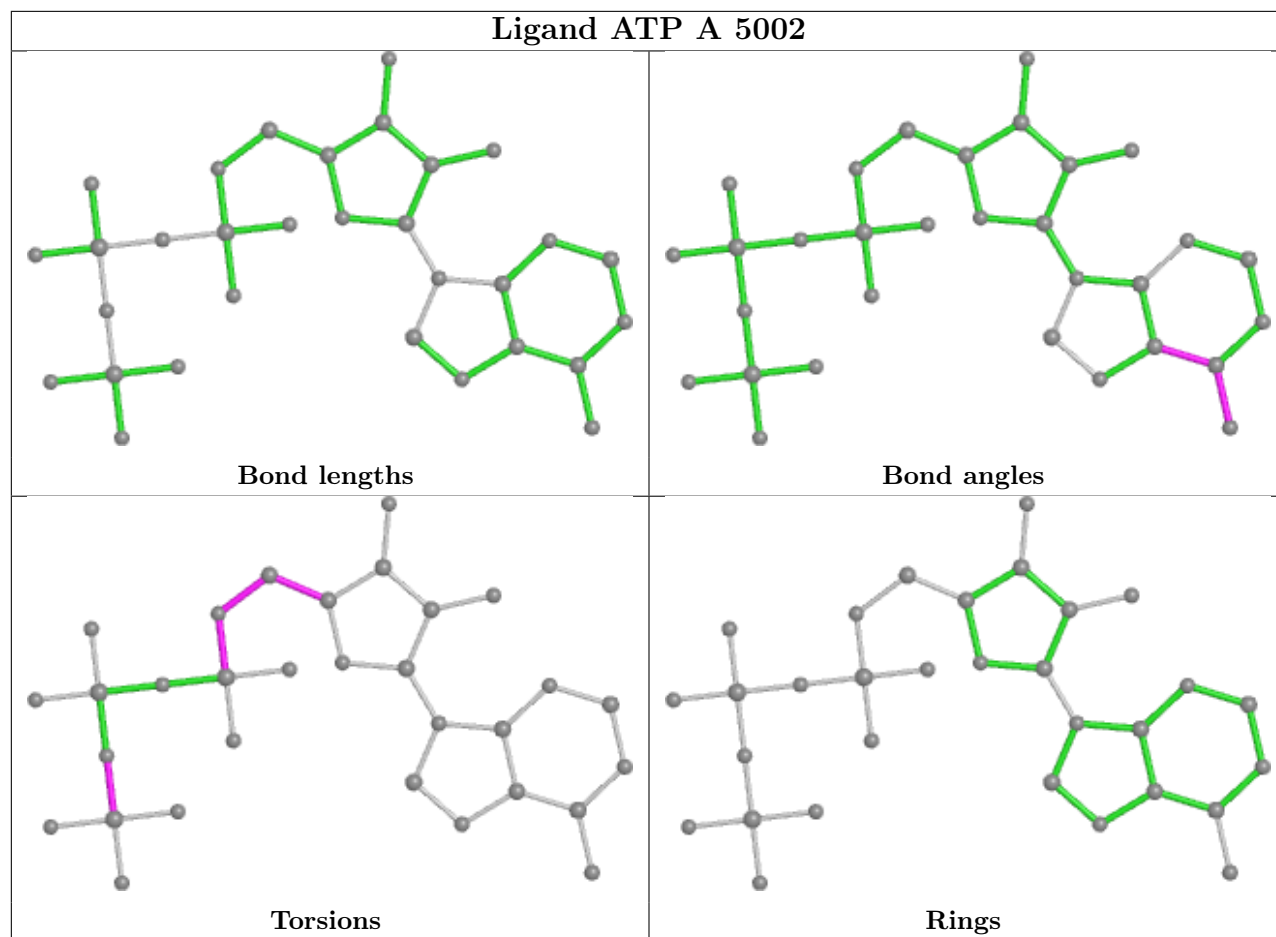
There are no ring outliers.

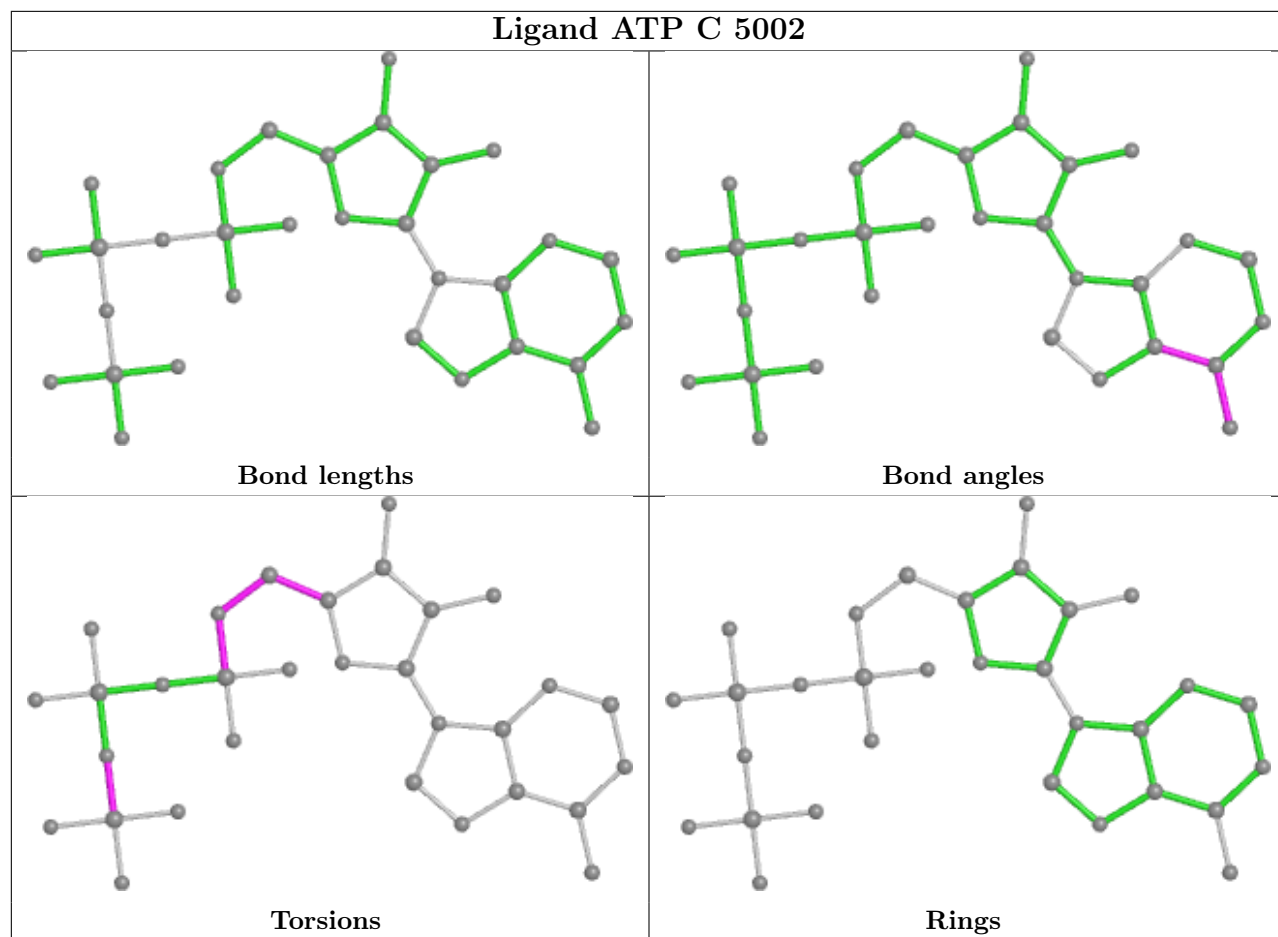
4 monomers are involved in 4 short contacts:

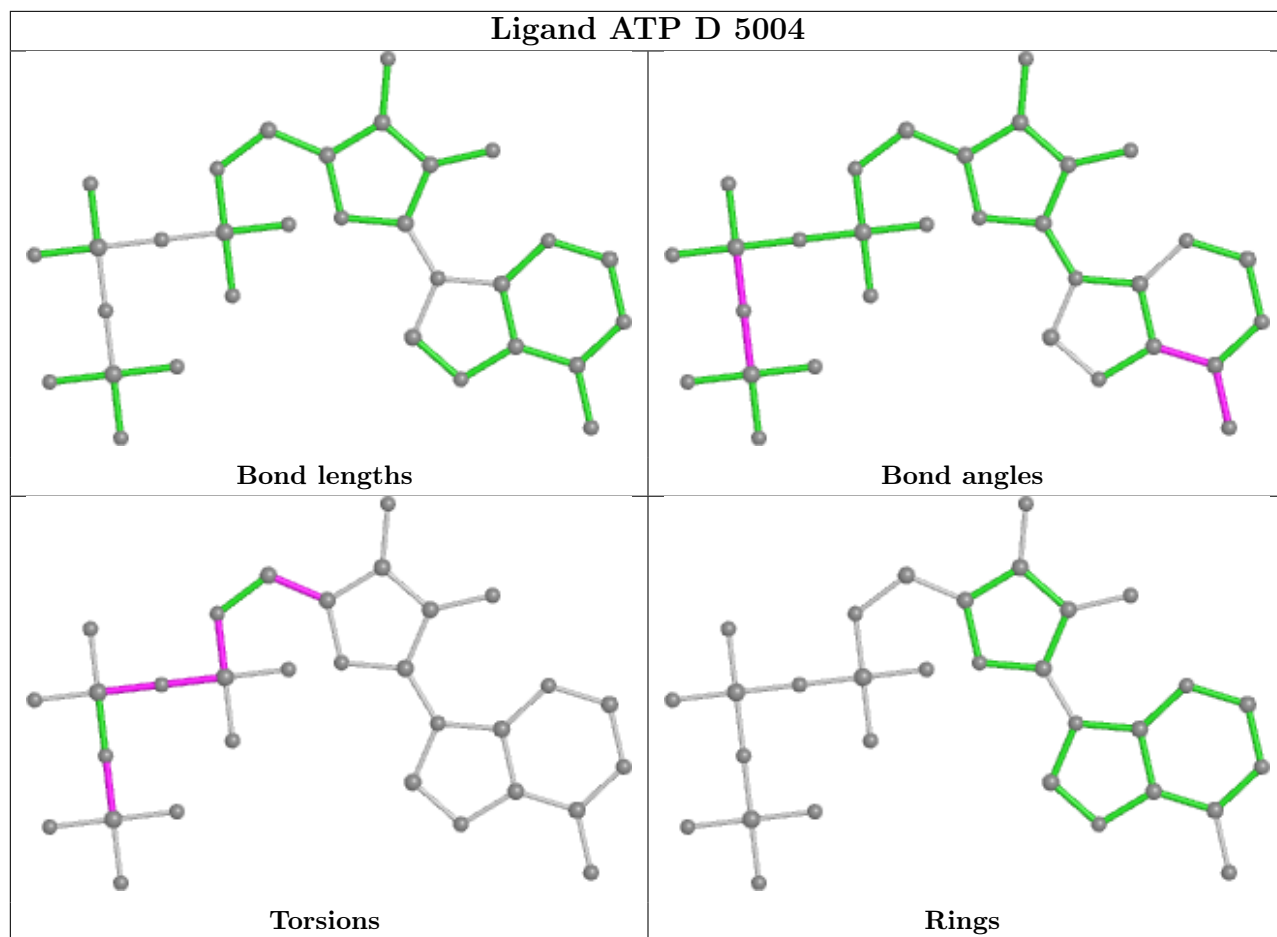
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	5004	ATP	1	0
6	C	5004	ATP	1	0
6	A	5004	ATP	1	0
6	B	5004	ATP	1	0

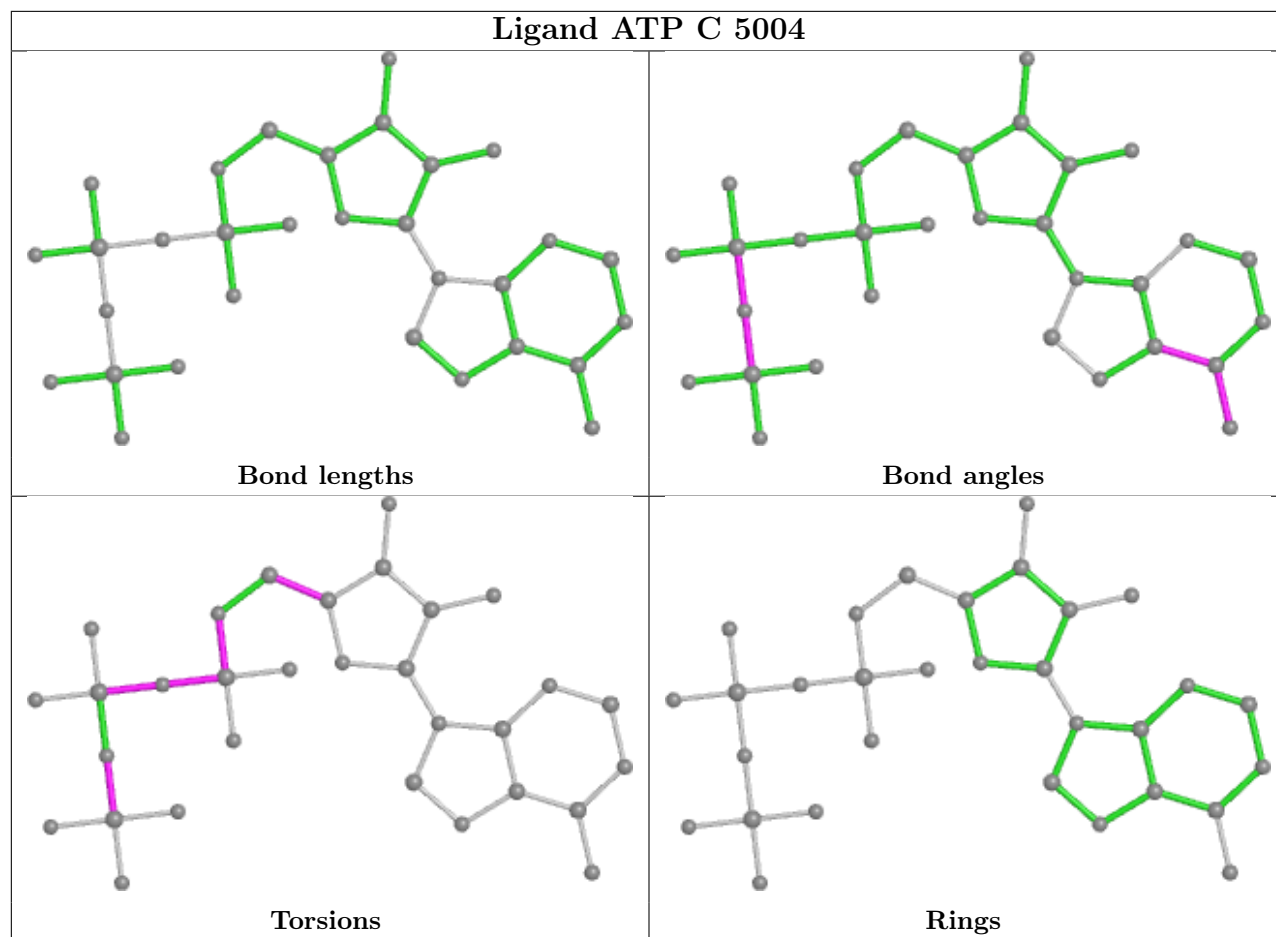
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

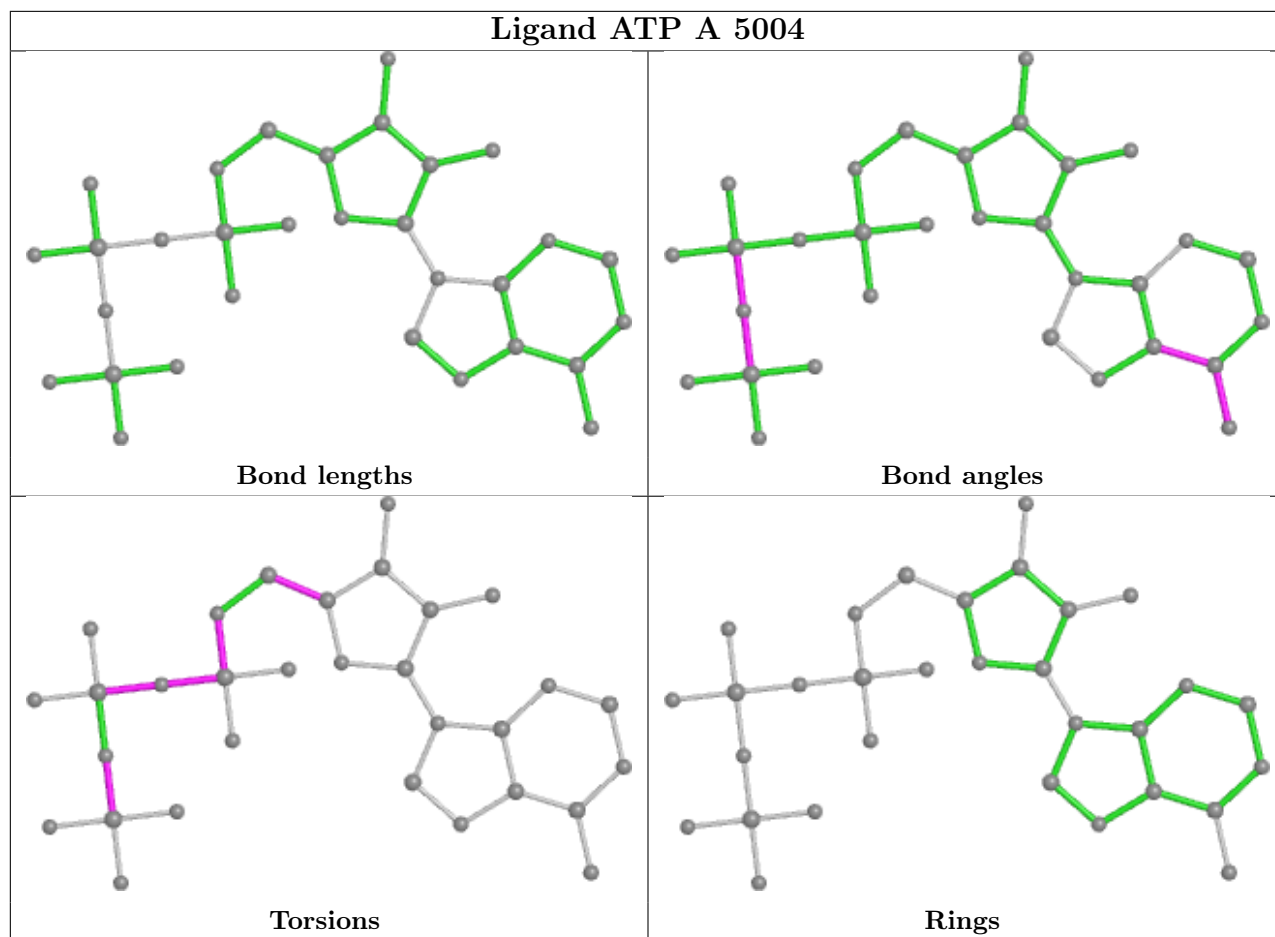


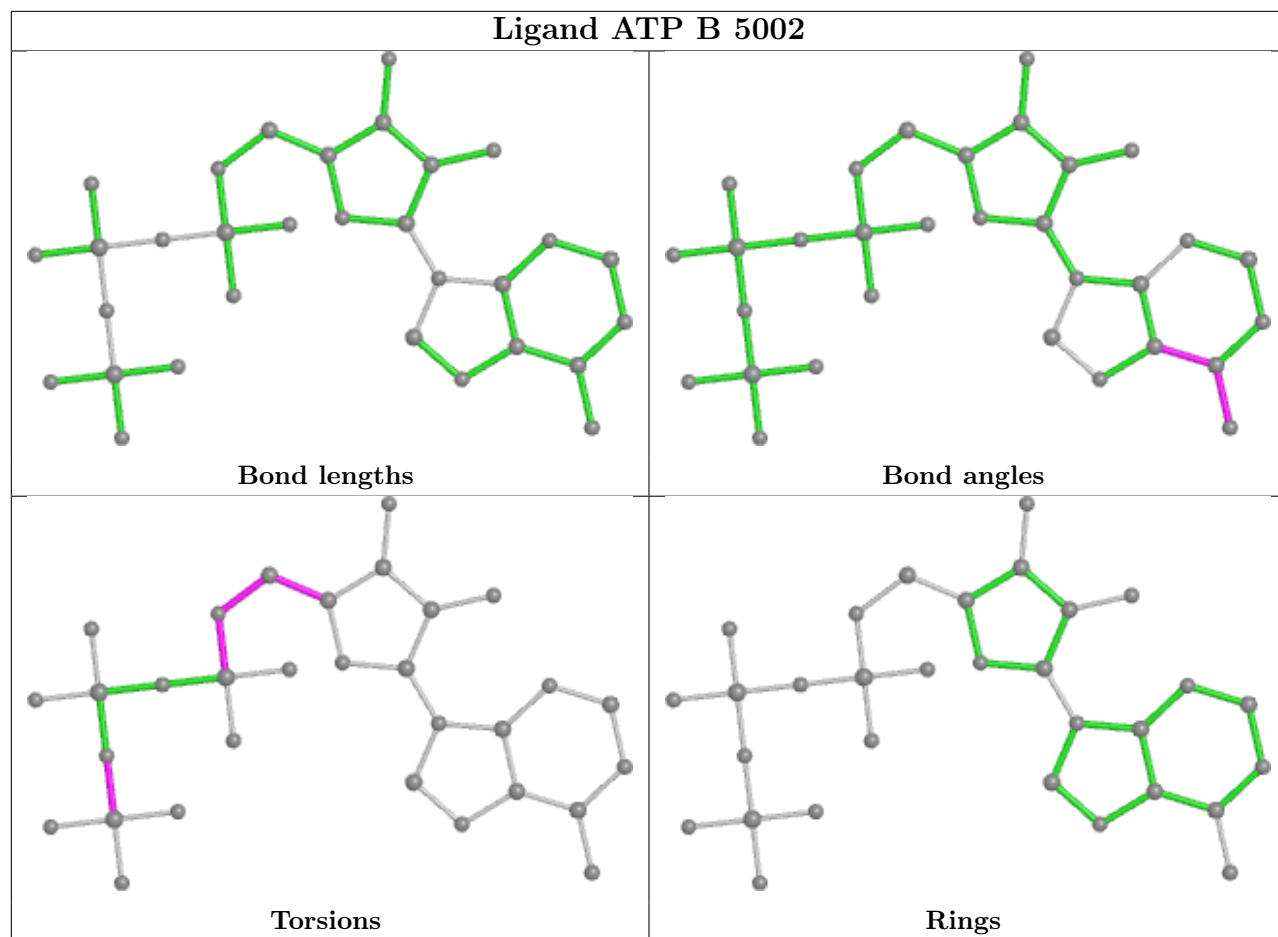


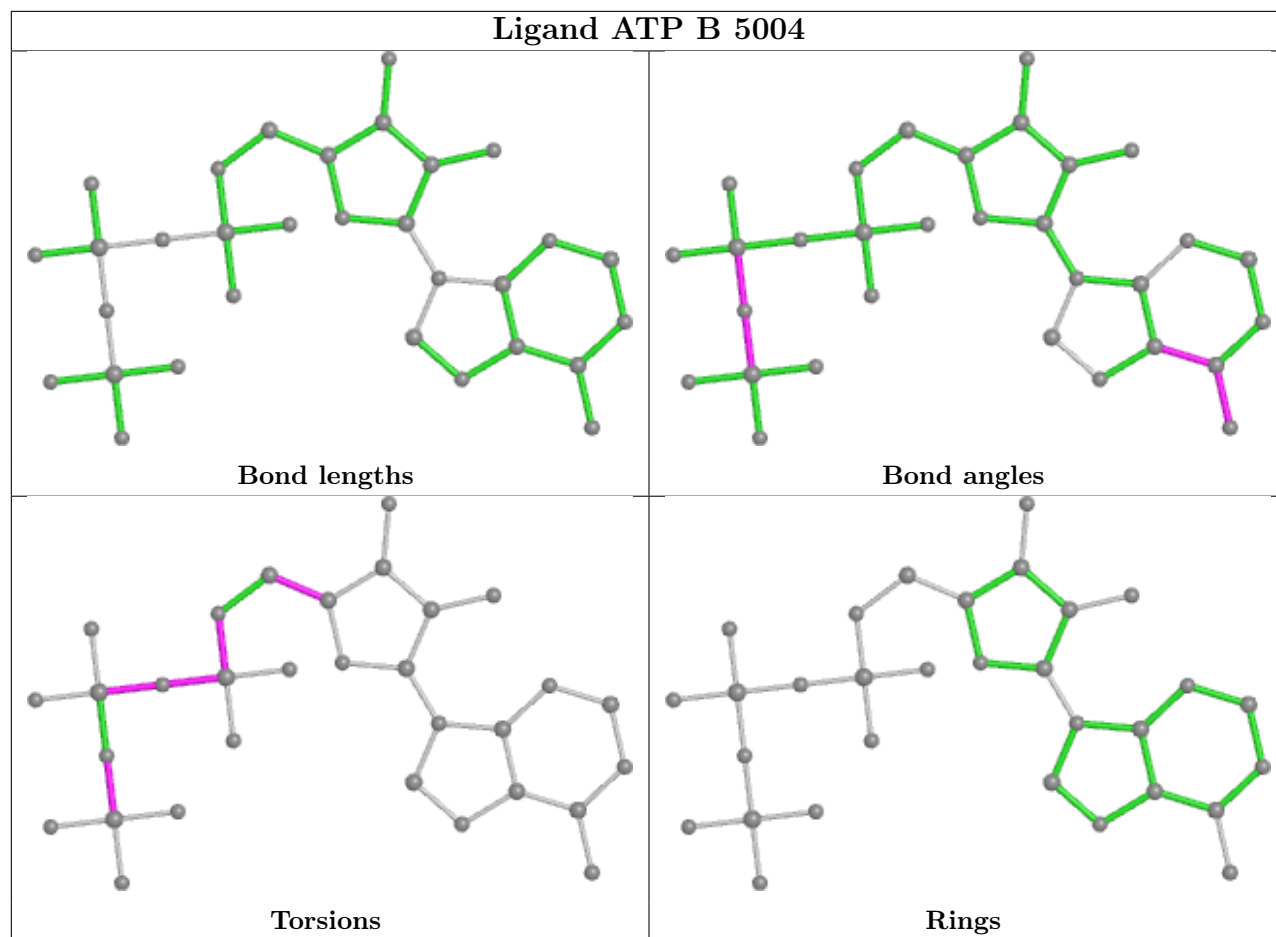












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

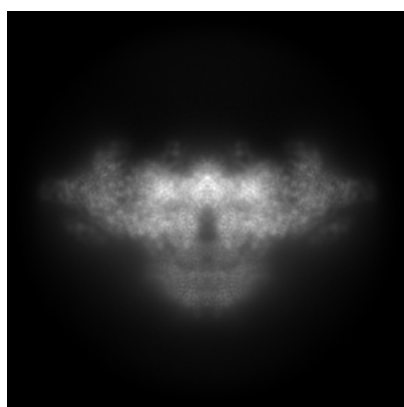
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42769. These allow visual inspection of the internal detail of the map and identification of artifacts.

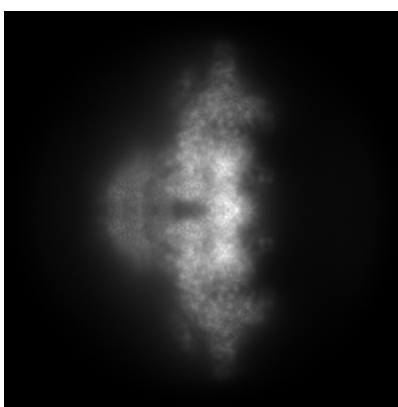
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

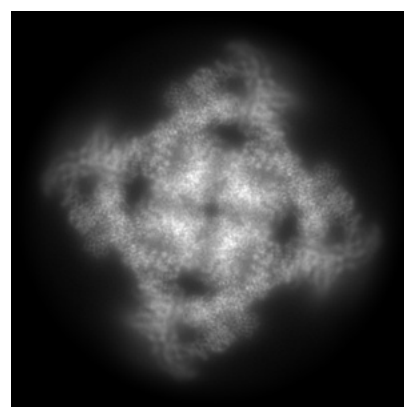
6.1.1 Primary map



X



Y

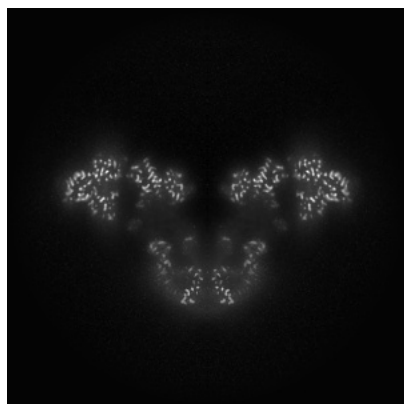


Z

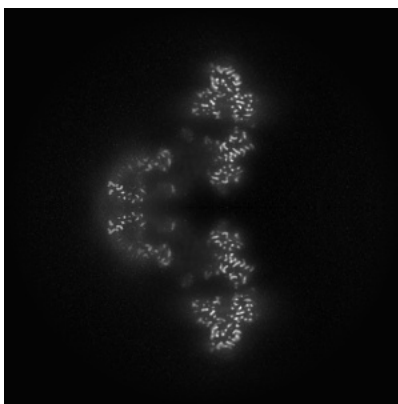
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

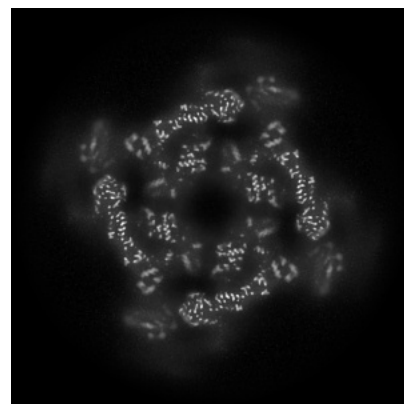
6.2.1 Primary map



X Index: 256



Y Index: 256

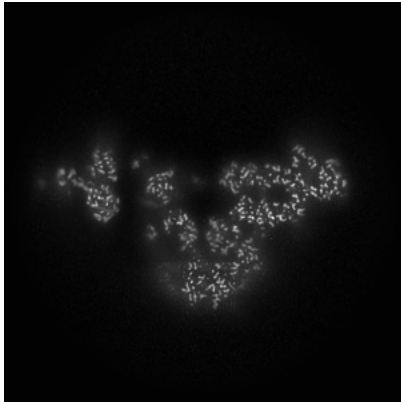


Z Index: 256

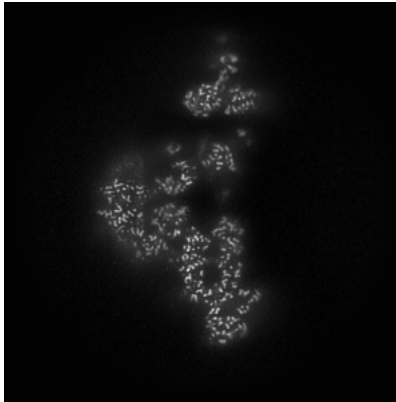
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

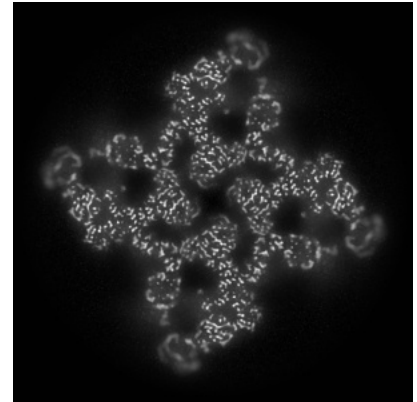
6.3.1 Primary map



X Index: 239



Y Index: 239

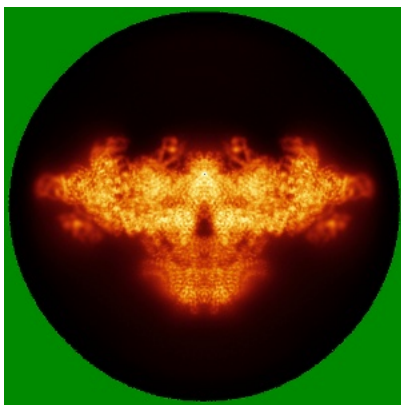


Z Index: 283

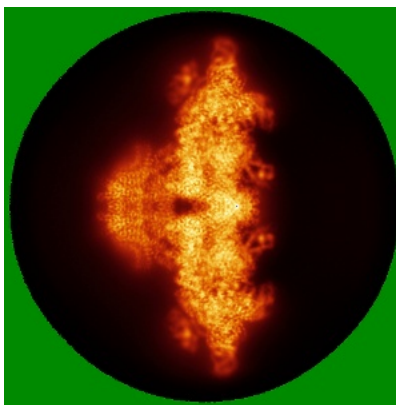
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

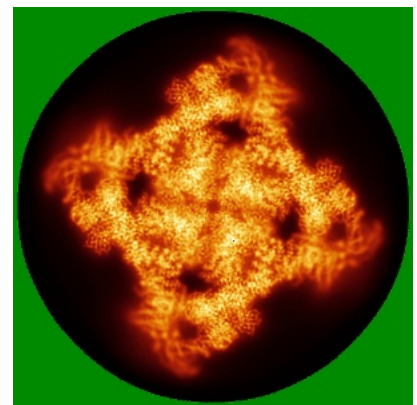
6.4.1 Primary map



X



Y

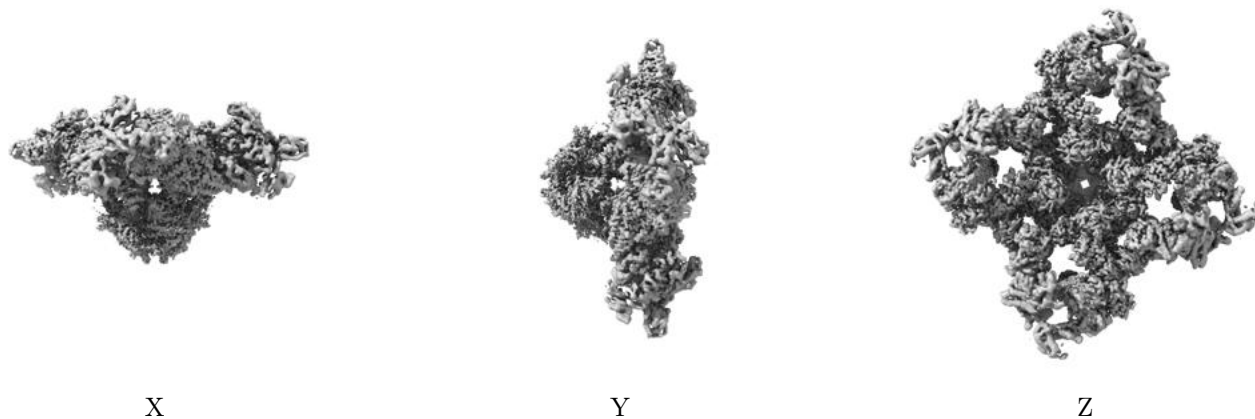


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

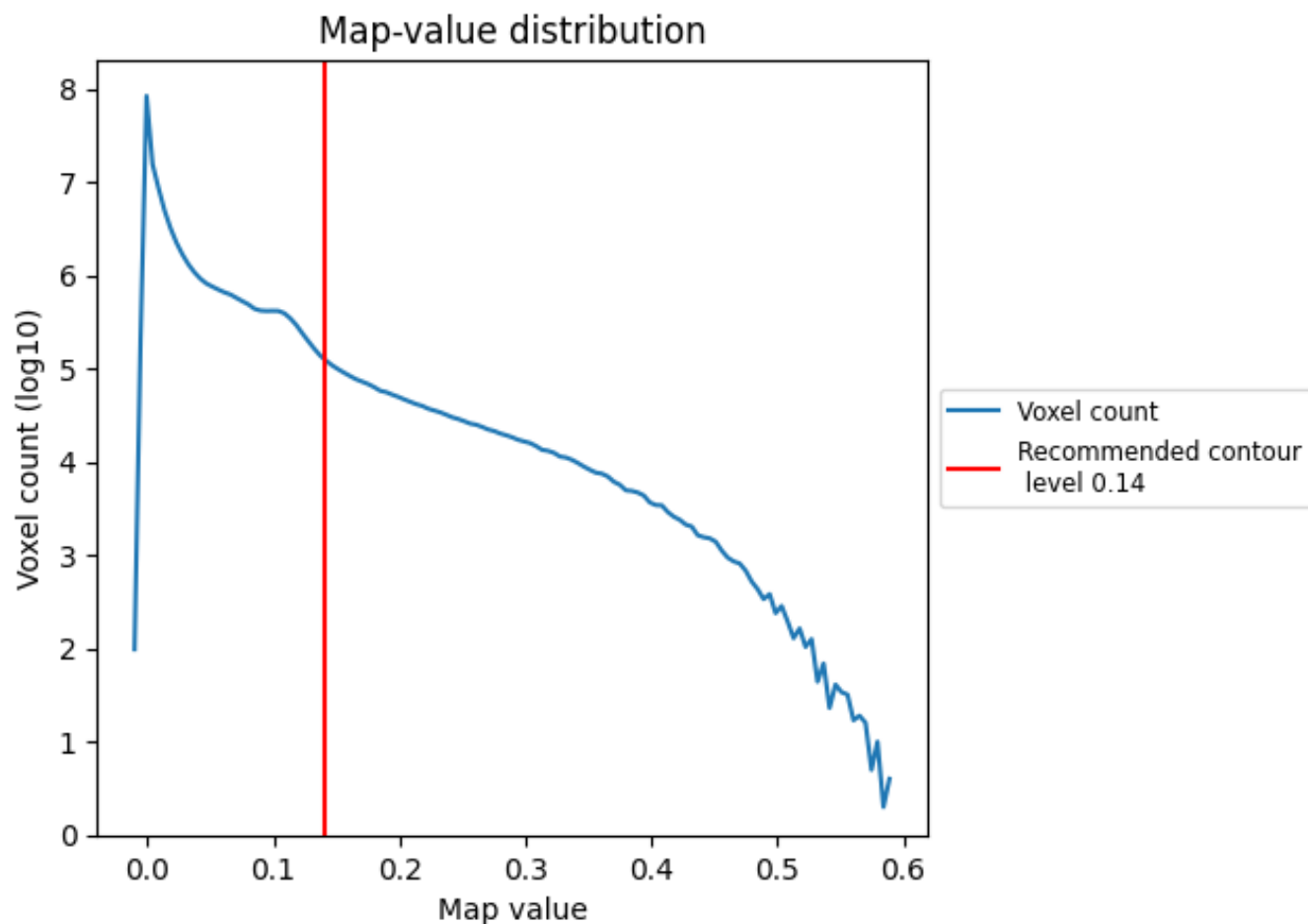
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

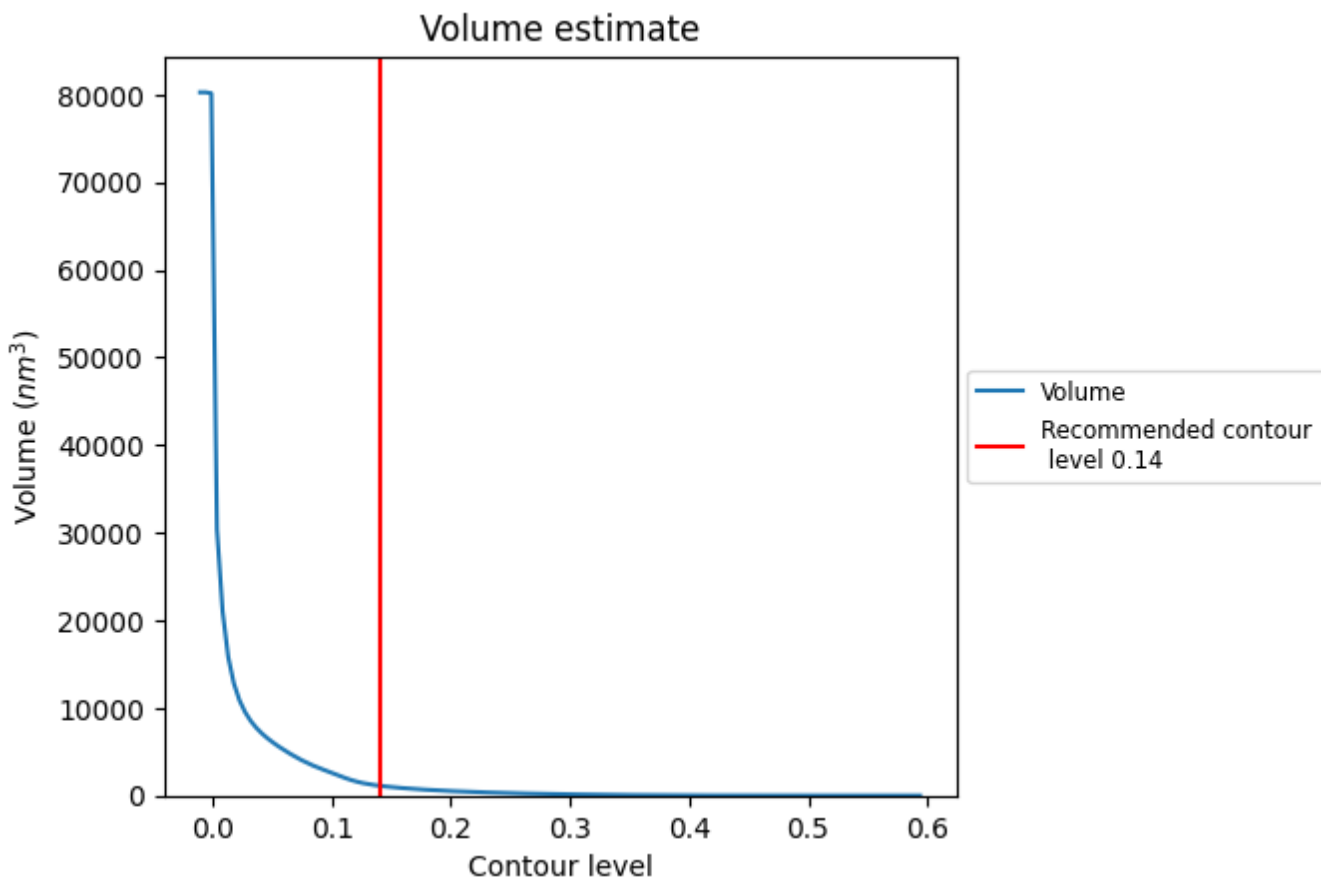
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

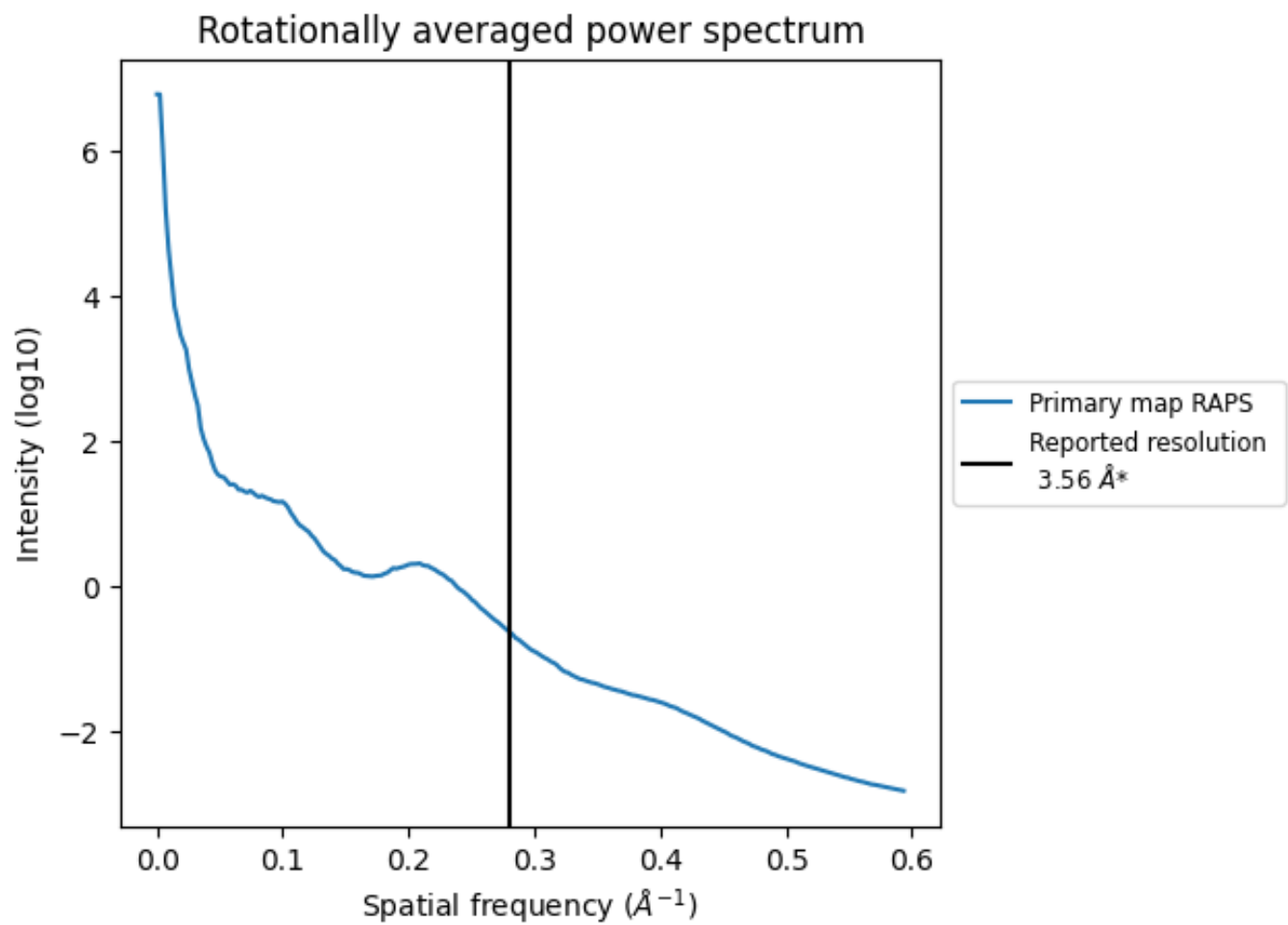
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 11220 nm^3 ; this corresponds to an approximate mass of 1014 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

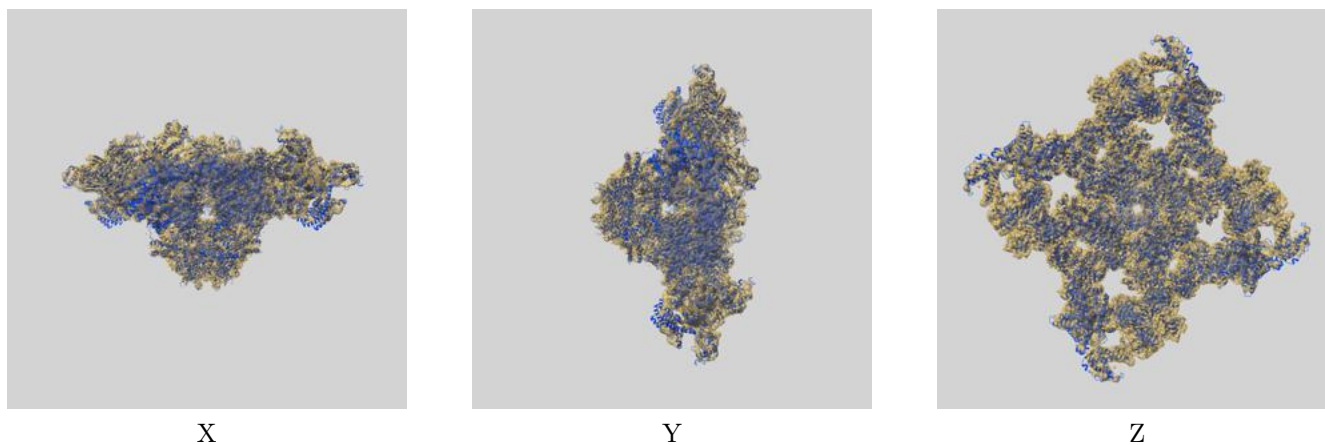
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

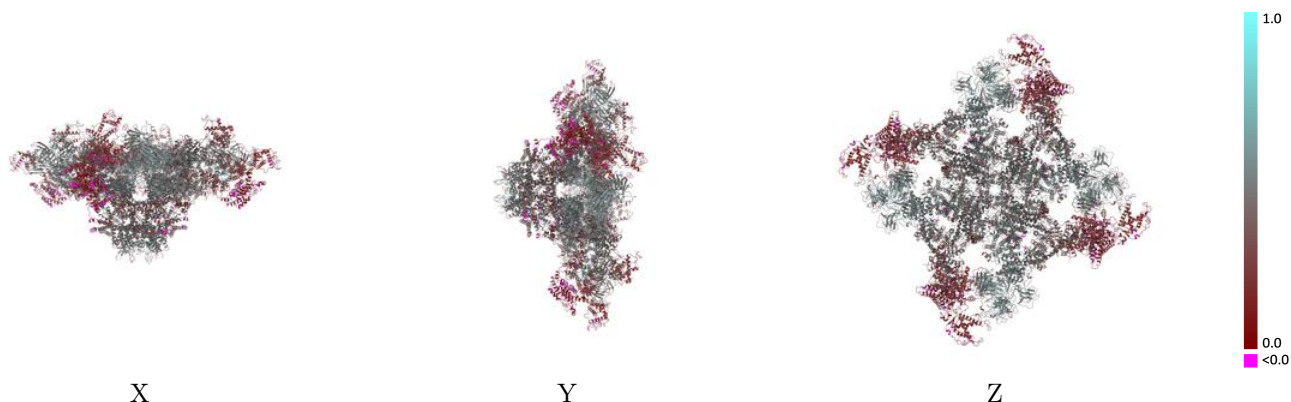
This section contains information regarding the fit between EMDB map EMD-42769 and PDB model 8UXM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



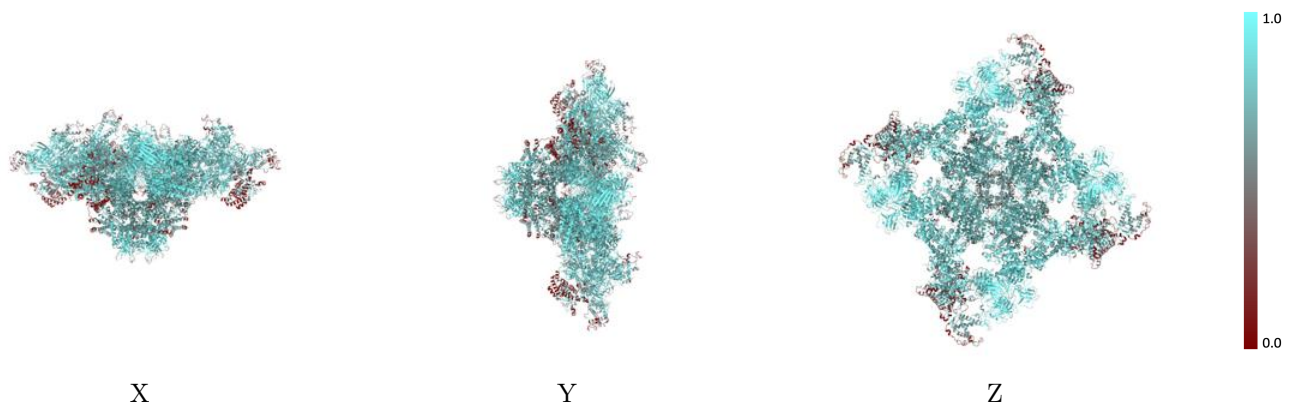
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



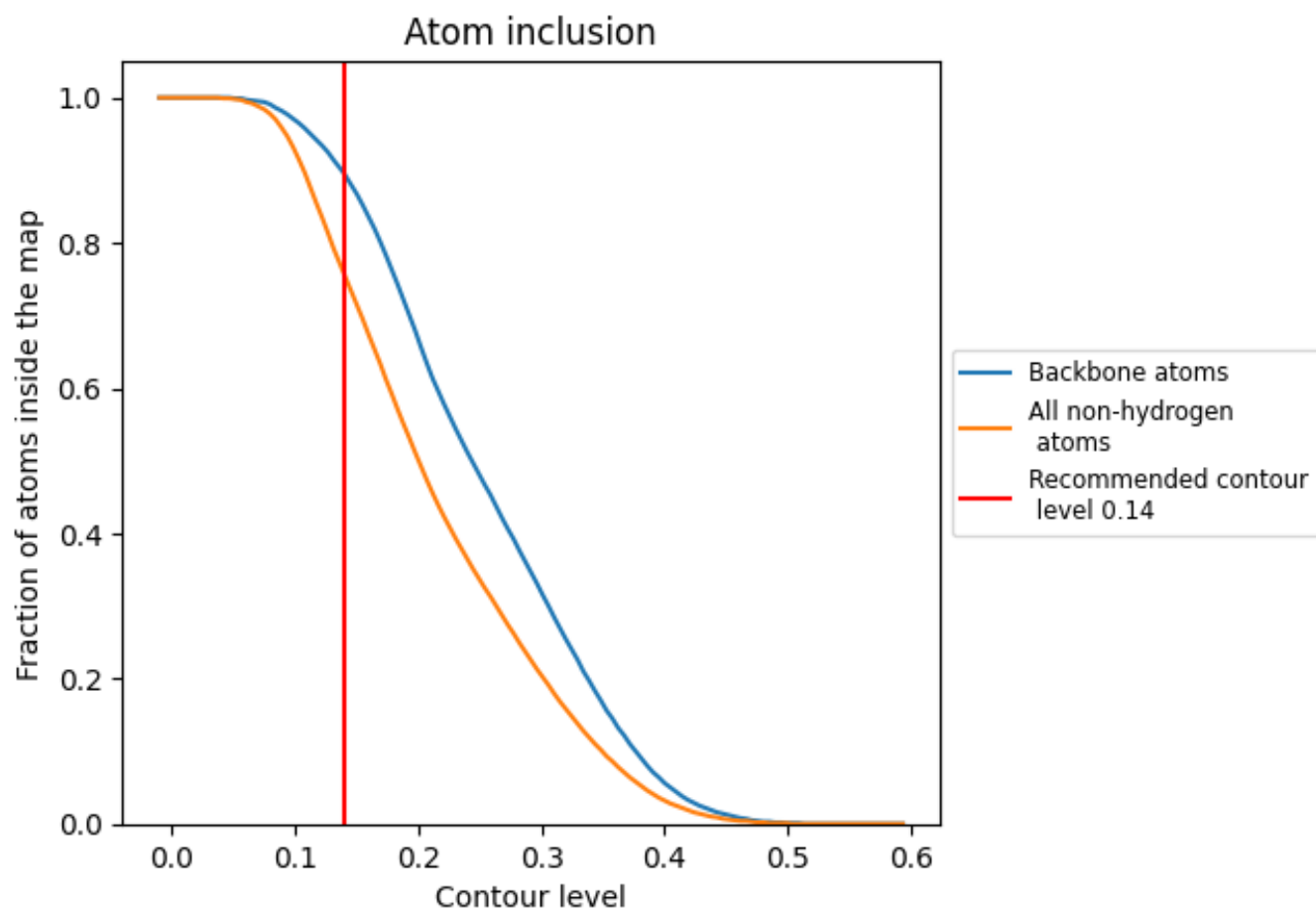
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.3810
A	 0.7540	 0.3840
B	 0.7560	 0.3860
C	 0.7520	 0.3800
D	 0.7540	 0.3820
E	 0.8920	 0.5130
F	 0.8910	 0.5110
G	 0.8960	 0.5120
H	 0.8970	 0.5110
I	 0.7240	 0.2220
J	 0.7320	 0.2220
K	 0.7240	 0.2220
L	 0.7310	 0.2190

