



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 11:58 pm GMT

PDB ID : 6TED
EMDB ID : EMD-10480
Title : Structure of complete, activated transcription complex Pol II-DSIF-PAF-SPT6
uncovers allosteric elongation activation by RTF1
Authors : Vos, S.M.; Farnung, L.; Cramer, P.
Deposited on : 2019-11-11
Resolution : 3.10 Å (reported)
Based on initial models : 4L1U, 6GMH, 6AFO

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:

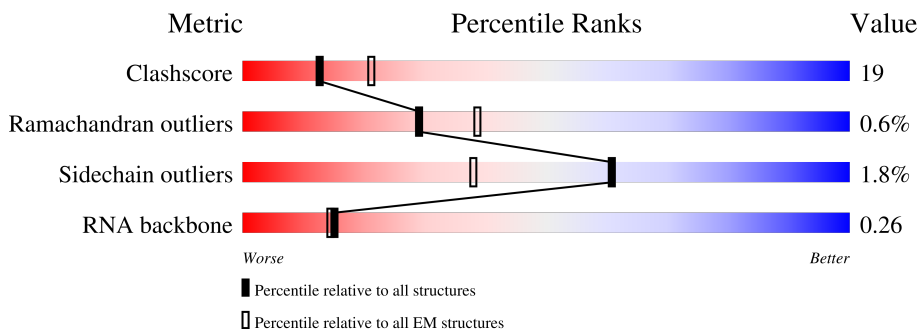
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.10 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.






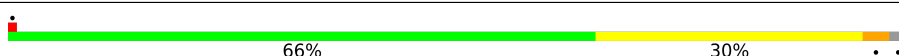
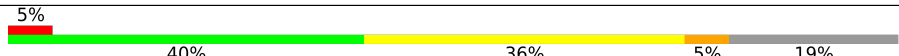

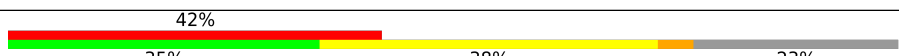
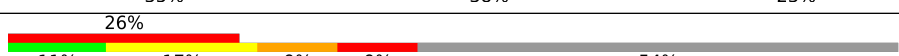
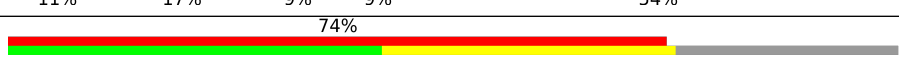

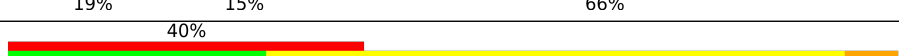
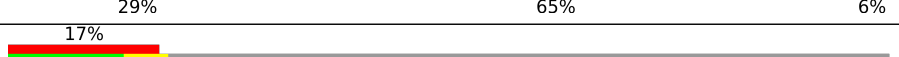

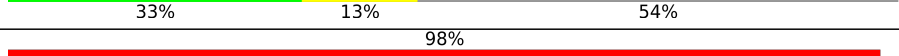

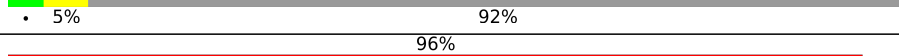

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1984	
2	B	1251	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	48	
15	P	46	
16	Q	1179	
17	R	713	
18	T	48	
19	U	666	
20	V	531	
21	W	305	
22	X	531	
23	Y	121	
24	Z	1087	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 57142 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
1	A	1426	11255	7074	2014	2095	2	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1122	8980	5684	1576	1656	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1004	630	170	200	4	0	0

- Molecule 5 is a protein called RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1333	866	214	245	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1197	759	195	238	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	942	582	168	181	11	0	0

- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	47	390	240	77	67	6	0	0

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	1002	4737	2583	1071	1076	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total	C	N	O	P	0	0
			773	361	158	217	37		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	890	Total	C	N	O	S	0	0
			7226	4579	1264	1352	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	244	Total	C	N	O	S	0	0
			1832	1148	340	337	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	48	974	462	168	296	48	0	0

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	125	852	534	151	166	1	0	0

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	244	1703	1061	305	333	4	0	0

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	300	2333	1483	392	454	4	0	0

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	43	353	220	69	64	0	0

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	116	911	570	159	173	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
24	Z	510	4023	2550	709	745	1	18	0	0

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total 2	Zn 2	0
25	B	1	Total 1	Zn 1	0
25	C	1	Total 1	Zn 1	0
25	I	2	Total 2	Zn 2	0
25	J	1	Total 1	Zn 1	0
25	L	1	Total 1	Zn 1	0
25	Y	1	Total 1	Zn 1	0

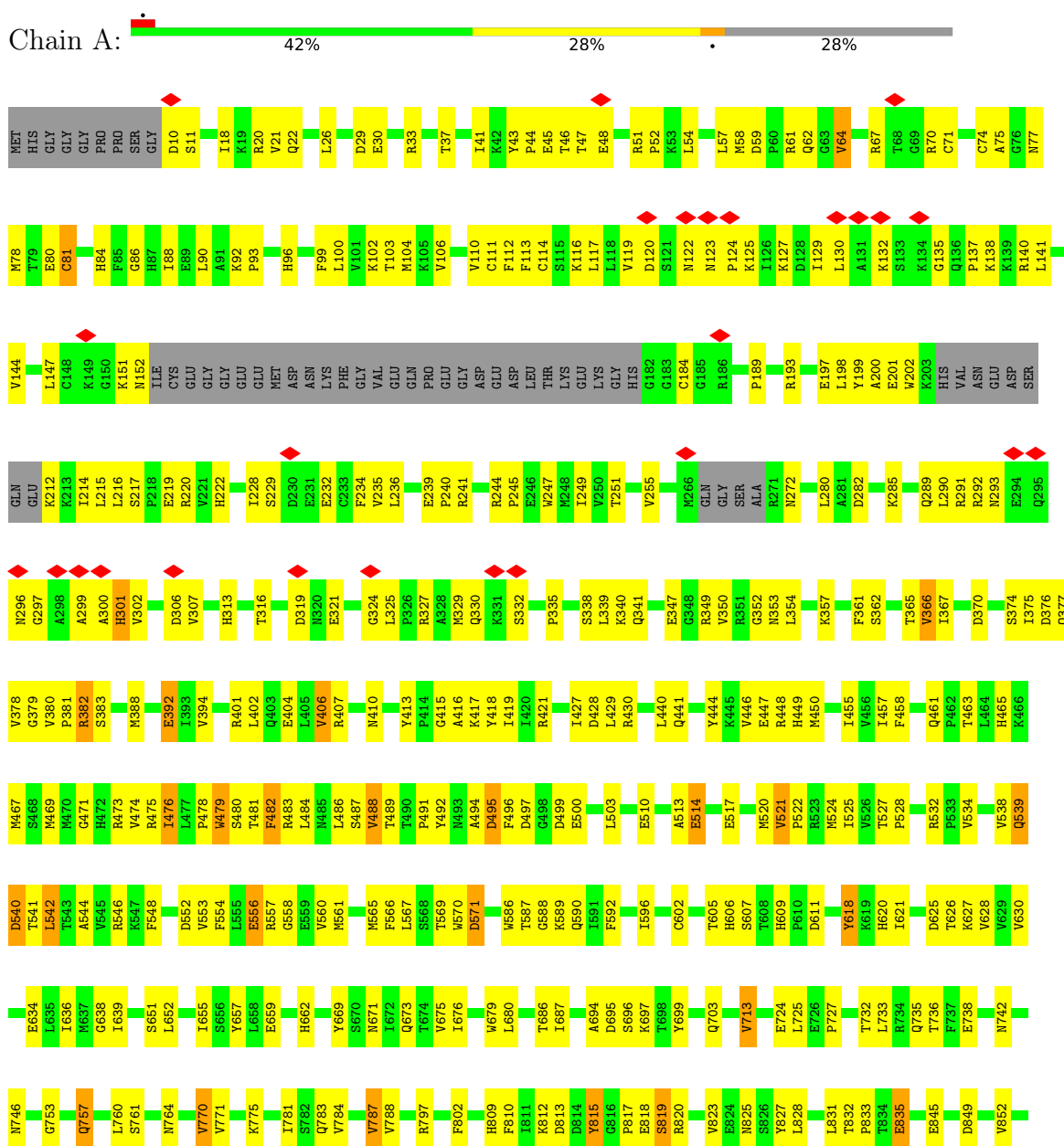
- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total 1	Mg 1	0

3 Residue-property plots

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.

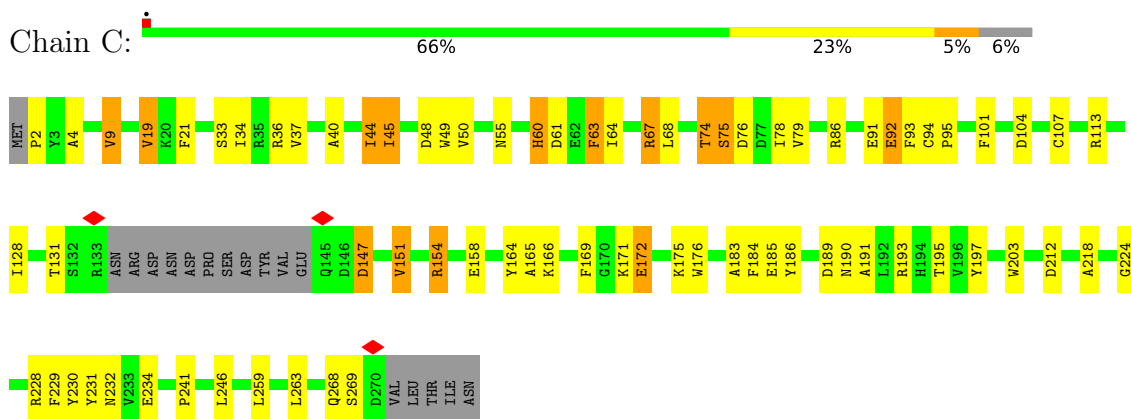
- Molecule 1: DNA-directed RNA polymerase subunit



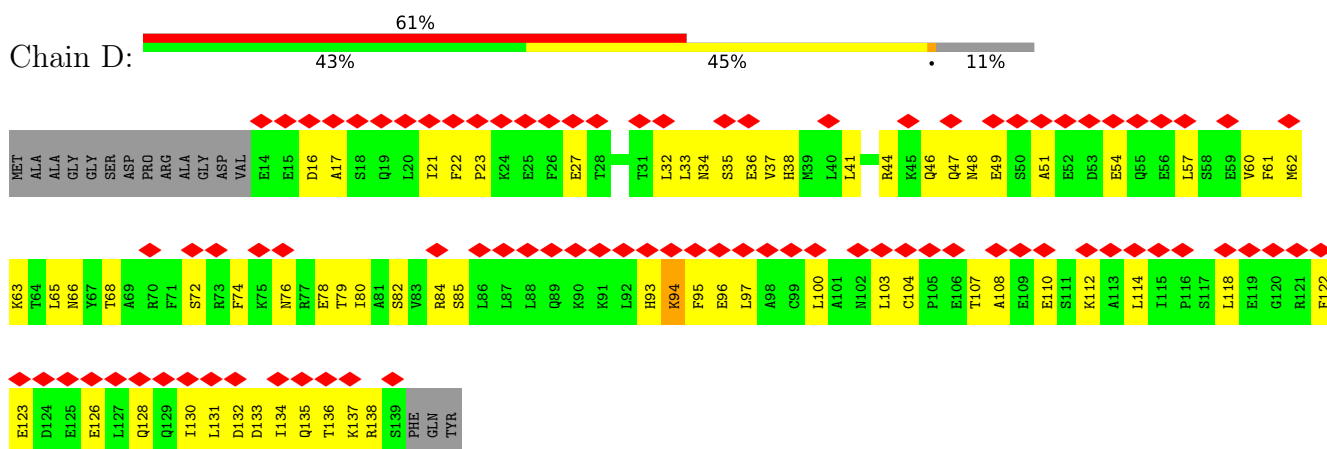


MET	VAL	GLN	K146	ALA	A339	R438	E544	L634	P720	F810	S899	D1004	M1125
CYS	SER	ALA	T147	LYS	Y342	1439	L545	R638	R721	Y811	E900	A1005	M1129
THR	VAL	ALA	F148	LYS	M347	G451	E546	R639	M728	Y814	T901	M1006	M1130
ASN	GLN	GLN	P153	SER	K346	G452	M548	L643	Q731	E815	V904	M1007	R1131
LEU	SER	GLN	H154	ALA	M347	W452	E551	R646	V735	E816	V907	K1010	T1134
SER	ARG	ALA	I155	CYS	P349	W453	R552	E647	Y736	R821	T910	L1014	Y1135
GLN	ARG	ALA	M155	ALA	R348	G454	L553	E648	Y737	G822	L911	L1015	E1136
ALA	GLY	SER	L156	SER	P349	Q454	R554	E649	T738	F823	N912	L1016	E1137
LEU	GLY	GLY	R157	GLY	H350	D455	L555	R650	Y739	F824	N913	L1017	N1142
GLY	GLY	GLY	L158	VAL	V351	Q456	R556	R651	W740	D824	F918	Y1018	K1143
ALA	ALA	ALA	T159	VAL	S354	K457	R557	S652	H741	E825	C919	G1019	T1144
TYR	PRO	GLU	L163	GLU	D355	K458	R558	S653	V742	E826	R920	F1020	Q1145
PHE	GLY	GLY	M164	GLY	F356	K459	A559	S654	W743	R834	K921	H1021	L1148
ARG	SER	SER	G165	TYR	C357	H460	E565	D655	R744	E835	R922	L1022	V1149
ALA	CYS	ALA	L166	ASN	C358	H461	T565	D656	R745	E836	R923	R1023	R1150
ALA	ALA	ALA	R167	ASN	T359	Q461	K566	S659	P746	G839	R924	Y1027	R1151
ALA	MET	MET	R168	LEU	K360	Q462	L567	G660	R747	H840	V925	L1028	F1152
LEU	LEU	TYR	L170	TYR	K361	W466	F568	G661	Y750	H841	R926	Y1029	K1156
THR	ASP	ASP	D170	ASP	Y367	S467	M573	V661	L751	R842	V927	L1030	L1157
ALA	ALA	ASP	E176	ALA	K368	R472	V574	V662	Y752	H843	I931	T1038	E1161
ALA	ASP	ASP	C177	ASP	V369	L473	G575	E663	Y753	H844	G932	S1039	M1171
ALA	GLU	GLU	P178	GLU	H370	L479	H577	E664	P754	R847	D833	S1040	M1172
SER	LEU	LEU	L179	LEU	R371	L479	H578	E665	R755	L848	D834	Q1040	S1173
SER	LEU	LEU	D180	LEU	R372	L479	H579	D666	K756	L849	D835	Q1041	V1174
TRP	TRP	TRP	D181	TRP	R373	L479	H580	D667	P757	D851	S937	Y1047	
ALA	ALA	ALA	Y184	ALA	L377	R483	L583	E671	T760	R859	R938	Y1048	
GLY	PHE	ASP	F185	ASP	D386	R484	L584	E672	E765	R860	H939	Y1049	
PHE	PHE	ASP	I186	ASP	H387	L485	L585	E673	Y766	D864	H940	Q1049	
GLU	GLY	ASP	I187	ASP	Y388	L485	L586	E674	Y767	D865	G941	Q1050	
TRP	TRP	TRP	E191	ASP	L393	D492	L587	E675	R768	D866	K942	R1062	
ARG	ARG	ASP	K192	ASP	L394	G493	R588	E676	R769	D867	K943	G1065	
ARG	ARG	ASP	V193	ASP	L395	K494	R589	E677	F769	D868	C945	G1066	
LYS	LYS	LYS	E198	LYS	L396	L495	R592	E678	R770	D869	Y949	M1071	
ARG	ARG	LYS	K199	LYS	L397	L496	L595	E679	R771	D870	R950	M1072	
ARG	ARG	LYS	K211	LYS	L403	L497	L596	E680	E771	D871	R951	Q1073	
ARG	ARG	LYS	D212	LYS	F404	R498	L597	E681	E772	D872	D953	P1074	
SER	SER	LYS	T218	LYS	R405	R499	L601	E682	Y783	Y783	T957	E1088	
LEU	LEU	LYS	R222	LYS	F408	L501	V601	E683	S784	S784	C958	C1093	
LEU	LEU	LYS	S223	LYS	L411	L502	E609	E684	Y785	Y785	E959	Q1101	
LEU	LEU	LEU	R224	LEU	L412	L503	R610	E685	G786	G786	Y968	Q1102	
ALA	ALA	LEU	S228	LEU	L413	L504	R611	E686	Y787	Y787	S974	R1104	
ARG	ARG	LEU	S229	LEU	L414	L505	R612	E687	Y788	Y788	R975	E1105	
PRO	PRO	ARG	R230	PRO	E414	L506	R613	E688	Y789	Y789	C984	F1108	
GLY	GLY	GLY	E135	PRO	Q420	L507	R614	E689	Y790	Y790	K993	D1112	
GLY	GLY	GLY	G136	PRO	F422	L508	R615	E690	Y791	Y791	G994	Q1115	
ALA	ALA	ALA	E137	PRO	F423	L509	R616	E691	Y792	Y792	P996	Q1116	
ALA	ALA	ALA	E138	PRO	F424	L510	R617	E692	Y793	Y793	G997	H1117	
CYS	CYS	CYS	E139	PRO	F425	L511	R618	E693	Y794	Y794	R997	V1118	
ARG	ARG	ARG	E140	PRO	F426	L512	R619	E694	Y795	Y795	P1001	C1119	
TRP	TRP	TRP	E141	PRO	F427	L513	R620	E695	Y796	Y796	F1002	M1120	
TRP	TRP	TRP	E142	PRO	F428	L514	R621	E696	Y797	Y797	F1003		
LEU	LEU	LEU	E143	PRO	F429	L515	R622	E697	Y798	Y798			
LEU	LEU	LEU	H144	PRO	F430	L516	R623	E698	Y799	Y799			
ALA	ALA	ALA	Q145	PRO	F431	L517	R624	E699	Y800	Y800			

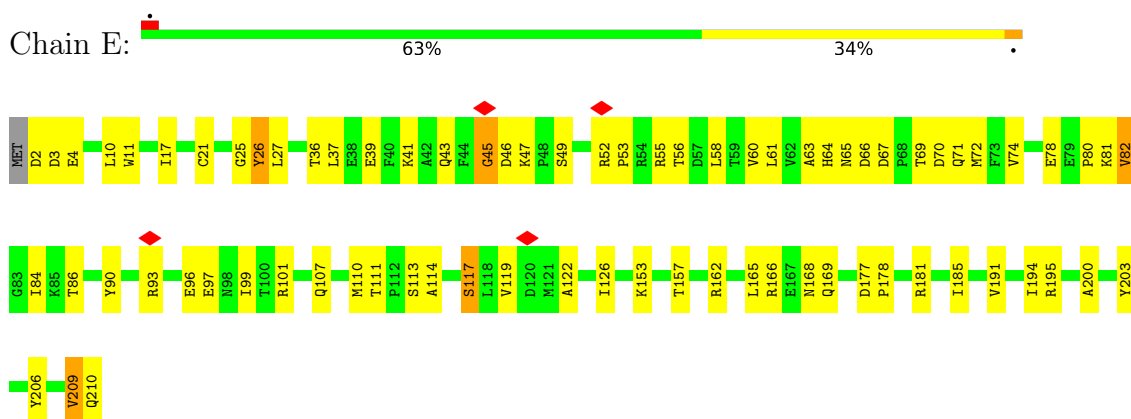
• Molecule 3: RNA polymerase II subunit C



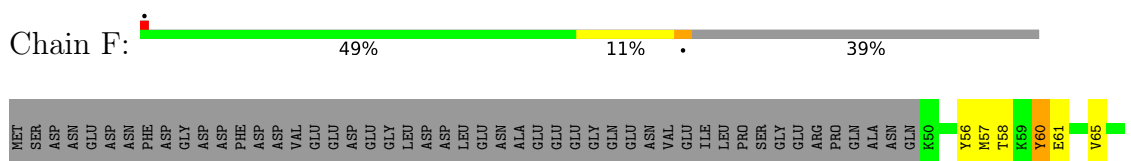
• Molecule 4: RNA polymerase II subunit D



• Molecule 5: RNA polymerase II subunit E

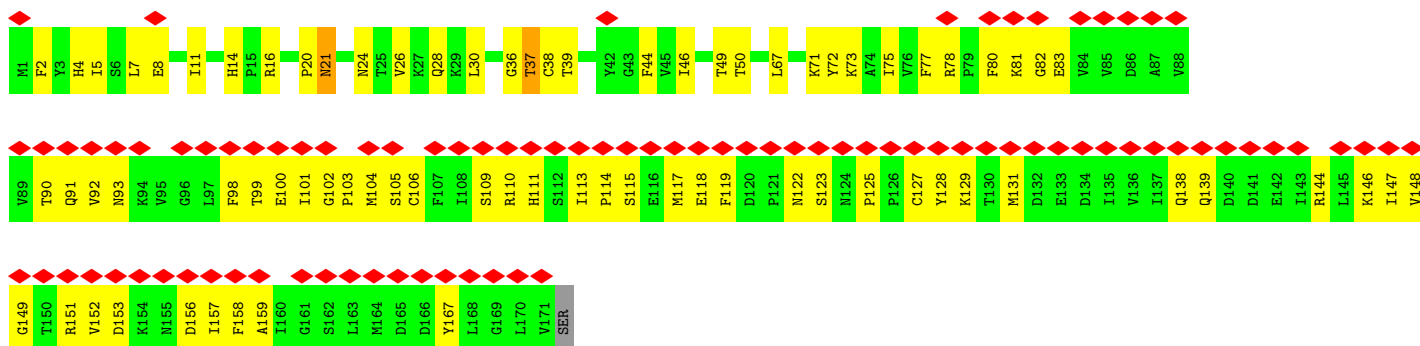


• Molecule 6: RNA polymerase II subunit F

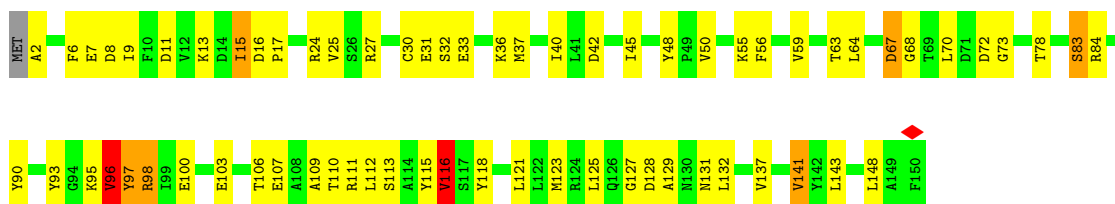




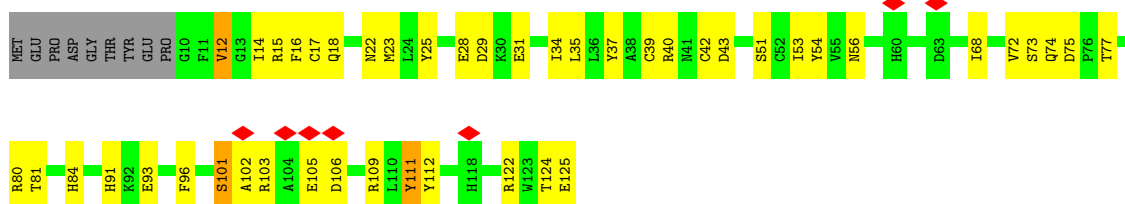
• Molecule 7: RNA polymerase II subunit G



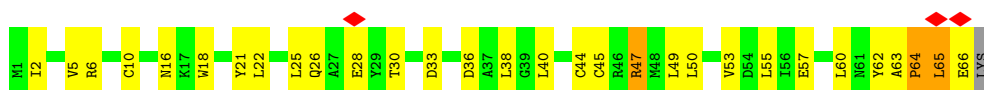
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

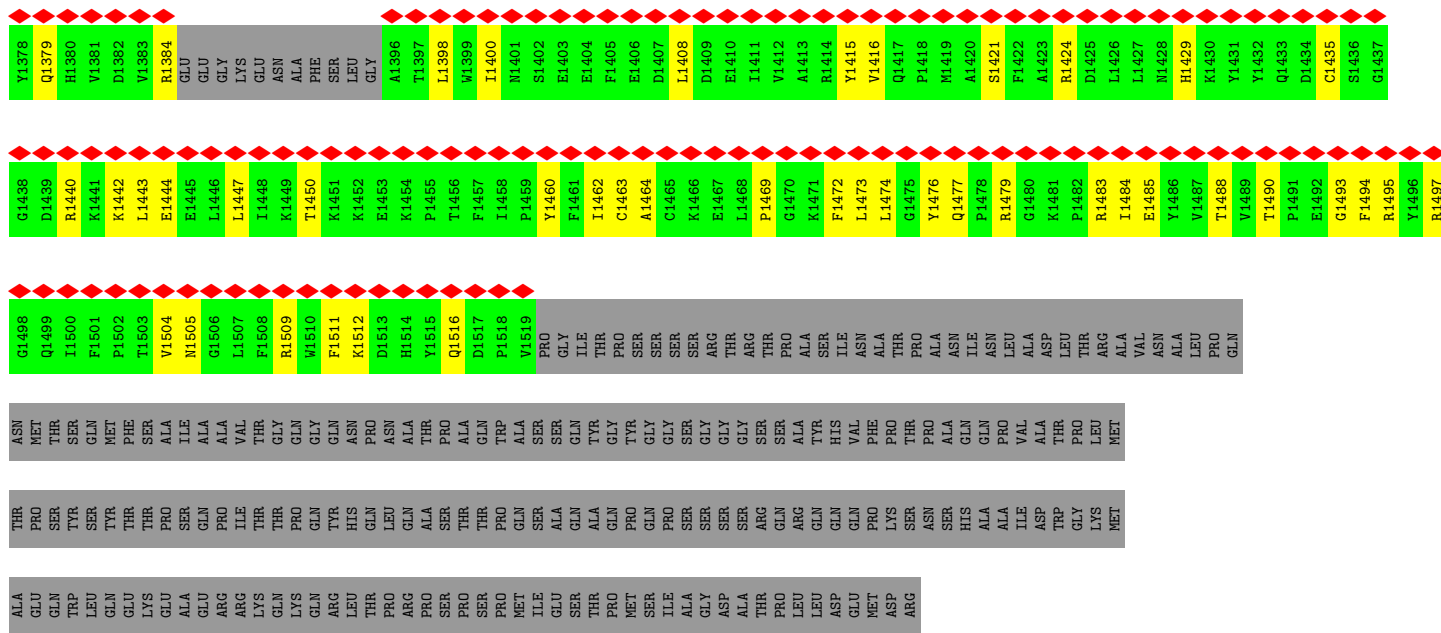


• Molecule 10: Uncharacterized protein

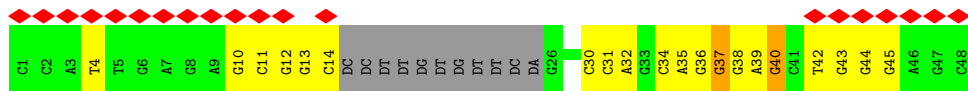


• Molecule 11: Uncharacterized protein

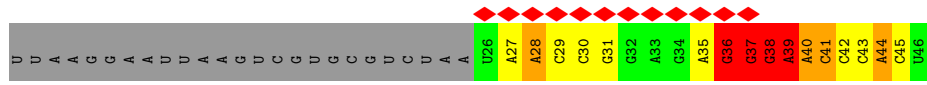
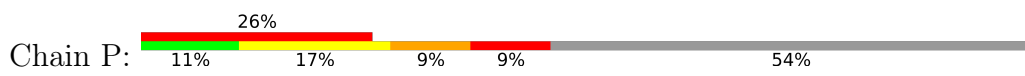
ARG	L658	Q718	G778	K638	K898	L958	V1018	E1078	R1138	CYS	K1258	I1327	ARG
LYS	A659	Q719	I779	F839	S899	Y959	T1019	S1079	T1139	PRO	V1259	A1328	LYS
GLN	E660	Q720	R780	L840	E900	C960	M1020	A1080	A1140	PHE	G1260	A1329	GLN
ARG	D661	L721	V781	L841	A901	E961	C1021	E1081	Y1141	GLN	M1261	I1330	ARG
THR	E662	L722	G783	N842	E902	F962	H1022	A1082	R1142	GLN	T1262	I1331	THR
THR	G663	Y723	L784	K843	F903	I963	M1023	A1083	S1143	ASP	V1263	I1332	THR
ASN	Q604	Q724	I785	K944	R904	N964	G1024	N1084	P1144	ASN	H1264	I1333	ASN
PRO	V605	M725	A785	P845	D905	R965	P1025	P1085	M1145	PRO	C1265	I1334	PRO
LYS	L606	A726	F786	H846	Y906	V966	K1026	A1086	T1146	LEU	L1266	I1335	LYS
ARG	R607	K727	S787	V847	P907	E967	M1027	G1087	E1147	SER	I1267	I1336	ARG
VAL	Q608	E728	S788	V848	P908	E968	F1028	A1088	E1148	GLU	M1268	I1337	VAL
TRP	T609	L729	A789	T849	V909	V969	M1029	L1089	I1149	TRP	K1269	I1338	TRP
ASN	F610	K730	R790	V850	L910	F970	M1030	E1090	F1150	ASN	I1270	I1339	ASN
HIS	E611	N731	D791	A851	R911	G971	C1031	I1091	M1151	HIS	D1271	I1340	HIS
PHE	E612	K732	H792	G852	Q912	D972	A1032	I1092	M1152	PHE	I1272	I1341	PHE
ASP	R613	L733	P793	E853	A913	V973	G1033	L1093	L1153	ASP	E1273	I1342	ASP
GLY	A614	L734	P794	N854	V914	N974	F1034	E1094	T1154	GLY	K1274	I1343	GLY
CYS	K615	A735	F795	R855	S915	R975	L1035	N1095	K1155	CYS	F1275	I1344	CYS
PRO	L616	E736	C796	D856	L916	A976	K1036	P1096	E1156	PRO	S1276	I1345	PRO
GLY	N617	A737	A797	A857	A917	I977	I1037	E1097	T1157	GLY	A1277	I1346	GLY
TYR	T619	K738	L798	Q858	R918	A978	D1038	R1098	P1158	TYR	L1278	I1347	TYR
GLY	L619	E739	V799	N859	R919	H979	T1039	L1099	E1159	GLY	L1279	I1348	GLY
ASN	P620	Y740	N800	L860	I920	P980	ALA	K1100	T1160	ASN	I1226	I1349	ASN
ASP	T621	V741	G801	I861	Q921	Y981	SER	D1101	F1161	ASP	G1227	I1350	ASP
GLM	K622	I742	E802	E862	D922	S982	GLY	L1102	F1162	GLM	V1228	I1351	GLM
K623	T884	K743	G803	D863	P923	Q983	ASP	D1103	I1163	K623	K1229	I1352	K623
G624	F885	A744	E904	V864	L924	A984	SER	L1104	G1164	G624	S1230	I1353	G624
R625	E887	C745	V905	K865	I925	L985	THR	D1105	K1165	R625	R1231	I1354	R625
K626	E888	S746	T806	R866	E926	I986	ASP	D1106	L1166	K626	L1232	I1355	K626
D627	E889	R747	D807	I867	F927	Q987	TYR	A1107	I1167	D627	L1233	I1356	D627
V628	K890	K748	F808	V868	A928	Y988	ILE	A1108	I1168	V628	N1234	I1357	V628
D629	Q891	L749	L809	H869	Q929	V989	V1051	E1109	C1169	D629	G1235	I1358	D629
E630	F892	Y750	R810	E870	V930	C990	E1052	E1110	M1170	E630	V1236	I1359	E630
A631	Y893	N751	L811	L871	V931	G991	L1053	E1111	V1171	A631	T1237	I1360	A631
H632	Y894	W752	P812	D872	S832	L982	D1054	E1112	T1172	H632	G1238	I1361	H632
Y633	R895	L753	H813	Q873	SER	G983	G1055	R1113	G1173	Y633	F1239	I1362	Y633
Y635	D896	R754	H814	G874	ASP	P994	S1056	Q1114	I1174	Y635	I1240	I1363	Y635
S636	F897	A756	T815	Q875	E935	D936	R1057	G1115	A1175	S636	P1241	I1364	S636
F637	S899	W757	LYS	Q876	D936	I937	V1058	Y1116	H1176	F637	T1242	I1365	F637
K638	H700	Y758	ARG	L877	L938	T988	H1059	G1117	ARG	K638	K1243	I1366	K638
Y639	W701	R759	THR	S878	L938	T988	P1060	D1118	PRO	Y639	F1244	I1367	Y639
L640	Q702	P760	ALA	S879	C939	H999	E1061	K1119	GLN	L640	L1245	I1368	L640
K641	V701	D761	TRP	I880	L940	L1000	T1062	H1120	GLY	K641	S1246	I1369	K641
W642	Q703	Q762	ARG	G881	K941	L1001	Y1063	I1121	GLU	W642	D1247	I1370	W642
K643	E704	Q763	GLU	V882	F942	K1002	E1064	T1122	TYR	K643	K1248	I1371	K643
P644	W705	Q763	VAL	E883	H943	I1003	M1065	L1123	ASP	P644	V1249	I1372	P644
V645	N706	GLU	GLU	L884	P944	L1004	A1066	Y1124	GLN	V645	V1250	I1373	V645
K646	R707	GLU	GLU	V885	L945	L1004	A1067	D1125	ALA	K646	I1251	I1374	K646
E647	Q708	ASP	ASP	V886	Q946	K1006	R1068	I1126	ILE	E647	R1252	I1375	E647
L648	R709	ASP	ASP	N887	E947	M1007	M1069	R1127	ARG	L648	P1253	I1376	L648
R649	T710	PHE	PHE	E888	H948	M1008	A1070	A1128	ASN	R649	E1254	I1377	R649
D650	M711	MET	MET	L889	V949	T1009	V1071	I1129	THR	D650	E1255	I1378	D650
Q652	A712	ASP	ASP	A890	V950	R1010	D1072	L1130	GLY	Q652	R1256	I1379	Q652
F653	I713	GLU	GLU	I891	K951	L1011	A1073	S1131	LEU	F653	V1257	I1380	F653
L654	E714	ASN	ASN	L892	E952	E1012	L1074	C1132	TRP	L654		I1381	L654
I656	R715	ASN	ASN	Y893	E953	S1013	E1076	R1133	GLN	I656		I1382	I656
C657	A716	ASP	ASP	M894	L955	T1015	D1077	K1135		C657		I1383	C657
	L717	K777	K837	S896	A857	L1017		L1137					



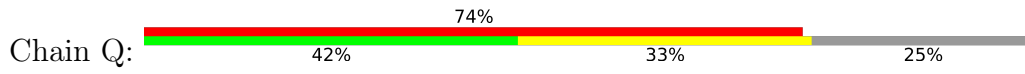
• Molecule 14: DNA (37-MER)

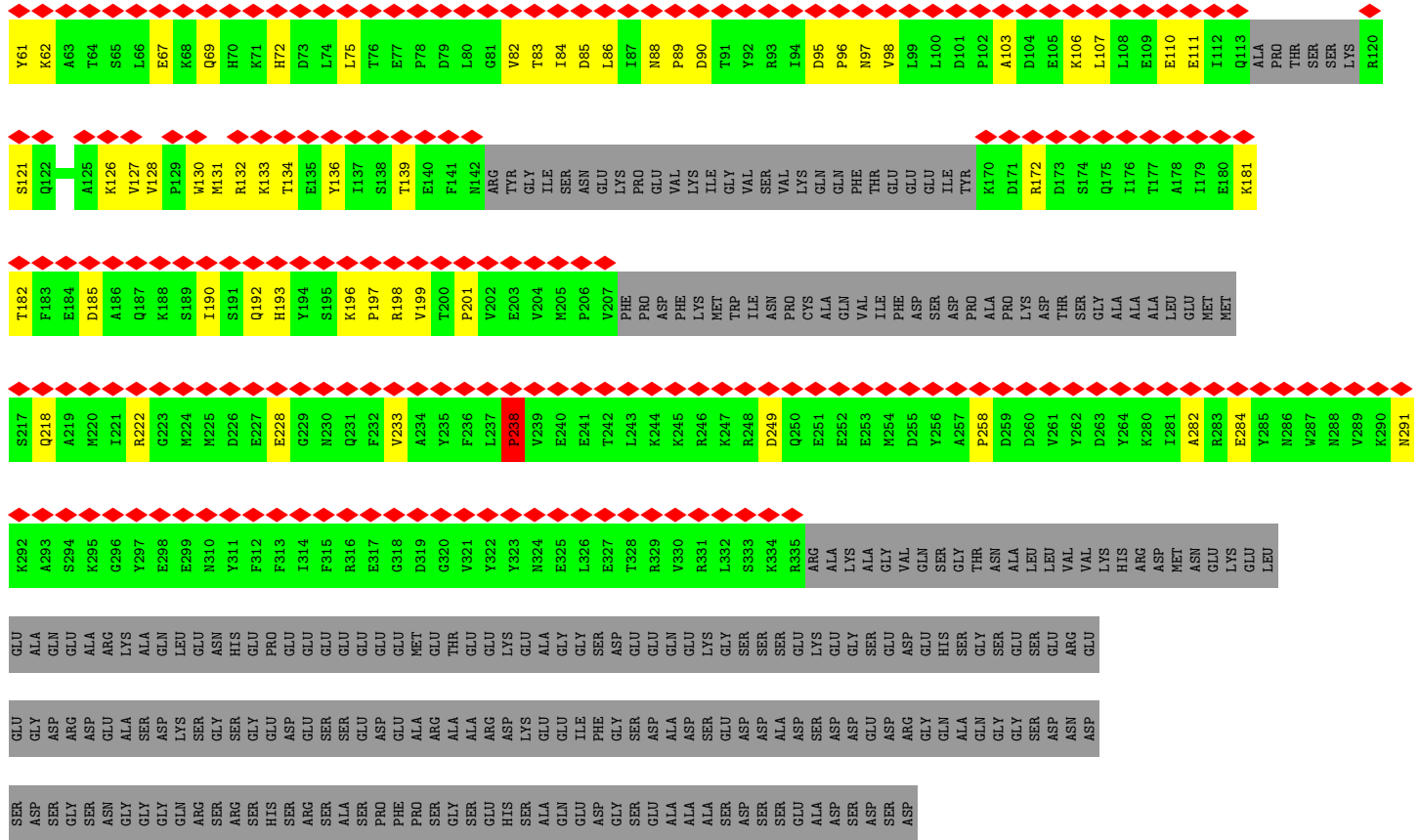


• Molecule 15: RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')

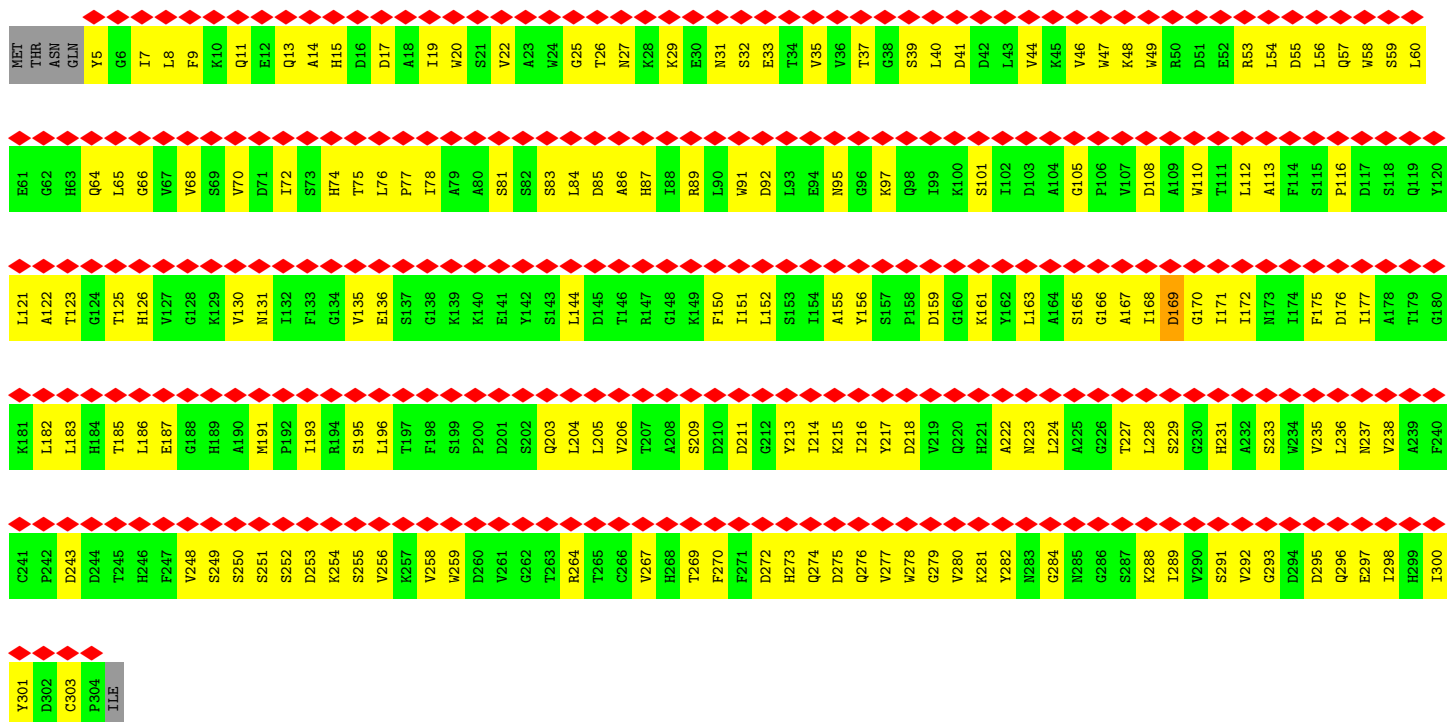


• Molecule 16: RNA polymerase-associated protein CTR9 homolog





● Molecule 21: WD repeat-containing protein 61



THR ASP ILE GLN VAL ASP THR TYR LEU ASP THR GLN VAL VAL GLY GLN THR GLY VAL ILE ARG SER VAL THR GLY GLY MET CYS SER VAL TYR LEU LYS ASP SER GLU LYS VAL VAL SER ILE SER SER HIS LEU GLU PRO ILE THR PRO THR LYS ASN ASN VAL

LYS VAL ILE LEU GLY ASP ARG GLU ALA THR GLY VAL LEU LEU SER ILE ASP GLY GLU ASP GLY ILE VAL ARG MET ASP LEU ASP GLU GLN LEU LYS ILE LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	446195	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.049, 1.049, 1.049	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: MG, TPO, SEP, ZN

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	A	1.40	97/11437 (0.8%)	0.89	18/15433 (0.1%)
2	B	1.63	126/9158 (1.4%)	0.97	28/12360 (0.2%)
3	C	1.77	44/2115 (2.1%)	0.96	7/2873 (0.2%)
4	D	0.42	0/1017	0.51	0/1368
5	E	1.29	10/1751 (0.6%)	0.81	1/2366 (0.0%)
6	F	1.69	9/636 (1.4%)	0.89	0/859
7	G	0.75	0/1364	0.62	0/1853
8	H	1.78	31/1219 (2.5%)	0.92	1/1644 (0.1%)
9	I	1.25	4/964 (0.4%)	0.79	0/1305
10	J	1.82	9/533 (1.7%)	1.03	3/719 (0.4%)
11	K	1.68	8/939 (0.9%)	0.92	2/1271 (0.2%)
12	L	1.57	5/395 (1.3%)	1.00	2/525 (0.4%)
13	M	0.26	0/4763	0.48	1/6084 (0.0%)
14	N	0.98	1/870 (0.1%)	0.87	1/1341 (0.1%)
15	P	1.34	3/506 (0.6%)	1.82	22/787 (2.8%)
16	Q	0.36	0/7365	0.51	0/9927
17	R	0.39	0/1860	0.56	2/2509 (0.1%)
18	T	1.68	11/1087 (1.0%)	1.13	6/1674 (0.4%)
19	U	0.34	0/864	0.58	2/1173 (0.2%)
20	V	0.32	0/1728	0.52	2/2357 (0.1%)
21	W	0.37	0/2392	0.53	0/3257
22	X	0.34	0/356	0.52	0/478
23	Y	0.27	0/927	0.48	0/1250
24	Z	0.45	0/4081	0.55	1/5493 (0.0%)
All	All	1.15	358/58327 (0.6%)	0.79	99/78906 (0.1%)

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
1	A	0	2
2	B	0	3
17	R	0	1
All	All	0	6

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-15.42	1.20	1.53
2	B	94	SER	C-N	-11.45	1.07	1.34
8	H	116	VAL	CB-CG1	-9.52	1.32	1.52
2	B	690	CYS	CB-SG	-8.84	1.67	1.82
2	B	1047	TYR	CD1-CE1	-8.57	1.26	1.39
2	B	753	TYR	CD2-CE2	-8.37	1.26	1.39
2	B	548	TRP	CB-CG	-8.34	1.35	1.50
1	A	999	ARG	C-N	-8.25	1.15	1.34
8	H	118	TYR	CD1-CE1	-8.14	1.27	1.39
1	A	1050	CYS	CB-SG	-8.09	1.68	1.82
1	A	886	VAL	CB-CG1	-8.08	1.35	1.52
8	H	118	TYR	CD2-CE2	-8.05	1.27	1.39
2	B	29	VAL	CB-CG2	-8.01	1.36	1.52
1	A	827	TYR	CD1-CE1	-7.83	1.27	1.39
3	C	19	VAL	CB-CG2	-7.76	1.36	1.52
2	B	664	TYR	CD1-CE1	-7.73	1.27	1.39
1	A	1374	VAL	CB-CG2	-7.68	1.36	1.52
1	A	492	TYR	CE2-CZ	-7.61	1.28	1.38
10	J	10	CYS	CB-SG	-7.54	1.69	1.82
1	A	492	TYR	CD2-CE2	-7.50	1.28	1.39
18	T	25	DA	C3'-O3'	-7.48	1.34	1.44
2	B	664	TYR	CD2-CE2	-7.39	1.28	1.39
10	J	62	TYR	CD1-CE1	-7.36	1.28	1.39
1	A	514	GLU	CB-CG	-7.34	1.38	1.52
8	H	118	TYR	CE1-CZ	-7.25	1.29	1.38
2	B	1047	TYR	CD2-CE2	-7.21	1.28	1.39
1	A	1396	ARG	CB-CG	-7.17	1.33	1.52
8	H	48	TYR	CD1-CE1	-7.14	1.28	1.39
9	I	72	VAL	CB-CG1	-7.11	1.38	1.52
2	B	108	MET	C-N	-7.10	1.17	1.34
2	B	1047	TYR	CE1-CZ	-7.09	1.29	1.38
1	A	380	VAL	CB-CG2	-7.06	1.38	1.52
2	B	809	VAL	CB-CG1	-7.01	1.38	1.52
2	B	615	TYR	CD1-CE1	-7.01	1.28	1.39
1	A	1379	GLU	CB-CG	-6.96	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	VAL	CB-CG1	-6.96	1.38	1.52
2	B	184	TYR	CD2-CE2	-6.95	1.28	1.39
18	T	28	DG	C3'-O3'	-6.95	1.34	1.44
2	B	753	TYR	CE2-CZ	-6.90	1.29	1.38
2	B	755	GLN	C-N	-6.90	1.18	1.34
3	C	176	TRP	CE3-CZ3	-6.89	1.26	1.38
1	A	560	VAL	CB-CG2	-6.86	1.38	1.52
10	J	45	CYS	CB-SG	-6.86	1.70	1.82
1	A	492	TYR	CD1-CE1	-6.85	1.29	1.39
2	B	662	VAL	CB-CG2	-6.85	1.38	1.52
2	B	693	TYR	CE1-CZ	-6.83	1.29	1.38
2	B	1029	TYR	CD2-CE2	-6.83	1.29	1.39
5	E	191	VAL	CB-CG1	-6.83	1.38	1.52
2	B	615	TYR	CD2-CE2	-6.79	1.29	1.39
3	C	184	PHE	CD1-CE1	-6.79	1.25	1.39
2	B	1029	TYR	CE1-CZ	-6.79	1.29	1.38
2	B	120	TYR	CD2-CE2	-6.77	1.29	1.39
2	B	753	TYR	CE1-CZ	-6.76	1.29	1.38
2	B	1047	TYR	CE2-CZ	-6.75	1.29	1.38
2	B	509	VAL	CB-CG1	-6.74	1.38	1.52
3	C	186	TYR	CD1-CE1	-6.73	1.29	1.39
2	B	753	TYR	CD1-CE1	-6.72	1.29	1.39
2	B	177	CYS	CB-SG	-6.70	1.70	1.82
2	B	504	THR	CB-CG2	-6.69	1.30	1.52
2	B	1105	GLU	CB-CG	-6.66	1.39	1.52
6	F	60	TYR	CD1-CE1	-6.63	1.29	1.39
2	B	1029	TYR	CD1-CE1	-6.61	1.29	1.39
6	F	109	TYR	CD1-CE1	-6.61	1.29	1.39
8	H	115	TYR	CD1-CE1	-6.61	1.29	1.39
3	C	184	PHE	CD2-CE2	-6.60	1.26	1.39
1	A	815	TYR	CD2-CE2	-6.60	1.29	1.39
1	A	815	TYR	CD1-CE1	-6.59	1.29	1.39
8	H	97	TYR	CE1-CZ	-6.58	1.29	1.38
18	T	33	DC	N1-C2	-6.58	1.33	1.40
2	B	801	VAL	CB-CG1	-6.57	1.39	1.52
12	L	55	PHE	CB-CG	-6.56	1.40	1.51
2	B	750	VAL	CB-CG2	-6.55	1.39	1.52
2	B	806	PHE	CD1-CE1	-6.54	1.26	1.39
3	C	229	PHE	CD1-CE1	-6.51	1.26	1.39
18	T	27	DT	C3'-O3'	-6.51	1.35	1.44
2	B	811	TYR	CE1-CZ	-6.48	1.30	1.38
3	C	172	GLU	CB-CG	-6.48	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	CYS	CB-SG	-6.47	1.71	1.82
8	H	115	TYR	CE1-CZ	-6.46	1.30	1.38
3	C	186	TYR	CD2-CE2	-6.46	1.29	1.39
2	B	193	VAL	CB-CG2	-6.45	1.39	1.52
2	B	693	TYR	CD1-CE1	-6.45	1.29	1.39
8	H	90	TYR	CD1-CE1	-6.44	1.29	1.39
1	A	787	VAL	CB-CG2	-6.43	1.39	1.52
3	C	169	PHE	CD1-CE1	-6.43	1.26	1.39
2	B	622	CYS	CB-SG	-6.37	1.71	1.82
1	A	871	VAL	CB-CG1	-6.37	1.39	1.52
3	C	169	PHE	CD2-CE2	-6.35	1.26	1.39
1	A	835	GLU	CB-CG	-6.34	1.40	1.52
1	A	827	TYR	CD2-CE2	-6.34	1.29	1.39
1	A	1140	THR	CA-CB	-6.33	1.36	1.53
1	A	521	VAL	CB-CG2	-6.33	1.39	1.52
2	B	922	ARG	CB-CG	-6.30	1.35	1.52
10	J	5	VAL	CB-CG2	-6.29	1.39	1.52
5	E	191	VAL	CB-CG2	-6.28	1.39	1.52
2	B	919	CYS	CB-SG	-6.28	1.71	1.82
3	C	231	TYR	CD1-CE1	-6.27	1.29	1.39
10	J	62	TYR	CE1-CZ	-6.26	1.30	1.38
6	F	109	TYR	CD2-CE2	-6.26	1.29	1.39
1	A	891	TYR	CD1-CE1	-6.23	1.30	1.39
1	A	630	VAL	CB-CG1	-6.22	1.39	1.52
1	A	590	GLN	CG-CD	-6.22	1.36	1.51
2	B	33	TYR	CE1-CZ	-6.21	1.30	1.38
11	K	56	VAL	CB-CG1	-6.21	1.39	1.52
18	T	33	DC	N1-C6	-6.21	1.33	1.37
2	B	805	PHE	CD2-CE2	-6.21	1.26	1.39
2	B	752	TYR	CE2-CZ	-6.21	1.30	1.38
6	F	60	TYR	CE1-CZ	-6.20	1.30	1.38
2	B	984	CYS	CB-SG	-6.20	1.71	1.82
2	B	809	VAL	CB-CG2	-6.19	1.39	1.52
8	H	90	TYR	CD2-CE2	-6.18	1.30	1.39
2	B	949	TYR	CD1-CE1	-6.18	1.30	1.39
12	L	45	TYR	CE1-CZ	-6.17	1.30	1.38
2	B	1029	TYR	CE2-CZ	-6.17	1.30	1.38
18	T	26	DG	C3'-O3'	-6.17	1.35	1.44
1	A	669	TYR	CD1-CE1	-6.14	1.30	1.39
8	H	115	TYR	CE2-CZ	-6.11	1.30	1.38
8	H	98	ARG	CB-CG	-6.10	1.36	1.52
2	B	236	TRP	CB-CG	-6.10	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	33	DC	C1'-N1	-6.09	1.38	1.47
1	A	474	VAL	CB-CG1	-6.08	1.40	1.52
12	L	45	TYR	CD1-CE1	-6.07	1.30	1.39
2	B	193	VAL	CB-CG1	-6.06	1.40	1.52
2	B	198	GLU	CB-CG	-6.06	1.40	1.52
2	B	924	ARG	CB-CG	-6.06	1.36	1.52
2	B	923	VAL	CB-CG1	-6.05	1.40	1.52
11	K	75	VAL	CB-CG2	-6.05	1.40	1.52
1	A	590	GLN	CB-CG	-6.04	1.36	1.52
3	C	104	ASP	CA-CB	-6.02	1.40	1.53
1	A	873	VAL	CB-CG2	-6.01	1.40	1.52
2	B	707	CYS	CB-SG	-6.01	1.72	1.82
8	H	141	VAL	CB-CG2	-6.00	1.40	1.52
2	B	367	TYR	CD1-CE1	-6.00	1.30	1.39
3	C	186	TYR	CE2-CZ	-5.97	1.30	1.38
1	A	827	TYR	CE1-CZ	-5.97	1.30	1.38
2	B	184	TYR	CE2-CZ	-5.96	1.30	1.38
8	H	115	TYR	CD2-CE2	-5.94	1.30	1.39
18	T	24	DG	C3'-O3'	-5.94	1.36	1.44
18	T	33	DC	N3-C4	-5.93	1.29	1.33
3	C	151	VAL	CB-CG1	-5.90	1.40	1.52
1	A	366	VAL	CB-CG1	-5.89	1.40	1.52
2	B	92	TYR	CD2-CE2	-5.89	1.30	1.39
10	J	6	ARG	CB-CG	-5.89	1.36	1.52
3	C	197	TYR	CE1-CZ	-5.88	1.30	1.38
1	A	458	PHE	CD1-CE1	-5.87	1.27	1.39
3	C	186	TYR	CE1-CZ	-5.87	1.30	1.38
2	B	184	TYR	CD1-CE1	-5.86	1.30	1.39
3	C	197	TYR	CE2-CZ	-5.86	1.30	1.38
2	B	806	PHE	CD2-CE2	-5.85	1.27	1.39
3	C	231	TYR	CD2-CE2	-5.85	1.30	1.39
1	A	377	GLN	CB-CG	-5.84	1.36	1.52
1	A	657	TYR	CD1-CE1	-5.83	1.30	1.39
8	H	96	VAL	CB-CG1	-5.82	1.40	1.52
1	A	669	TYR	CE1-CZ	-5.80	1.31	1.38
8	H	90	TYR	CE2-CZ	-5.80	1.31	1.38
15	P	44	A	N9-C4	-5.80	1.34	1.37
2	B	697	GLU	CG-CD	-5.80	1.43	1.51
2	B	1020	TYR	CD1-CE1	-5.80	1.30	1.39
1	A	669	TYR	CD2-CE2	-5.79	1.30	1.39
1	A	771	VAL	CB-CG2	-5.77	1.40	1.52
2	B	794	VAL	CB-CG2	-5.76	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	907	VAL	CB-CG1	-5.76	1.40	1.52
2	B	184	TYR	CE1-CZ	-5.75	1.31	1.38
2	B	788	TYR	CE2-CZ	-5.74	1.31	1.38
2	B	1093	CYS	CB-SG	-5.74	1.72	1.81
2	B	811	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	1047	TYR	CG-CD1	-5.74	1.31	1.39
12	L	45	TYR	CD2-CE2	-5.72	1.30	1.39
1	A	482	PHE	CD2-CE2	-5.72	1.27	1.39
1	A	784	VAL	CB-CG1	-5.72	1.40	1.52
2	B	1149	VAL	CB-CG2	-5.71	1.40	1.52
2	B	788	TYR	CD1-CE1	-5.71	1.30	1.39
3	C	197	TYR	CD1-CE1	-5.70	1.30	1.39
1	A	556	GLU	CB-CG	-5.69	1.41	1.52
1	A	447	GLU	CB-CG	-5.68	1.41	1.52
8	H	48	TYR	CE1-CZ	-5.68	1.31	1.38
5	E	209	VAL	CB-CG2	-5.67	1.41	1.52
2	B	120	TYR	CD1-CE1	-5.67	1.30	1.39
15	P	40	A	N9-C4	-5.66	1.34	1.37
1	A	556	GLU	CG-CD	-5.66	1.43	1.51
2	B	697	GLU	CB-CG	-5.66	1.41	1.52
1	A	406	VAL	CB-CG1	-5.65	1.41	1.52
1	A	1375	ARG	CG-CD	-5.65	1.37	1.51
11	K	97	GLU	CB-CG	-5.64	1.41	1.52
1	A	901	VAL	CB-CG2	-5.64	1.41	1.52
3	C	169	PHE	CB-CG	-5.63	1.41	1.51
2	B	510	CYS	CB-SG	-5.63	1.72	1.81
2	B	191	GLU	CG-CD	-5.63	1.43	1.51
2	B	785	TYR	CD2-CE2	-5.63	1.30	1.39
5	E	203	TYR	CD2-CE2	-5.63	1.30	1.39
1	A	810	PHE	CD2-CE2	-5.62	1.28	1.39
2	B	788	TYR	CD2-CE2	-5.62	1.30	1.39
2	B	568	PHE	CD1-CE1	-5.61	1.28	1.39
2	B	814	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	815	TYR	CE2-CZ	-5.60	1.31	1.38
11	K	63	VAL	CB-CG1	-5.60	1.41	1.52
2	B	1027	VAL	CB-CG2	-5.60	1.41	1.52
3	C	19	VAL	CB-CG1	-5.59	1.41	1.52
2	B	949	TYR	CD2-CE2	-5.59	1.30	1.39
3	C	185	GLU	CB-CG	-5.59	1.41	1.52
2	B	176	GLU	CB-CG	-5.59	1.41	1.52
11	K	61	TYR	CD1-CE1	-5.57	1.30	1.39
2	B	814	TYR	CE1-CZ	-5.57	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	115	TYR	CG-CD2	-5.57	1.31	1.39
5	E	26	TYR	CD2-CE2	-5.56	1.31	1.39
8	H	50	VAL	CB-CG2	-5.56	1.41	1.52
2	B	671	GLU	CB-CG	-5.56	1.41	1.52
3	C	229	PHE	CD2-CE2	-5.56	1.28	1.39
2	B	367	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	500	GLU	CB-CG	-5.54	1.41	1.52
3	C	230	TYR	CD1-CE1	-5.54	1.31	1.39
3	C	45	ILE	CB-CG2	-5.54	1.35	1.52
2	B	1153	TYR	CE2-CZ	-5.53	1.31	1.38
6	F	102	ILE	C-N	-5.53	1.23	1.34
1	A	479	TRP	CB-CG	-5.53	1.40	1.50
1	A	554	PHE	CD1-CE1	-5.52	1.28	1.39
1	A	810	PHE	CD1-CE1	-5.52	1.28	1.39
1	A	446	VAL	CB-CG2	-5.50	1.41	1.52
9	I	111	TYR	CD1-CE1	-5.50	1.31	1.39
1	A	1471	PHE	CD1-CE1	-5.50	1.28	1.39
3	C	37	VAL	CB-CG1	-5.49	1.41	1.52
1	A	378	VAL	CB-CG1	-5.48	1.41	1.52
2	B	466	VAL	CB-CG2	-5.48	1.41	1.52
2	B	791	GLU	CB-CG	-5.48	1.41	1.52
1	A	618	TYR	CD2-CE2	-5.48	1.31	1.39
15	P	45	C	N1-C6	-5.48	1.33	1.37
3	C	224	GLY	C-N	-5.47	1.21	1.34
3	C	231	TYR	CE1-CZ	-5.46	1.31	1.38
2	B	1018	TYR	CD1-CE1	-5.46	1.31	1.39
2	B	1048	TYR	CB-CG	-5.46	1.43	1.51
1	A	891	TYR	CD2-CE2	-5.46	1.31	1.39
8	H	93	TYR	CD1-CE1	-5.45	1.31	1.39
2	B	752	TYR	CD2-CE2	-5.45	1.31	1.39
1	A	970	PHE	CB-CG	-5.44	1.42	1.51
1	A	548	PHE	CD2-CE2	-5.44	1.28	1.39
6	F	60	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	1085	GLU	CB-CG	-5.43	1.41	1.52
2	B	1088	GLU	CB-CG	-5.43	1.41	1.52
6	F	60	TYR	CE2-CZ	-5.43	1.31	1.38
1	A	64	VAL	CB-CG1	-5.42	1.41	1.52
3	C	231	TYR	CE2-CZ	-5.40	1.31	1.38
11	K	61	TYR	CD2-CE2	-5.40	1.31	1.39
1	A	657	TYR	CD2-CE2	-5.40	1.31	1.39
1	A	891	TYR	CE1-CZ	-5.39	1.31	1.38
1	A	1087	VAL	CB-CG1	-5.39	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	661	VAL	CB-CG1	-5.38	1.41	1.52
11	K	102	GLU	CB-CG	-5.38	1.42	1.52
1	A	566	PHE	CD2-CE2	-5.38	1.28	1.39
8	H	118	TYR	CE2-CZ	-5.38	1.31	1.38
1	A	978	VAL	CB-CG1	-5.37	1.41	1.52
1	A	553	VAL	CB-CG2	-5.36	1.41	1.52
3	C	158	GLU	CB-CG	-5.36	1.42	1.52
8	H	25	VAL	CB-CG1	-5.35	1.41	1.52
2	B	766	TYR	CD2-CE2	-5.35	1.31	1.39
1	A	514	GLU	CG-CD	-5.35	1.44	1.51
8	H	90	TYR	CE1-CZ	-5.34	1.31	1.38
8	H	137	VAL	CB-CG2	-5.34	1.41	1.52
5	E	206	TYR	CD1-CE1	-5.33	1.31	1.39
1	A	886	VAL	CB-CG2	-5.33	1.41	1.52
2	B	615	TYR	CE1-CZ	-5.33	1.31	1.38
1	A	634	GLU	CB-CG	-5.33	1.42	1.52
1	A	382	ARG	CB-CG	-5.31	1.38	1.52
2	B	766	TYR	CD1-CE1	-5.31	1.31	1.39
2	B	664	TYR	CB-CG	-5.30	1.43	1.51
2	B	860	VAL	CB-CG2	-5.30	1.41	1.52
3	C	101	PHE	CD1-CE1	-5.30	1.28	1.39
2	B	568	PHE	CD2-CE2	-5.30	1.28	1.39
1	A	21	VAL	CB-CG2	-5.29	1.41	1.52
10	J	62	TYR	CD2-CE2	-5.29	1.31	1.39
11	K	68	GLU	CB-CG	-5.29	1.42	1.52
2	B	752	TYR	CB-CG	-5.28	1.43	1.51
1	A	26	LEU	C-N	-5.28	1.22	1.34
1	A	787	VAL	CB-CG1	-5.27	1.41	1.52
3	C	197	TYR	CG-CD1	-5.27	1.32	1.39
9	I	111	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	679	TRP	CE3-CZ3	-5.26	1.29	1.38
6	F	56	TYR	CD1-CE1	-5.25	1.31	1.39
5	E	194	ILE	C-N	-5.25	1.22	1.34
2	B	176	GLU	CG-CD	-5.25	1.44	1.51
3	C	197	TYR	CD2-CE2	-5.25	1.31	1.39
1	A	458	PHE	CD2-CE2	-5.25	1.28	1.39
2	B	1006	VAL	CB-CG2	-5.25	1.41	1.52
3	C	184	PHE	CB-CG	-5.25	1.42	1.51
2	B	1153	TYR	CD2-CE2	-5.23	1.31	1.39
3	C	9	VAL	CB-CG2	-5.23	1.41	1.52
2	B	736	TYR	CD2-CE2	-5.23	1.31	1.39
1	A	970	PHE	CD1-CE1	-5.23	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	VAL	CB-CG2	-5.22	1.41	1.52
3	C	176	TRP	CB-CG	-5.22	1.40	1.50
14	N	37	DG	N9-C4	-5.22	1.33	1.38
2	B	743	ARG	CG-CD	-5.22	1.39	1.51
9	I	112	TYR	CD1-CE1	-5.21	1.31	1.39
12	L	54	VAL	CB-CG2	-5.21	1.42	1.52
1	A	713	VAL	CB-CG2	-5.21	1.42	1.52
3	C	234	GLU	CB-CG	-5.21	1.42	1.52
2	B	735	VAL	CB-CG2	-5.21	1.42	1.52
18	T	27	DT	N1-C6	-5.21	1.34	1.38
1	A	770	VAL	CB-CG1	-5.21	1.42	1.52
8	H	115	TYR	CG-CD1	-5.20	1.32	1.39
5	E	206	TYR	CD2-CE2	-5.20	1.31	1.39
5	E	11	TRP	CB-CG	-5.20	1.40	1.50
6	F	65	VAL	CB-CG1	-5.19	1.42	1.52
3	C	50	VAL	CB-CG2	-5.18	1.42	1.52
2	B	1048	TYR	CD1-CE1	-5.18	1.31	1.39
1	A	827	TYR	CG-CD1	-5.17	1.32	1.39
2	B	523	VAL	CB-CG1	-5.17	1.42	1.52
8	H	97	TYR	CD1-CE1	-5.17	1.31	1.39
18	T	32	DT	N1-C2	-5.16	1.33	1.38
2	B	923	VAL	CB-CG2	-5.16	1.42	1.52
2	B	369	VAL	CB-CG2	-5.16	1.42	1.52
1	A	669	TYR	CG-CD2	-5.15	1.32	1.39
2	B	753	TYR	CG-CD2	-5.15	1.32	1.39
1	A	492	TYR	CG-CD2	-5.14	1.32	1.39
2	B	33	TYR	CD1-CE1	-5.14	1.31	1.39
2	B	750	VAL	CB-CG1	-5.14	1.42	1.52
1	A	978	VAL	CB-CG2	-5.13	1.42	1.52
5	E	203	TYR	CD1-CE1	-5.13	1.31	1.39
3	C	101	PHE	CD2-CE2	-5.12	1.29	1.39
3	C	230	TYR	CD2-CE2	-5.12	1.31	1.39
8	H	48	TYR	CD2-CE2	-5.12	1.31	1.39
2	B	918	PHE	CD2-CE2	-5.12	1.29	1.39
3	C	203	TRP	CB-CG	-5.11	1.41	1.50
3	C	21	PHE	CD2-CE2	-5.11	1.29	1.39
10	J	18	TRP	CB-CG	-5.11	1.41	1.50
1	A	1402	CYS	CB-SG	-5.10	1.73	1.81
2	B	666	ASP	CB-CG	-5.10	1.41	1.51
1	A	392	GLU	CB-CG	-5.10	1.42	1.52
1	A	548	PHE	CE1-CZ	-5.09	1.27	1.37
1	A	1392	TYR	CD2-CE2	-5.08	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	TYR	CE2-CZ	-5.07	1.31	1.38
2	B	811	TYR	CG-CD1	-5.07	1.32	1.39
8	H	98	ARG	CG-CD	-5.07	1.39	1.51
2	B	782	ILE	CB-CG2	-5.07	1.37	1.52
10	J	53	VAL	CB-CG2	-5.07	1.42	1.52
1	A	570	TRP	CE3-CZ3	-5.06	1.29	1.38
3	C	49	TRP	CB-CG	-5.06	1.41	1.50
1	A	554	PHE	CD2-CE2	-5.06	1.29	1.39
1	A	618	TYR	CD1-CE1	-5.06	1.31	1.39
1	A	570	TRP	CB-CG	-5.05	1.41	1.50
1	A	521	VAL	CB-CG1	-5.04	1.42	1.52
1	A	675	VAL	CB-CG1	-5.04	1.42	1.52
3	C	164	TYR	CD2-CE2	-5.04	1.31	1.39
2	B	926	VAL	CB-CG1	-5.04	1.42	1.52
1	A	586	TRP	CD2-CE2	-5.04	1.35	1.41
2	B	945	CYS	CB-SG	-5.03	1.73	1.81
8	H	116	VAL	CB-CG2	-5.03	1.42	1.52
2	B	736	TYR	CD1-CE1	-5.03	1.31	1.39
2	B	801	VAL	CB-CG2	-5.03	1.42	1.52
8	H	97	TYR	CE2-CZ	-5.02	1.32	1.38
1	A	81	CYS	CB-SG	-5.02	1.73	1.81
2	B	1018	TYR	CD2-CE2	-5.02	1.31	1.39
2	B	785	TYR	CD1-CE1	-5.01	1.31	1.39
2	B	807	ARG	CG-CD	-5.01	1.39	1.51
8	H	115	TYR	CB-CG	-5.01	1.44	1.51
1	A	479	TRP	CE3-CZ3	-5.01	1.29	1.38
2	B	466	VAL	CB-CG1	-5.01	1.42	1.52
1	A	458	PHE	CB-CG	-5.01	1.42	1.51
1	A	788	VAL	CB-CG1	-5.00	1.42	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	40	A	C8-N9-C4	-13.77	100.29	105.80
15	P	40	A	N7-C8-N9	12.63	120.11	113.80
15	P	41	C	C6-N1-C2	-11.07	115.87	120.30
3	C	224	GLY	C-N-CA	10.22	147.25	121.70
15	P	40	A	C5-N7-C8	-9.32	99.24	103.90
15	P	39	A	C8-N9-C4	-9.26	102.10	105.80
18	T	34	DT	O5'-P-OP1	-9.09	97.52	105.70
1	A	457	ILE	CG1-CB-CG2	-8.95	91.72	111.40
15	P	39	A	N1-C2-N3	8.41	133.51	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	33	DC	OP1-P-O3'	8.23	123.31	105.20
2	B	473	LEU	CB-CG-CD2	-8.05	97.32	111.00
2	B	411	LEU	CB-CG-CD2	-7.96	97.46	111.00
15	P	40	A	N9-C4-C5	7.60	108.84	105.80
2	B	583	LEU	CB-CG-CD1	-7.48	98.28	111.00
14	N	40	DG	O4'-C1'-N9	7.36	113.15	108.00
15	P	39	A	N9-C4-C5	7.34	108.74	105.80
2	B	567	ILE	CG1-CB-CG2	-7.31	95.31	111.40
1	A	484	LEU	CB-CG-CD2	-7.25	98.67	111.00
2	B	545	LEU	CB-CG-CD2	-7.25	98.68	111.00
15	P	42	C	C6-N1-C2	-7.21	117.42	120.30
1	A	524	MET	CG-SD-CE	-7.09	88.86	100.20
3	C	68	LEU	CB-CG-CD1	-6.96	99.16	111.00
2	B	668	LEU	CB-CG-CD2	-6.96	99.17	111.00
17	R	507	PRO	N-CA-CB	6.88	111.56	103.30
15	P	41	C	N3-C2-O2	-6.85	117.11	121.90
1	A	542	LEU	CB-CG-CD2	-6.75	99.52	111.00
15	P	39	A	C6-N1-C2	-6.57	114.66	118.60
1	A	1396	ARG	CG-CD-NE	-6.55	98.03	111.80
15	P	37	G	O4'-C1'-N9	6.53	113.43	108.20
18	T	29	DG	O4'-C4'-C3'	-6.53	101.89	104.50
3	C	67	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	A	1090	LEU	CB-CG-CD2	-6.48	99.98	111.00
15	P	40	A	N3-C4-N9	-6.43	122.25	127.40
2	B	848	LEU	CB-CG-CD1	-6.39	100.13	111.00
18	T	26	DG	O4'-C4'-C3'	-6.36	101.96	104.50
20	V	258	PRO	N-CA-CB	6.33	110.89	103.30
2	B	505	LEU	CA-CB-CG	6.30	129.80	115.30
2	B	501	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	A	486	LEU	CB-CG-CD2	-6.23	100.42	111.00
17	R	506	PRO	N-CA-CB	6.17	110.71	103.30
18	T	27	DT	O4'-C4'-C3'	-6.16	102.04	104.50
1	A	1463	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	A	1095	LEU	CB-CG-CD2	-6.09	100.64	111.00
2	B	163	LEU	CB-CG-CD2	-6.08	100.66	111.00
2	B	411	LEU	CA-CB-CG	6.07	129.27	115.30
11	K	100	LEU	CB-CG-CD2	-6.07	100.69	111.00
15	P	38	G	C6-C5-N7	-5.97	126.82	130.40
5	E	165	LEU	CB-CG-CD2	-5.96	100.86	111.00
13	M	1330	PRO	N-CA-CB	5.95	110.44	103.30
1	A	26	LEU	C-N-CA	-5.94	106.86	121.70
20	V	238	PRO	N-CA-CB	5.92	110.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	41	C	O4'-C1'-N1	5.92	112.94	108.20
2	B	395	LEU	CB-CG-CD2	-5.91	100.96	111.00
10	J	55	LEU	CB-CG-CD2	-5.90	100.98	111.00
1	A	1400	LEU	CB-CG-CD2	-5.88	101.00	111.00
15	P	38	G	N7-C8-N9	5.88	116.04	113.10
19	U	463	PRO	N-CA-CB	5.78	110.23	103.30
15	P	38	G	C4-N9-C1'	5.76	133.98	126.50
2	B	556	ILE	C-N-CA	-5.73	107.38	121.70
18	T	32	DT	O4'-C1'-N1	5.71	112.00	108.00
1	A	979	LEU	CB-CG-CD1	-5.68	101.35	111.00
11	K	93	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	B	1014	LEU	CB-CG-CD2	-5.63	101.43	111.00
15	P	41	C	C6-N1-C1'	5.60	127.52	120.80
2	B	866	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	A	1398	LEU	CB-CG-CD2	-5.55	101.56	111.00
15	P	41	C	C5-C6-N1	5.54	123.77	121.00
19	U	493	PRO	N-CA-CB	5.50	109.90	103.30
3	C	228	ARG	NE-CZ-NH1	-5.49	117.56	120.30
2	B	1015	LEU	CB-CG-CD2	-5.48	101.68	111.00
2	B	115	LEU	CB-CG-CD2	-5.44	101.76	111.00
24	Z	758	PRO	N-CA-CB	5.43	109.82	103.30
2	B	542	LEU	CB-CG-CD2	-5.42	101.78	111.00
2	B	576	ILE	CG1-CB-CG2	-5.39	99.54	111.40
2	B	21	LEU	CA-CB-CG	5.39	127.70	115.30
15	P	36	G	P-O3'-C3'	5.37	126.15	119.70
1	A	938	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	B	403	LEU	CB-CG-CD1	-5.32	101.96	111.00
8	H	121	LEU	CB-CG-CD2	-5.30	101.99	111.00
10	J	50	LEU	CB-CG-CD2	-5.25	102.08	111.00
2	B	751	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	80	GLU	C-N-CA	-5.23	108.63	121.70
2	B	371	ARG	NE-CZ-NH1	-5.22	117.69	120.30
12	L	44	MET	CG-SD-CE	-5.21	91.86	100.20
2	B	959	GLU	C-N-CA	-5.18	111.42	122.30
2	B	395	LEU	CA-CB-CG	-5.16	103.43	115.30
15	P	39	A	N7-C8-N9	5.16	116.38	113.80
10	J	65	LEU	CA-CB-CG	5.14	127.13	115.30
3	C	67	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	565	MET	CG-SD-CE	-5.12	92.01	100.20
2	B	377	LEU	CB-CG-CD1	-5.10	102.32	111.00
2	B	146	LYS	CA-CB-CG	5.10	124.62	113.40
1	A	567	LEU	CB-CG-CD1	-5.05	102.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	38	G	C8-N9-C4	-5.04	104.38	106.40
1	A	484	LEU	CA-CB-CG	5.03	126.86	115.30
2	B	665	ILE	CG1-CB-CG2	-5.02	100.35	111.40
12	L	20	GLY	N-CA-C	-5.02	100.56	113.10
3	C	44	ILE	CG1-CB-CG2	-5.00	100.40	111.40
3	C	154	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide
17	R	592	ASP	Peptide

5.2 Too-close contacts [i](#)

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	A	11255	0	11374	435	0
2	B	8980	0	9017	295	0
3	C	2072	0	2019	45	0
4	D	1004	0	980	55	0
5	E	1720	0	1737	73	0
6	F	626	0	657	11	0
7	G	1333	0	1321	80	0
8	H	1197	0	1156	44	0
9	I	942	0	873	38	0
10	J	524	0	541	19	0
11	K	920	0	942	28	0
12	L	390	0	397	13	0
13	M	4737	0	2262	46	0
14	N	773	0	412	38	0
15	P	452	0	229	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	7226	0	7169	355	0
17	R	1832	0	1687	114	0
18	T	974	0	541	39	0
19	U	852	0	668	31	0
20	V	1703	0	1426	85	0
21	W	2333	0	2246	155	0
22	X	353	0	371	28	0
23	Y	911	0	908	27	0
24	Z	4023	0	4035	181	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	Y	1	0	0	0	0
26	A	1	0	0	0	0
All	All	57142	0	52968	2040	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 19.

All (2040) 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)
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.42	0.99
2:B:953:ASP:OD1	3:C:36:ARG:NH2	1.96	0.98
1:A:609:HIS:HD1	1:A:626:THR:HG1	1.04	0.94
16:Q:505:ARG:HH21	20:V:44:PHE:HB2	1.32	0.93
1:A:904:GLN:NE2	1:A:981:CYS:O	2.01	0.91
2:B:105:PRO:HG2	19:U:512:THR:HA	1.51	0.91
16:Q:830:ARG:HA	16:Q:833:LYS:HE2	1.54	0.90
21:W:278:TRP:HB2	21:W:293:GLY:HA2	1.51	0.90
1:A:1227:THR:H	1:A:1230:GLN:HE21	1.19	0.90
14:N:30:DC:H42	18:T:19:DG:H1	1.18	0.89
23:Y:7:PRO:HG3	23:Y:23:LYS:HA	1.53	0.89
2:B:332:LYS:NZ	2:B:333:GLU:OE1	2.07	0.88
21:W:40:LEU:HD12	21:W:66:GLY:HA3	1.53	0.88
16:Q:727:LEU:HB3	16:Q:732:LYS:HB3	1.57	0.87
17:R:388:ARG:NH1	17:R:446:GLU:O	2.08	0.87
16:Q:768:VAL:HG21	16:Q:778:GLU:HG3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:ARG:NH2	9:I:105:GLU:OE2	2.08	0.86
17:R:387:VAL:HG13	17:R:405:ILE:HD11	1.58	0.86
24:Z:478:VAL:HB	24:Z:518:LEU:HD11	1.58	0.85
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.10	0.85
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.40	0.85
18:T:41:DC:H4'	24:Z:283:ARG:HE	1.41	0.85
3:C:193:ARG:NH2	3:C:218:ALA:O	2.09	0.85
21:W:35:VAL:HB	21:W:47:TRP:HB2	1.59	0.85
8:H:98:ARG:NH2	8:H:100:GLU:OE1	2.09	0.85
2:B:85:LEU:HB2	2:B:131:THR:HB	1.59	0.85
23:Y:75:GLN:O	23:Y:111:ARG:NH1	2.09	0.85
16:Q:682:ASP:O	16:Q:686:ASN:ND2	2.09	0.84
1:A:197:GLU:HB2	1:A:215:LEU:HD11	1.60	0.84
17:R:570:TRP:HB3	20:V:133:LYS:HE2	1.61	0.83
1:A:404:GLU:OE2	1:A:407:ARG:NH1	2.12	0.82
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.12	0.82
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.12	0.82
4:D:107:THR:HG23	4:D:110:GLU:H	1.43	0.82
14:N:37:DG:N1	18:T:12:DC:N3	2.27	0.82
1:A:392:GLU:OE2	1:A:401:ARG:NH2	2.11	0.81
5:E:166:ARG:HH22	5:E:168:ASN:HD22	1.26	0.81
16:Q:387:ALA:N	16:Q:390:ASP:OD2	2.13	0.81
21:W:14:ALA:N	21:W:296:GLN:O	2.13	0.81
21:W:172:ILE:HB	21:W:186:LEU:HB2	1.61	0.81
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.62	0.81
16:Q:643:ASP:OD2	22:X:239:GLN:NE2	2.11	0.81
4:D:76:ASN:HD22	4:D:79:THR:HG23	1.45	0.81
10:J:25:LEU:HB3	17:R:563:ILE:HD11	1.61	0.81
21:W:237:ASN:HD22	21:W:279:GLY:HA2	1.45	0.81
23:Y:3:LEU:O	23:Y:8:LYS:NZ	2.12	0.81
21:W:95:ASN:O	21:W:97:LYS:NZ	2.12	0.81
16:Q:276:ALA:HB1	16:Q:288:VAL:HG23	1.61	0.81
16:Q:737:LYS:HZ2	16:Q:764:LEU:HD13	1.46	0.80
1:A:1182:GLN:O	1:A:1192:TRP:NE1	2.14	0.80
21:W:35:VAL:N	21:W:47:TRP:O	2.12	0.80
2:B:756:LYS:NZ	20:V:134:THR:OG1	2.15	0.80
1:A:1525:TPO:O3P	13:M:1358:ARG:NH2	2.15	0.80
15:P:39:A:H3'	15:P:40:A:H8	1.47	0.80
16:Q:268:ASN:HD22	16:Q:271:VAL:H	1.29	0.79
1:A:1536:GLY:O	13:M:1483:ARG:NH2	2.16	0.79
7:G:111:HIS:HB3	24:Z:494:ARG:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:237:ASN:HB3	21:W:280:VAL:HG22	1.65	0.79
16:Q:41:LEU:HD23	16:Q:81:ASP:HB3	1.65	0.79
16:Q:534:TYR:HH	16:Q:553:TRP:HD1	1.31	0.79
1:A:1180:ASN:O	1:A:1183:SER:OG	2.00	0.79
20:V:47:LYS:HB3	22:X:228:GLU:HB2	1.63	0.79
1:A:539:GLN:O	1:A:541:THR:N	2.16	0.78
2:B:297:MET:HG2	2:B:377:LEU:HD11	1.65	0.78
3:C:154:ARG:NH1	10:J:63:ALA:HB2	1.98	0.78
1:A:349:ARG:HE	2:B:1157:LEU:HD22	1.46	0.78
15:P:38:G:H2'	15:P:39:A:H8	1.49	0.78
15:P:40:A:H2'	15:P:41:C:C6	2.19	0.78
1:A:1189:ASP:HA	1:A:1192:TRP:HE3	1.49	0.78
14:N:14:DC:N4	18:T:35:DG:O6	2.16	0.78
16:Q:268:ASN:HD21	16:Q:270:MET:HB3	1.49	0.78
1:A:413:TYR:O	1:A:415:GLY:N	2.17	0.78
16:Q:568:TRP:HE1	16:Q:591:ILE:HD12	1.49	0.78
24:Z:216:VAL:HB	24:Z:226:TYR:HB2	1.65	0.77
9:I:101:SER:OG	9:I:102:ALA:O	2.03	0.77
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.66	0.77
19:U:394:TYR:O	20:V:172:ARG:NH2	2.17	0.77
24:Z:728:THR:O	24:Z:747:ARG:NH1	2.18	0.77
16:Q:624:LYS:HG3	16:Q:627:ARG:HH21	1.47	0.76
1:A:272:ASN:ND2	18:T:34:DT:O2	2.19	0.76
1:A:1189:ASP:HA	1:A:1192:TRP:CE3	2.20	0.76
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.68	0.76
1:A:571:ASP:OD1	1:A:571:ASP:N	2.13	0.76
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.66	0.76
11:K:77:THR:OG1	11:K:81:TYR:O	2.04	0.76
17:R:562:TYR:O	17:R:566:ARG:NE	2.18	0.76
20:V:47:LYS:HE3	22:X:230:VAL:HG22	1.67	0.76
16:Q:353:TYR:OH	20:V:57:ARG:O	2.04	0.76
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.19	0.75
1:A:1434:GLU:O	1:A:1436:VAL:N	2.19	0.75
16:Q:314:ARG:HH12	16:Q:349:GLN:HE22	1.33	0.75
2:B:834:ARG:NH2	2:B:841:ARG:O	2.20	0.75
1:A:819:SER:O	1:A:819:SER:OG	2.05	0.74
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.52	0.74
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.67	0.74
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.68	0.74
14:N:37:DG:O6	18:T:12:DC:N4	2.20	0.74
1:A:296:ASN:OD1	1:A:297:GLY:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.69	0.74
1:A:1467:GLY:O	1:A:1469:GLY:N	2.20	0.74
2:B:677:MET:H	2:B:682:LEU:HD22	1.52	0.74
20:V:193:HIS:HB2	20:V:199:VAL:HG12	1.70	0.74
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.21	0.74
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.21	0.74
24:Z:438:GLY:HA3	24:Z:452:PRO:HB2	1.68	0.74
2:B:388:TYR:H	2:B:504:THR:HG21	1.51	0.73
24:Z:492:ILE:HG22	24:Z:502:LEU:HB3	1.70	0.73
24:Z:554:GLU:OE2	24:Z:559:GLN:NE2	2.21	0.73
15:P:39:A:C3'	15:P:40:A:H8	2.01	0.73
21:W:214:ILE:N	21:W:228:LEU:O	2.21	0.73
24:Z:353:ALA:HB3	24:Z:360:ILE:HB	1.69	0.73
16:Q:424:GLN:HB2	22:X:231:TRP:CE3	2.24	0.73
24:Z:188:GLU:O	24:Z:192:THR:OG1	2.05	0.73
24:Z:295:TYR:N	24:Z:304:SER:OG	2.17	0.73
1:A:1184:THR:O	1:A:1186:VAL:N	2.22	0.73
21:W:169:ASP:N	21:W:169:ASP:OD1	2.22	0.73
2:B:898:THR:O	2:B:899:SER:OG	2.05	0.72
8:H:32:SER:HB3	8:H:37:MET:H	1.52	0.72
2:B:84:TYR:HB3	2:B:132:VAL:HG23	1.70	0.72
2:B:309:PHE:O	9:I:40:ARG:NH2	2.22	0.72
2:B:650:ASN:N	19:U:460:TYR:OH	2.17	0.72
4:D:131:LEU:HA	4:D:134:ILE:HD12	1.71	0.72
5:E:81:LYS:NZ	14:N:39:DA:OP1	2.19	0.72
1:A:539:GLN:O	1:A:542:LEU:N	2.21	0.72
21:W:272:ASP:O	21:W:274:GLN:NE2	2.22	0.72
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.71	0.72
19:U:438:ALA:O	19:U:439:ARG:NH1	2.20	0.72
20:V:110:GLU:HG3	20:V:111:GLU:H	1.53	0.72
1:A:289:GLN:O	1:A:293:ASN:HB2	1.89	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.72
21:W:251:SER:OG	21:W:253:ASP:OD1	2.05	0.72
2:B:348:LEU:O	2:B:361:LYS:NZ	2.22	0.72
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.70	0.72
23:Y:93:LEU:HD22	23:Y:97:ILE:HD11	1.70	0.72
2:B:595:ASP:OD1	2:B:596:ILE:N	2.20	0.71
16:Q:163:ILE:HB	16:Q:194:PRO:HG3	1.72	0.71
21:W:81:SER:HB3	21:W:91:TRP:HE1	1.55	0.71
16:Q:302:GLU:HG3	16:Q:305:GLN:HE21	1.55	0.71
8:H:128:ASP:OD1	8:H:131:ASN:ND2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:401:LEU:HD22	16:Q:418:LEU:HG	1.72	0.71
17:R:405:ILE:HG23	17:R:426:LEU:HD11	1.72	0.71
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.72	0.71
10:J:64:PRO:O	12:L:23:HIS:NE2	2.23	0.71
18:T:8:DG:H1'	18:T:9:DC:H5'	1.73	0.71
21:W:256:VAL:HB	21:W:270:PHE:HB2	1.72	0.71
24:Z:504:SER:OG	24:Z:507:THR:O	2.08	0.71
16:Q:384:LEU:HD13	16:Q:397:ALA:HB2	1.73	0.71
19:U:507:THR:O	19:U:509:ARG:N	2.24	0.71
24:Z:470:LYS:HB2	24:Z:516:ARG:HA	1.72	0.71
5:E:36:THR:N	5:E:39:GLU:OE2	2.16	0.70
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.72	0.70
16:Q:799:VAL:O	16:Q:802:LYS:NZ	2.23	0.70
17:R:405:ILE:HG12	17:R:426:LEU:HD21	1.72	0.70
7:G:151:ARG:O	7:G:158:PHE:N	2.22	0.70
10:J:44:CYS:O	10:J:47:ARG:NH1	2.25	0.70
1:A:77:ASN:OD1	1:A:78:MET:N	2.25	0.70
16:Q:729:LYS:HE2	16:Q:732:LYS:HD2	1.72	0.70
1:A:244:ARG:HE	1:A:245:PRO:HD2	1.57	0.70
3:C:74:THR:OG1	3:C:74:THR:O	2.09	0.70
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.25	0.70
7:G:110:ARG:HH21	7:G:118:GLU:HA	1.56	0.70
9:I:42:CYS:SG	9:I:43:ASP:N	2.65	0.70
24:Z:563:MET:HA	24:Z:637:VAL:HG11	1.73	0.70
24:Z:759:GLY:O	24:Z:761:MET:N	2.24	0.70
2:B:85:LEU:N	2:B:131:THR:O	2.25	0.70
1:A:100:LEU:HD23	1:A:193:ARG:HE	1.57	0.69
19:U:450:LEU:HD21	19:U:452:LEU:HD23	1.73	0.69
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.27	0.69
1:A:357:LYS:NZ	2:B:1112:ASP:OD1	2.26	0.69
1:A:686:THR:OG1	1:A:687:ILE:N	2.25	0.69
16:Q:624:LYS:HG3	16:Q:627:ARG:NH2	2.07	0.69
5:E:97:GLU:HB2	5:E:99:ILE:HG12	1.74	0.69
13:M:1379:GLN:HG2	13:M:1469:PRO:HB2	1.73	0.69
17:R:428:LEU:HB2	17:R:437:PHE:CD2	2.27	0.69
21:W:231:HIS:HD1	21:W:235:VAL:HG22	1.57	0.69
24:Z:502:LEU:HG	24:Z:511:LEU:HB3	1.75	0.69
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.25	0.69
7:G:91:GLN:HG2	7:G:93:ASN:HD21	1.58	0.69
24:Z:525:ALA:HB1	24:Z:552:ARG:HH22	1.58	0.69
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1462:ILE:HD11	13:M:1472:PHE:HB3	1.74	0.69
21:W:113:ALA:HB3	21:W:122:ALA:HB3	1.74	0.69
1:A:999:ARG:NH2	8:H:103:GLU:OE2	2.24	0.69
4:D:34:ASN:O	4:D:68:THR:OG1	2.09	0.69
17:R:564:ASN:HD21	20:V:136:TYR:C	1.96	0.69
1:A:1212:LEU:HD21	1:A:1289:GLU:HB3	1.75	0.69
16:Q:752:VAL:HG22	16:Q:803:MET:HE2	1.75	0.69
24:Z:450:ILE:HG23	24:Z:452:PRO:HD3	1.74	0.69
5:E:2:ASP:OD2	5:E:4:GLU:N	2.25	0.69
7:G:152:VAL:HG22	7:G:157:ILE:HG22	1.74	0.69
17:R:410:GLU:OE1	17:R:423:ASN:ND2	2.25	0.69
8:H:36:LYS:HG3	16:Q:709:ARG:HH22	1.57	0.68
17:R:366:ARG:NH1	24:Z:775:TPO:OG1	2.26	0.68
4:D:23:PRO:HG2	7:G:78:ARG:HH12	1.58	0.68
13:M:1488:THR:HB	13:M:1495:ARG:HB3	1.75	0.68
17:R:570:TRP:HD1	20:V:133:LYS:HD2	1.57	0.68
20:V:192:GLN:HB2	20:V:197:PRO:HB3	1.74	0.68
13:M:1512:LYS:O	13:M:1516:GLN:NE2	2.24	0.68
16:Q:886:LYS:O	16:Q:890:MET:HG2	1.94	0.68
15:P:39:A:H3'	15:P:40:A:C8	2.29	0.68
1:A:487:SER:OG	1:A:673:GLN:NE2	2.26	0.68
24:Z:433:LEU:HB3	24:Z:436:LEU:HD12	1.75	0.68
24:Z:478:VAL:HG21	24:Z:502:LEU:HD22	1.74	0.68
21:W:289:ILE:HB	21:W:301:TYR:HB2	1.74	0.68
16:Q:86:LEU:HD11	16:Q:116:LEU:HB3	1.76	0.68
7:G:123:SER:OG	7:G:125:PRO:O	2.11	0.68
16:Q:590:ARG:HA	16:Q:593:LYS:HG3	1.76	0.67
2:B:633:LEU:HD11	2:B:679:PRO:HB2	1.76	0.67
2:B:649:ASN:HB2	19:U:460:TYR:OH	1.93	0.67
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.17	0.67
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.77	0.67
16:Q:394:ARG:HB3	16:Q:398:LYS:HE3	1.76	0.67
24:Z:419:ASN:OD1	24:Z:516:ARG:NH1	2.27	0.67
1:A:140:ARG:HH22	1:A:234:PHE:HD1	1.41	0.67
1:A:611:ASP:N	1:A:611:ASP:OD1	2.25	0.67
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.28	0.67
5:E:82:VAL:HG22	5:E:86:THR:OG1	1.93	0.67
21:W:13:GLN:NE2	21:W:15:HIS:O	2.27	0.67
17:R:406:THR:OG1	17:R:427:GLN:O	2.11	0.67
1:A:112:PHE:O	1:A:113:PHE:HB2	1.93	0.67
1:A:116:LYS:NZ	1:A:184:CYS:SG	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:TRP:CE2	2:B:679:PRO:HG3	2.30	0.67
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.77	0.67
2:B:1136:GLU:HB2	2:B:1143:LYS:HG2	1.77	0.67
16:Q:484:GLU:HB3	16:Q:487:HIS:HB2	1.76	0.66
24:Z:295:TYR:H	24:Z:304:SER:HG	1.42	0.66
2:B:1157:LEU:O	2:B:1161:GLU:HG3	1.95	0.66
4:D:128:GLN:NE2	4:D:132:ASP:OD1	2.27	0.66
24:Z:184:CYS:SG	24:Z:185:LYS:N	2.68	0.66
7:G:21:ASN:OD1	7:G:21:ASN:N	2.23	0.66
7:G:109:SER:HB3	24:Z:493:VAL:HG21	1.77	0.66
19:U:474:ARG:H	20:V:218:GLN:HA	1.60	0.66
21:W:236:LEU:N	21:W:250:SER:O	2.27	0.66
21:W:292:VAL:HG12	21:W:298:ILE:HG12	1.76	0.66
1:A:200:ALA:HB3	1:A:214:ILE:HG12	1.78	0.66
14:N:37:DG:N2	18:T:12:DC:O2	2.26	0.66
1:A:413:TYR:O	1:A:449:HIS:HD2	1.77	0.66
1:A:1118:THR:O	1:A:1123:ARG:HB2	1.96	0.66
2:B:1003:ASN:O	2:B:1005:ALA:N	2.27	0.66
16:Q:534:TYR:OH	16:Q:556:GLU:OE1	2.12	0.66
3:C:212:ASP:OD1	3:C:212:ASP:N	2.28	0.66
13:M:1373:VAL:HG21	13:M:1379:GLN:HG3	1.76	0.66
21:W:66:GLY:O	21:W:83:SER:OG	2.11	0.66
1:A:539:GLN:NE2	2:B:790:GLN:O	2.28	0.66
14:N:34:DC:H2''	14:N:35:DA:C8	2.30	0.66
16:Q:268:ASN:ND2	16:Q:271:VAL:H	1.93	0.66
16:Q:420:GLN:O	22:X:229:ARG:NH1	2.28	0.66
24:Z:613:GLU:O	24:Z:625:HIS:N	2.28	0.66
14:N:10:DG:H2''	14:N:11:DC:C5	2.30	0.66
21:W:46:VAL:HB	21:W:58:TRP:HB2	1.77	0.66
2:B:354:SER:OG	2:B:355:ASP:N	2.26	0.65
3:C:154:ARG:HH11	10:J:63:ALA:HB2	1.61	0.65
21:W:130:VAL:HB	21:W:144:LEU:HD12	1.78	0.65
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.78	0.65
11:K:13:PHE:HB2	11:K:16:GLU:HG3	1.77	0.65
16:Q:494:ALA:HB1	22:X:224:ILE:HG12	1.78	0.65
17:R:494:GLU:HA	17:R:497:LYS:HD2	1.79	0.65
23:Y:4:GLU:O	23:Y:27:GLN:NE2	2.29	0.65
5:E:27:LEU:O	16:Q:877:GLN:NE2	2.29	0.65
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.19	0.65
5:E:93:ARG:HA	5:E:96:GLU:OE1	1.97	0.65
14:N:30:DC:N3	18:T:19:DG:N2	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:342:LEU:HD11	20:V:67:GLU:HG2	1.78	0.65
16:Q:86:LEU:HG	16:Q:120:ALA:HB2	1.76	0.65
2:B:1071:ASN:O	2:B:1073:GLN:N	2.29	0.65
14:N:30:DC:N4	18:T:19:DG:H1	1.93	0.65
16:Q:211:LEU:HD12	16:Q:213:LYS:HZ1	1.62	0.65
1:A:1184:THR:C	1:A:1186:VAL:H	2.00	0.65
8:H:72:ASP:OD1	8:H:73:GLY:N	2.29	0.65
21:W:218:ASP:N	21:W:223:ASN:O	2.29	0.65
23:Y:14:ARG:HH21	23:Y:54:SER:HA	1.61	0.65
24:Z:539:LEU:HD22	24:Z:616:HIS:HB3	1.79	0.65
21:W:195:SER:OG	21:W:236:LEU:O	2.15	0.65
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.79	0.65
16:Q:856:LEU:HD23	16:Q:857:LEU:HD22	1.78	0.65
24:Z:558:PHE:N	24:Z:570:VAL:O	2.30	0.65
2:B:223:SER:OG	2:B:350:HIS:ND1	2.26	0.64
16:Q:605:LEU:O	16:Q:609:ASN:ND2	2.30	0.64
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.78	0.64
16:Q:568:TRP:CZ3	16:Q:592:LEU:HB2	2.32	0.64
20:V:45:ASP:N	20:V:45:ASP:OD1	2.30	0.64
24:Z:470:LYS:NZ	24:Z:518:LEU:O	2.31	0.64
4:D:76:ASN:HD21	4:D:78:GLU:HB2	1.61	0.64
5:E:113:SER:OG	14:N:40:DG:OP1	2.15	0.64
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.13	0.64
21:W:214:ILE:HB	21:W:228:LEU:HB3	1.78	0.64
24:Z:282:LYS:O	24:Z:287:LYS:NZ	2.28	0.64
17:R:569:GLU:O	17:R:573:VAL:HG23	1.97	0.64
20:V:48:PHE:HB2	22:X:229:ARG:HB2	1.78	0.64
1:A:329:MET:HA	1:A:335:PRO:HA	1.80	0.64
1:A:1140:THR:OG1	1:A:1140:THR:O	2.12	0.64
2:B:100:GLU:OE1	2:B:100:GLU:N	2.24	0.64
7:G:153:ASP:N	7:G:156:ASP:O	2.23	0.64
21:W:26:THR:HG23	21:W:284:GLY:HA2	1.80	0.64
16:Q:710:LYS:HB2	16:Q:712:TYR:CD1	2.32	0.64
2:B:497:LYS:HG3	2:B:498:PRO:HD3	1.80	0.64
14:N:31:DC:H2"	14:N:32:DA:C8	2.32	0.64
2:B:577:HIS:NE2	2:B:583:LEU:HD11	2.13	0.64
24:Z:519:GLN:NE2	24:Z:521:CYS:SG	2.71	0.64
1:A:376:ASP:CG	1:A:473:ARG:HH21	2.01	0.63
17:R:355:LEU:HG	17:R:357:GLU:H	1.62	0.63
2:B:787:GLY:O	2:B:790:GLN:HG3	1.98	0.63
21:W:92:ASP:HB3	21:W:95:ASN:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.33	0.63
2:B:184:TYR:CE2	2:B:191:GLU:HG2	2.33	0.63
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.79	0.63
14:N:38:DG:H2''	14:N:39:DA:C8	2.34	0.63
1:A:1540:THR:HG23	13:M:1479:ARG:HE	1.62	0.63
2:B:93:LEU:O	19:U:507:THR:HA	1.99	0.63
8:H:2:ALA:C	8:H:84:ARG:HH22	2.02	0.63
16:Q:123:ILE:HG13	16:Q:124:ILE:HG12	1.80	0.63
16:Q:398:LYS:O	16:Q:402:LYS:HD3	1.99	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.81	0.63
18:T:38:DG:H2''	18:T:39:DC:C5	2.33	0.63
21:W:48:LYS:N	21:W:55:ASP:O	2.27	0.63
5:E:166:ARG:NH2	5:E:168:ASN:HD22	1.95	0.63
7:G:36:GLY:O	24:Z:628:LYS:NZ	2.23	0.63
8:H:8:ASP:OD1	8:H:32:SER:OG	2.05	0.63
17:R:355:LEU:HD12	17:R:356:PRO:HD2	1.81	0.63
17:R:404:GLU:OE1	17:R:455:TRP:NE1	2.32	0.63
24:Z:733:ARG:NH1	24:Z:744:SER:OG	2.31	0.63
8:H:30:CYS:HG	8:H:56:PHE:HZ	1.47	0.63
16:Q:286:SER:O	16:Q:290:HIS:ND1	2.32	0.63
16:Q:611:TRP:HE1	16:Q:628:HIS:HA	1.63	0.63
2:B:67:LEU:H	2:B:83:ARG:HB2	1.64	0.63
16:Q:239:ALA:HB2	16:Q:257:LEU:HB3	1.81	0.63
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.34	0.62
16:Q:576:LEU:HD21	16:Q:585:GLN:HE22	1.64	0.62
16:Q:128:GLN:HE22	20:V:86:LEU:HD13	1.64	0.62
16:Q:835:ASP:OD1	16:Q:839:ARG:NE	2.32	0.62
21:W:206:VAL:HG11	21:W:238:VAL:HG21	1.81	0.62
5:E:64:HIS:N	5:E:70:ASP:O	2.31	0.62
1:A:481:THR:O	1:A:483:ARG:NH1	2.32	0.62
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.80	0.62
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.32	0.62
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.62
1:A:922:PHE:H	1:A:1052:ARG:HH11	1.48	0.62
8:H:110:THR:O	8:H:129:ALA:N	2.32	0.62
11:K:5:PRO:HG2	11:K:8:GLU:HG3	1.81	0.62
1:A:556:GLU:OE1	1:A:556:GLU:N	2.33	0.62
2:B:100:GLU:HA	2:B:105:PRO:HG3	1.82	0.62
5:E:55:ARG:HB2	5:E:78:GLU:HG3	1.82	0.62
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.11	0.62
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HG	2:B:84:TYR:OH	2.00	0.62
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.82	0.62
16:Q:394:ARG:HD2	16:Q:421:ILE:HG23	1.82	0.62
16:Q:849:LYS:O	16:Q:852:LEU:HG	2.00	0.62
24:Z:506:LEU:HD11	24:Z:552:ARG:HH21	1.63	0.62
8:H:83:SER:OG	8:H:84:ARG:N	2.33	0.62
9:I:12:VAL:HG21	9:I:53:ILE:O	2.00	0.62
21:W:206:VAL:HG22	21:W:216:ILE:HG12	1.81	0.62
8:H:32:SER:OG	8:H:33:GLU:N	2.33	0.61
12:L:56:ASP:O	12:L:58:ARG:N	2.33	0.61
17:R:564:ASN:OD1	20:V:136:TYR:N	2.29	0.61
1:A:797:ARG:NH2	1:A:815:TYR:O	2.32	0.61
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.82	0.61
5:E:39:GLU:OE1	5:E:39:GLU:N	2.24	0.61
8:H:2:ALA:O	8:H:84:ARG:NH2	2.30	0.61
16:Q:86:LEU:HD12	16:Q:89:LEU:HB2	1.80	0.61
1:A:30:GLU:HA	1:A:33:ARG:HE	1.63	0.61
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.81	0.61
1:A:1468:THR:H	6:F:60:TYR:HB3	1.66	0.61
2:B:19:PRO:O	2:B:21:LEU:N	2.32	0.61
16:Q:249:ASP:O	16:Q:253:ASN:ND2	2.33	0.61
17:R:364:LEU:HB2	17:R:387:VAL:HG12	1.81	0.61
24:Z:366:TYR:O	24:Z:373:PHE:N	2.28	0.61
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.34	0.61
16:Q:715:GLN:HB2	16:Q:746:VAL:HG11	1.83	0.61
20:V:110:GLU:HG3	20:V:111:GLU:N	2.14	0.61
1:A:88:ILE:O	1:A:90:LEU:N	2.33	0.61
16:Q:38:HIS:HE1	16:Q:73:LEU:HD13	1.66	0.61
16:Q:68:ARG:HE	16:Q:89:LEU:HD12	1.65	0.61
24:Z:390:LEU:HD12	24:Z:393:LEU:HD12	1.82	0.61
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.01	0.61
3:C:190:ASN:ND2	3:C:195:THR:O	2.20	0.61
16:Q:862:GLU:HA	16:Q:865:LEU:HG	1.82	0.61
2:B:228:SER:O	2:B:405:ARG:NH1	2.34	0.61
3:C:91:GLU:OE1	24:Z:713:SER:HB2	2.01	0.61
5:E:45:GLY:HA3	5:E:53:PRO:HD3	1.82	0.61
16:Q:729:LYS:HB2	16:Q:732:LYS:HD2	1.82	0.61
1:A:47:THR:HA	1:A:52:PRO:HA	1.81	0.61
1:A:1244:ASN:HB2	1:A:1262:MET:HE1	1.81	0.61
1:A:1481:LYS:O	13:M:1384:ARG:NH1	2.34	0.61
2:B:144:HIS:CD2	2:B:431:LEU:HD21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:158:GLN:HG3	16:Q:159:SER:H	1.66	0.61
1:A:1301:ILE:HG22	1:A:1345:ARG:HH21	1.65	0.60
16:Q:379:LYS:HZ1	20:V:61:TYR:HE2	1.47	0.60
21:W:26:THR:HA	21:W:284:GLY:HA2	1.83	0.60
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.82	0.60
16:Q:646:ASN:HA	22:X:239:GLN:HA	1.82	0.60
20:V:196:LYS:O	20:V:198:ARG:HG3	2.01	0.60
21:W:53:ARG:NH1	21:W:54:LEU:O	2.34	0.60
23:Y:66:PRO:HB2	23:Y:78:SER:HA	1.82	0.60
24:Z:554:GLU:OE1	24:Z:557:THR:OG1	2.18	0.60
7:G:151:ARG:HB3	7:G:158:PHE:O	2.01	0.60
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.66	0.60
16:Q:65:GLU:OE1	16:Q:93:TYR:OH	2.15	0.60
1:A:123:ASN:O	1:A:127:LYS:HG2	2.02	0.60
16:Q:80:LYS:O	16:Q:83:MET:HG3	2.01	0.60
16:Q:222:SER:O	16:Q:226:GLU:HG2	2.01	0.60
21:W:27:ASN:O	21:W:32:SER:OG	2.19	0.60
6:F:114:SER:OG	6:F:115:TYR:N	2.33	0.60
16:Q:163:ILE:HG21	16:Q:189:ALA:HA	1.83	0.60
16:Q:313:ALA:HB2	16:Q:328:TYR:HB2	1.83	0.60
23:Y:19:CYS:SG	23:Y:21:LEU:HB2	2.42	0.60
3:C:55:ASN:ND2	3:C:60:HIS:O	2.34	0.60
16:Q:48:ALA:HB2	16:Q:63:LEU:HD11	1.84	0.60
16:Q:65:GLU:HA	16:Q:89:LEU:HD11	1.82	0.60
21:W:176:ASP:HB2	21:W:183:LEU:HD11	1.83	0.60
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.16	0.60
20:V:233:VAL:O	20:V:238:PRO:N	2.35	0.60
2:B:784:SER:O	2:B:784:SER:OG	2.14	0.60
10:J:36:ASP:OD1	10:J:36:ASP:N	2.28	0.60
21:W:125:THR:OG1	21:W:131:ASN:ND2	2.34	0.60
1:A:217:SER:OG	1:A:220:ARG:N	2.35	0.60
5:E:45:GLY:CA	5:E:53:PRO:HD3	2.32	0.60
16:Q:581:TRP:O	16:Q:585:GLN:HB2	2.02	0.60
16:Q:620:ARG:HG3	16:Q:625:GLU:HB2	1.84	0.60
24:Z:629:LEU:HB2	24:Z:634:GLY:HA2	1.83	0.60
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.35	0.59
1:A:1222:THR:O	1:A:1225:LYS:N	2.34	0.59
3:C:189:ASP:O	3:C:191:ALA:N	2.34	0.59
1:A:1210:TRP:CZ2	1:A:1281:ASP:HB3	2.37	0.59
4:D:60:VAL:HA	4:D:63:LYS:HG2	1.82	0.59
7:G:109:SER:HB2	24:Z:503:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:CYS:O	2:B:691:SER:OG	2.21	0.59
2:B:743:ARG:NH1	2:B:745:ASP:OD1	2.35	0.59
16:Q:351:TYR:HB2	16:Q:360:ALA:HB2	1.83	0.59
16:Q:708:LEU:HD21	16:Q:719:VAL:HG21	1.83	0.59
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.84	0.59
11:K:49:GLN:NE2	11:K:93:ASP:OD2	2.34	0.59
1:A:64:VAL:HG11	1:A:78:MET:HA	1.84	0.59
24:Z:365:ARG:HD3	24:Z:374:LYS:HD2	1.84	0.59
24:Z:499:PHE:HD1	24:Z:512:LYS:HB3	1.67	0.59
16:Q:776:LEU:O	16:Q:779:VAL:HG22	2.03	0.59
1:A:379:GLY:HA2	1:A:475:ARG:O	2.02	0.59
1:A:1231:ILE:O	1:A:1235:ILE:HB	2.03	0.59
2:B:650:ASN:N	2:B:650:ASN:OD1	2.36	0.59
3:C:60:HIS:HB2	3:C:63:PHE:HB2	1.83	0.59
16:Q:371:TYR:HE2	16:Q:373:ASN:HD21	1.51	0.59
16:Q:505:ARG:NH2	20:V:44:PHE:HB2	2.12	0.59
16:Q:419:ALA:HB2	16:Q:433:ALA:HB3	1.83	0.59
1:A:620:HIS:O	8:H:97:TYR:OH	2.15	0.59
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.85	0.59
16:Q:201:ARG:HH12	16:Q:227:LEU:HD13	1.68	0.59
1:A:1005:HIS:HD2	1:A:1007:ILE:H	1.49	0.59
2:B:177:CYS:SG	2:B:180:ASP:N	2.74	0.59
4:D:103:LEU:O	7:G:144:ARG:NH2	2.36	0.59
16:Q:24:LEU:HD11	16:Q:56:LYS:HZ3	1.68	0.59
16:Q:624:LYS:HA	16:Q:627:ARG:HH21	1.67	0.59
15:P:39:A:C2	15:P:40:A:C5	2.91	0.58
21:W:8:LEU:N	21:W:300:ILE:O	2.30	0.58
1:A:476:ILE:O	1:A:476:ILE:HG13	2.00	0.58
2:B:912:ASN:OD1	2:B:912:ASN:N	2.26	0.58
9:I:17:CYS:N	9:I:22:ASN:O	2.27	0.58
14:N:11:DC:H2''	14:N:12:DG:C8	2.38	0.58
16:Q:884:LYS:O	16:Q:887:ASN:N	2.34	0.58
16:Q:774:SER:H	16:Q:830:ARG:NH1	1.99	0.58
17:R:574:GLU:HA	17:R:577:LYS:HG2	1.84	0.58
2:B:565:THR:HA	2:B:610:ARG:HB3	1.86	0.58
5:E:93:ARG:HB2	16:Q:891:PHE:CE1	2.38	0.58
8:H:63:THR:HG21	8:H:68:GLY:HA2	1.85	0.58
8:H:78:THR:O	8:H:78:THR:OG1	2.21	0.58
17:R:353:VAL:HG12	17:R:469:LEU:HD13	1.86	0.58
19:U:445:ASP:OD2	19:U:447:SER:OG	2.19	0.58
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.36	0.58
15:P:37:G:HO2'	15:P:38:G:H8	1.52	0.58
20:V:88:ASN:OD1	20:V:89:PRO:HD3	2.04	0.58
24:Z:562:ASN:HD21	24:Z:566:LYS:HG3	1.67	0.58
1:A:367:ILE:HA	1:A:482:PHE:O	2.04	0.58
1:A:394:VAL:HG23	1:A:444:TYR:O	2.04	0.58
2:B:743:ARG:HB3	2:B:743:ARG:HH11	1.69	0.58
5:E:66:ASP:OD1	5:E:67:ASP:N	2.36	0.58
17:R:363:ARG:NH2	17:R:365:SER:OG	2.36	0.58
1:A:11:SER:O	2:B:1135:TYR:OH	2.14	0.58
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.36	0.58
2:B:577:HIS:CD2	2:B:583:LEU:HD11	2.38	0.58
2:B:646:ARG:C	2:B:648:TYR:H	2.07	0.58
1:A:552:ASP:OD1	8:H:24:ARG:NH1	2.37	0.58
2:B:83:ARG:O	2:B:83:ARG:NH2	2.37	0.58
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.58
1:A:1244:ASN:HB2	1:A:1262:MET:CE	2.34	0.58
4:D:46:GLN:HA	4:D:49:GLU:CD	2.24	0.58
13:M:1356:ILE:HG22	13:M:1370:THR:HB	1.85	0.58
15:P:37:G:O2'	15:P:38:G:H8	1.86	0.58
15:P:38:G:H2'	15:P:39:A:C8	2.35	0.58
16:Q:95:GLN:NE2	20:V:84:ILE:O	2.37	0.58
17:R:493:GLU:OE1	17:R:493:GLU:N	2.22	0.58
2:B:715:ASP:OD1	2:B:715:ASP:N	2.19	0.58
24:Z:416:ARG:HE	24:Z:466:GLN:HE21	1.52	0.57
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.86	0.57
16:Q:156:LEU:HD11	16:Q:169:LYS:HE2	1.87	0.57
16:Q:504:ALA:HB2	16:Q:519:LEU:HB3	1.86	0.57
17:R:407:GLY:H	17:R:427:GLN:HB3	1.69	0.57
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.84	0.57
1:A:1177:TYR:OH	1:A:1282:ASP:HA	2.04	0.57
2:B:721:ARG:NH1	2:B:940:GLY:O	2.36	0.57
5:E:90:TYR:HA	16:Q:891:PHE:HZ	1.69	0.57
1:A:392:GLU:HG2	1:A:402:LEU:HD11	1.86	0.57
1:A:699:TYR:O	1:A:703:GLN:HG2	2.05	0.57
2:B:235:ILE:HG13	2:B:348:LEU:HD13	1.85	0.57
7:G:37:THR:HA	24:Z:628:LYS:NZ	2.20	0.57
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.57
7:G:122:ASN:OD1	7:G:123:SER:N	2.38	0.57
16:Q:384:LEU:HG	16:Q:386:ALA:H	1.69	0.57
24:Z:280:ARG:HH21	24:Z:288:ASP:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.86	0.57
21:W:27:ASN:HB2	21:W:31:ASN:HD21	1.70	0.57
24:Z:192:THR:HG23	24:Z:245:LEU:HD21	1.85	0.57
1:A:96:HIS:HD2	1:A:99:PHE:CD2	2.23	0.57
1:A:546:ARG:HG2	1:A:546:ARG:O	2.04	0.57
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.36	0.57
1:A:1484:MET:HB2	13:M:1362:LYS:HE3	1.87	0.57
11:K:39:ASP:OD1	11:K:39:ASP:N	2.35	0.57
16:Q:474:PHE:HB2	16:Q:503:LEU:HD13	1.85	0.57
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.87	0.57
1:A:962:ASP:CG	1:A:1046:ARG:HH21	2.08	0.57
16:Q:208:PHE:HD1	16:Q:213:LYS:HD2	1.70	0.57
21:W:48:LYS:HB2	21:W:57:GLN:HB2	1.85	0.57
1:A:282:ASP:HB3	1:A:313:HIS:CE1	2.39	0.57
1:A:1146:GLN:OE1	1:A:1153:ARG:HD3	2.05	0.57
20:V:55:GLN:OE1	20:V:57:ARG:NE	2.35	0.57
24:Z:450:ILE:HG21	24:Z:468:LEU:HD11	1.86	0.57
1:A:92:LYS:HD2	1:A:307:VAL:HG11	1.87	0.56
1:A:117:LEU:HG	1:A:232:GLU:OE2	2.05	0.56
21:W:152:LEU:HD12	21:W:168:ILE:HA	1.85	0.56
1:A:1005:HIS:CD2	1:A:1007:ILE:H	2.23	0.56
3:C:4:ALA:HB2	11:K:93:ASP:HB2	1.86	0.56
16:Q:188:LYS:HB3	16:Q:191:ARG:HH11	1.70	0.56
16:Q:678:ALA:O	16:Q:684:TRP:NE1	2.38	0.56
17:R:560:ILE:HA	17:R:563:ILE:HG22	1.87	0.56
24:Z:501:ILE:HD11	24:Z:510:GLU:HB3	1.87	0.56
1:A:140:ARG:NH2	1:A:234:PHE:HD1	2.03	0.56
1:A:299:ALA:O	1:A:301:HIS:N	2.39	0.56
1:A:538:VAL:O	1:A:538:VAL:HG12	2.06	0.56
1:A:809:HIS:HE1	2:B:506:TRP:CZ2	2.23	0.56
2:B:177:CYS:HB2	2:B:738:THR:OG1	2.06	0.56
2:B:995:GLU:OE1	20:V:131:MET:HB3	2.05	0.56
5:E:55:ARG:O	5:E:56:THR:OG1	2.23	0.56
13:M:1505:ASN:O	13:M:1509:ARG:HG2	2.05	0.56
2:B:285:LEU:HD23	9:I:16:PHE:HZ	1.70	0.56
7:G:110:ARG:HH12	7:G:115:SER:HA	1.69	0.56
14:N:12:DG:H2''	14:N:13:DG:H8	1.70	0.56
21:W:68:VAL:HG13	21:W:83:SER:HA	1.87	0.56
9:I:25:TYR:O	9:I:37:TYR:HA	2.04	0.56
18:T:33:DC:H2''	18:T:34:DT:OP1	2.04	0.56
20:V:61:TYR:N	20:V:62:LYS:HA	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:384:VAL:HA	19:U:418:ASN:HB3	1.86	0.56
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.39	0.56
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.88	0.56
16:Q:802:LYS:HE2	16:Q:807:LEU:HB2	1.87	0.56
23:Y:14:ARG:NH1	23:Y:55:SER:OG	2.39	0.56
1:A:886:VAL:HG12	5:E:169:GLN:O	2.06	0.56
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.06	0.56
15:P:39:A:C3'	15:P:40:A:C8	2.87	0.56
16:Q:777:LYS:HE3	16:Q:781:ASN:HD21	1.71	0.56
19:U:395:GLU:HA	20:V:172:ARG:HH21	1.71	0.56
24:Z:478:VAL:HG11	24:Z:492:ILE:HG23	1.87	0.56
1:A:1211:LEU:HD12	1:A:1213:ARG:N	2.21	0.56
1:A:1234:LYS:HE2	1:A:1298:LEU:HA	1.87	0.56
2:B:639:HIS:O	2:B:643:LEU:HB2	2.06	0.56
4:D:104:CYS:HB3	4:D:135:GLN:HE22	1.70	0.56
17:R:415:TYR:CZ	17:R:438:ARG:HB3	2.41	0.56
24:Z:420:PHE:HB3	24:Z:440:ILE:HD13	1.88	0.56
2:B:218:THR:HG23	2:B:238:SER:HB3	1.88	0.56
2:B:1129:ASN:HB3	2:B:1134:THR:HG22	1.87	0.56
18:T:12:DC:H2''	18:T:13:DC:H5'	1.88	0.56
20:V:127:VAL:HG23	20:V:128:VAL:H	1.71	0.56
21:W:163:LEU:O	21:W:175:PHE:N	2.34	0.56
1:A:469:MET:HG3	2:B:1093:CYS:SG	2.46	0.55
3:C:60:HIS:HB2	3:C:63:PHE:H	1.71	0.55
14:N:39:DA:H2''	14:N:40:DG:O4'	2.07	0.55
20:V:95:ASP:OD1	20:V:95:ASP:N	2.39	0.55
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.38	0.55
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.87	0.55
21:W:81:SER:HB3	21:W:91:TRP:NE1	2.20	0.55
21:W:112:LEU:HD22	21:W:121:LEU:HD21	1.87	0.55
24:Z:472:PHE:HB3	24:Z:476:ASP:OD2	2.06	0.55
2:B:588:ARG:O	2:B:592:ARG:HD3	2.07	0.55
17:R:492:ILE:O	17:R:496:VAL:HG13	2.07	0.55
21:W:9:PHE:HB3	21:W:300:ILE:CG1	2.35	0.55
24:Z:364:ASN:O	24:Z:374:LYS:NZ	2.39	0.55
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.71	0.55
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.88	0.55
16:Q:302:GLU:HG3	16:Q:305:GLN:NE2	2.20	0.55
17:R:592:ASP:O	17:R:594:PHE:N	2.37	0.55
1:A:365:THR:HG22	1:A:366:VAL:H	1.70	0.55
7:G:118:GLU:O	7:G:128:TYR:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:108:ASP:HA	21:W:126:HIS:CE1	2.41	0.55
2:B:279:VAL:HG23	2:B:312:GLN:O	2.06	0.55
4:D:74:PHE:HE2	4:D:80:ILE:HG12	1.72	0.55
16:Q:451:PRO:HD3	16:Q:480:ARG:HG3	1.88	0.55
16:Q:772:GLU:HA	16:Q:773:LYS:HB2	1.88	0.55
24:Z:542:LEU:HD22	24:Z:570:VAL:HG11	1.87	0.55
1:A:528:PRO:HB3	1:A:899:GLU:HG3	1.87	0.55
17:R:363:ARG:NE	17:R:446:GLU:HA	2.21	0.55
18:T:31:DT:H2''	18:T:32:DT:H5'	1.89	0.55
22:X:250:PHE:CE1	22:X:253:LEU:HD22	2.42	0.55
1:A:1208:SER:O	1:A:1260:ARG:HD3	2.07	0.55
2:B:756:LYS:NZ	20:V:134:THR:HG1	2.02	0.55
7:G:46:ILE:HB	7:G:75:ILE:HG13	1.89	0.55
16:Q:772:GLU:HB3	16:Q:774:SER:CB	2.37	0.55
24:Z:416:ARG:NE	24:Z:466:GLN:HE21	2.04	0.55
1:A:874:LYS:HG3	1:A:880:ARG:HG3	1.89	0.55
2:B:649:ASN:ND2	19:U:460:TYR:OH	2.40	0.55
13:M:1369:VAL:HG11	13:M:1416:VAL:HG21	1.88	0.55
17:R:569:GLU:O	17:R:572:ILE:HG22	2.07	0.55
1:A:229:SER:OG	1:A:232:GLU:HB2	2.07	0.55
14:N:43:DG:H2''	14:N:44:DG:C8	2.42	0.55
16:Q:94:VAL:HG23	16:Q:140:LEU:HD11	1.89	0.55
16:Q:313:ALA:HB2	16:Q:328:TYR:CB	2.37	0.55
16:Q:761:LEU:HD22	16:Q:785:GLU:HB3	1.89	0.55
17:R:449:GLU:O	17:R:453:MET:HG2	2.07	0.55
7:G:7:LEU:N	7:G:72:TYR:O	2.40	0.54
9:I:17:CYS:HB3	9:I:22:ASN:H	1.72	0.54
13:M:1476:TYR:OH	13:M:1483:ARG:NH1	2.40	0.54
16:Q:568:TRP:CD2	16:Q:592:LEU:HD13	2.42	0.54
17:R:360:ASN:HA	17:R:363:ARG:HB2	1.89	0.54
21:W:31:ASN:HB2	21:W:72:ILE:HG21	1.90	0.54
21:W:41:ASP:OD1	21:W:41:ASP:N	2.40	0.54
1:A:350:VAL:HA	1:A:354:LEU:HB2	1.89	0.54
8:H:27:ARG:HD3	8:H:42:ASP:OD2	2.06	0.54
2:B:714:PRO:HD2	2:B:1001:PRO:HG3	1.88	0.54
2:B:859:ARG:HH12	2:B:901:THR:HG22	1.72	0.54
10:J:57:GLU:OE1	17:R:557:ILE:HG12	2.06	0.54
17:R:471:GLU:HG2	17:R:474:LYS:HE3	1.88	0.54
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.71	0.54
1:A:117:LEU:C	1:A:119:VAL:H	2.11	0.54
2:B:342:VAL:HG23	2:B:346:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:309:CYS:HB3	16:Q:328:TYR:HD1	1.73	0.54
16:Q:546:ASN:HD22	16:Q:577:ALA:HB2	1.73	0.54
24:Z:610:ARG:HD2	24:Z:629:LEU:HD21	1.89	0.54
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.90	0.54
1:A:522:PRO:O	1:A:662:HIS:HB2	2.07	0.54
2:B:309:PHE:HD2	9:I:40:ARG:NE	2.04	0.54
5:E:166:ARG:HH22	5:E:168:ASN:ND2	1.99	0.54
16:Q:316:PHE:HB2	16:Q:325:ALA:HB2	1.90	0.54
16:Q:525:ARG:HG3	16:Q:526:GLU:HG3	1.88	0.54
16:Q:776:LEU:HD22	16:Q:831:ALA:HA	1.88	0.54
21:W:76:LEU:HD12	21:W:77:PRO:HD2	1.89	0.54
24:Z:235:VAL:O	24:Z:239:ILE:HG12	2.07	0.54
1:A:48:GLU:OE1	1:A:51:ARG:HB2	2.08	0.54
1:A:606:HIS:HB3	1:A:626:THR:HB	1.89	0.54
5:E:111:THR:HG23	5:E:114:ALA:H	1.73	0.54
15:P:39:A:C2	18:T:33:DC:O2	2.61	0.54
17:R:385:CYS:O	17:R:405:ILE:HD12	2.08	0.54
21:W:236:LEU:HD13	21:W:278:TRP:CE3	2.42	0.54
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.38	0.54
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.54
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.40	0.54
16:Q:46:ALA:O	16:Q:50:GLU:HG2	2.08	0.54
19:U:450:LEU:CD2	19:U:452:LEU:HD23	2.37	0.54
21:W:19:ILE:HG12	21:W:39:SER:OG	2.06	0.54
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.89	0.54
16:Q:274:HIS:HA	16:Q:277:ASN:ND2	2.23	0.54
16:Q:505:ARG:HE	20:V:44:PHE:HB3	1.73	0.54
2:B:169:ARG:NH2	20:V:139:THR:OG1	2.40	0.54
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.38	0.54
4:D:133:ASP:O	4:D:136:THR:OG1	2.22	0.54
9:I:39:CYS:SG	9:I:40:ARG:N	2.81	0.54
16:Q:364:PHE:HB3	16:Q:380:ILE:HD11	1.90	0.54
21:W:29:LYS:O	21:W:77:PRO:HB3	2.08	0.54
2:B:159:THR:HA	2:B:164:ASN:ND2	2.22	0.54
17:R:452:PHE:CZ	17:R:456:LYS:HE2	2.43	0.54
19:U:379:PRO:HD2	19:U:382:LEU:HD12	1.89	0.54
21:W:233:SER:HG	21:W:251:SER:HB2	1.71	0.54
13:M:1463:CYS:O	13:M:1473:LEU:N	2.30	0.53
16:Q:147:GLN:O	16:Q:151:GLN:HG2	2.08	0.53
16:Q:392:GLU:HG2	16:Q:393:LYS:HG2	1.90	0.53
16:Q:553:TRP:HD1	16:Q:556:GLU:OE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.90	0.53
2:B:22:TRP:CH2	2:B:679:PRO:HD3	2.43	0.53
2:B:141:GLN:O	2:B:143:GLN:N	2.42	0.53
2:B:959:GLU:OE1	2:B:959:GLU:N	2.41	0.53
17:R:356:PRO:HB3	17:R:452:PHE:HB2	1.90	0.53
17:R:560:ILE:O	17:R:563:ILE:HG22	2.08	0.53
1:A:606:HIS:CG	1:A:607:SER:H	2.26	0.53
1:A:727:PRO:HA	1:A:736:THR:HG21	1.89	0.53
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.40	0.53
7:G:100:GLU:OE1	7:G:105:SER:HB3	2.08	0.53
7:G:117:MET:HB3	7:G:128:TYR:HB3	1.89	0.53
9:I:29:ASP:HB3	9:I:34:ILE:HG13	1.89	0.53
16:Q:772:GLU:HB3	16:Q:774:SER:HB3	1.89	0.53
21:W:228:LEU:HD13	21:W:264:ARG:HB3	1.90	0.53
21:W:256:VAL:O	21:W:269:THR:HA	2.07	0.53
1:A:64:VAL:HG12	1:A:81:CYS:SG	2.48	0.53
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.43	0.53
16:Q:190:LEU:O	16:Q:193:ASN:ND2	2.41	0.53
16:Q:454:LEU:HA	16:Q:457:VAL:HG12	1.91	0.53
16:Q:867:GLU:O	16:Q:871:GLN:HG3	2.08	0.53
20:V:45:ASP:HB3	22:X:232:ARG:HE	1.73	0.53
21:W:33:GLU:O	21:W:49:TRP:N	2.41	0.53
23:Y:40:LEU:HD22	23:Y:42:MET:HB3	1.89	0.53
24:Z:244:ASN:HB3	24:Z:245:LEU:HD22	1.90	0.53
1:A:141:LEU:HA	1:A:144:VAL:HG22	1.89	0.53
5:E:45:GLY:HA3	5:E:52:ARG:HB2	1.91	0.53
8:H:9:ILE:HD12	8:H:148:LEU:HD11	1.90	0.53
12:L:35:ARG:HH21	12:L:40:GLY:CA	2.20	0.53
13:M:1440:ARG:O	13:M:1444:GLU:HG2	2.08	0.53
16:Q:631:ARG:O	16:Q:635:ILE:HG12	2.09	0.53
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.36	0.53
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.74	0.53
1:A:1227:THR:N	1:A:1230:GLN:HE21	1.98	0.53
7:G:117:MET:N	7:G:117:MET:SD	2.80	0.53
22:X:233:THR:O	22:X:236:THR:OG1	2.22	0.53
24:Z:279:VAL:HA	24:Z:386:VAL:HG21	1.90	0.53
1:A:241:ARG:HB2	1:A:241:ARG:CZ	2.39	0.53
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.89	0.53
2:B:957:THR:HG22	2:B:1028:LEU:HD22	1.90	0.53
5:E:119:VAL:HA	5:E:122:ALA:HB2	1.90	0.53
2:B:395:LEU:HD11	2:B:532:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:623:GLU:O	16:Q:627:ARG:NE	2.42	0.53
16:Q:776:LEU:O	16:Q:780:LEU:HD12	2.08	0.53
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.42	0.53
2:B:741:HIS:CD2	2:B:742:VAL:HG23	2.43	0.53
2:B:789:ASN:O	2:B:968:ASN:HB2	2.09	0.53
2:B:833:THR:C	2:B:835:GLU:H	2.11	0.53
7:G:109:SER:HB3	24:Z:493:VAL:HG11	1.91	0.53
13:M:1352:GLN:HE22	13:M:1373:VAL:C	2.11	0.53
16:Q:769:LEU:HD13	16:Q:824:ALA:HB2	1.91	0.53
16:Q:777:LYS:HA	16:Q:780:LEU:HD13	1.91	0.53
21:W:9:PHE:H	21:W:300:ILE:HB	1.73	0.53
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.28	0.53
4:D:130:ILE:HA	4:D:133:ASP:OD2	2.09	0.53
9:I:68:ILE:HB	9:I:122:ARG:HD3	1.91	0.53
11:K:93:ASP:OD1	11:K:93:ASP:N	2.41	0.53
16:Q:26:GLU:HG3	16:Q:28:ASP:H	1.74	0.53
21:W:108:ASP:HA	21:W:126:HIS:ND1	2.23	0.53
21:W:248:VAL:HG12	21:W:258:VAL:HG22	1.90	0.53
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.07	0.52
7:G:8:GLU:HA	7:G:71:LYS:HA	1.91	0.52
7:G:37:THR:OG1	7:G:38:CYS:N	2.42	0.52
10:J:65:LEU:HD12	10:J:66:GLU:OE1	2.09	0.52
16:Q:244:ASN:ND2	20:V:69:GLN:HA	2.24	0.52
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.91	0.52
4:D:61:PHE:CE2	4:D:65:LEU:HD21	2.44	0.52
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.91	0.52
17:R:355:LEU:HD11	17:R:357:GLU:HG2	1.90	0.52
17:R:403:ALA:HB1	17:R:428:LEU:HB3	1.91	0.52
18:T:17:DT:H2"	18:T:18:DG:C8	2.44	0.52
18:T:35:DG:C2	18:T:36:DC:C2	2.97	0.52
16:Q:384:LEU:HD21	16:Q:386:ALA:HB3	1.91	0.52
16:Q:763:ARG:HG2	20:V:25:GLU:HG3	1.91	0.52
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.90	0.52
2:B:609:GLU:O	2:B:609:GLU:HG2	2.09	0.52
13:M:1447:LEU:HB3	13:M:1477:GLN:HG3	1.91	0.52
17:R:577:LYS:O	17:R:580:VAL:HG22	2.09	0.52
24:Z:422:PRO:HG3	24:Z:443:VAL:HG21	1.91	0.52
1:A:129:ILE:HD13	1:A:132:LYS:NZ	2.24	0.52
16:Q:420:GLN:HA	22:X:229:ARG:HH22	1.75	0.52
21:W:172:ILE:N	21:W:186:LEU:O	2.42	0.52
21:W:289:ILE:N	21:W:301:TYR:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:193:ALA:O	24:Z:197:MET:HG3	2.10	0.52
2:B:1136:GLU:HA	2:B:1143:LYS:HA	1.90	0.52
4:D:51:ALA:O	4:D:54:GLU:HB2	2.10	0.52
4:D:82:SER:O	4:D:85:SER:OG	2.25	0.52
5:E:209:VAL:O	5:E:210:GLN:HB2	2.10	0.52
7:G:93:ASN:O	7:G:128:TYR:OH	2.27	0.52
16:Q:239:ALA:HA	16:Q:257:LEU:HD13	1.92	0.52
16:Q:774:SER:O	16:Q:830:ARG:NH2	2.41	0.52
18:T:9:DC:C6	18:T:10:DT:H72	2.45	0.52
2:B:1010:LYS:HE3	20:V:130:TRP:CZ3	2.43	0.52
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.75	0.52
4:D:63:LYS:HE2	7:G:102:GLY:O	2.10	0.52
16:Q:380:ILE:HD12	16:Q:400:HIS:HE1	1.75	0.52
17:R:473:ASN:HA	17:R:476:GLU:CD	2.30	0.52
21:W:39:SER:HB2	21:W:41:ASP:OD1	2.10	0.52
21:W:217:TYR:HA	21:W:224:LEU:HA	1.91	0.52
1:A:525:ILE:O	1:A:534:VAL:HG22	2.09	0.52
1:A:1229:GLU:O	1:A:1233:GLU:HG3	2.10	0.52
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.52
7:G:7:LEU:O	7:G:72:TYR:N	2.27	0.52
16:Q:511:CYS:O	21:W:229:SER:OG	2.24	0.52
16:Q:790:HIS:HA	16:Q:793:PHE:CD2	2.45	0.52
17:R:452:PHE:HB3	17:R:453:MET:HE2	1.92	0.52
21:W:176:ASP:HB2	21:W:183:LEU:HD21	1.92	0.52
24:Z:588:ASP:HA	24:Z:640:THR:O	2.10	0.52
1:A:1546:PHE:HD2	13:M:1516:GLN:HG3	1.75	0.51
2:B:388:TYR:OH	2:B:524:LYS:HE3	2.10	0.51
2:B:651:TYR:HB2	19:U:460:TYR:CZ	2.44	0.51
5:E:36:THR:HG1	5:E:39:GLU:CD	2.13	0.51
5:E:67:ASP:OD2	5:E:69:THR:OG1	2.22	0.51
16:Q:768:VAL:HG13	16:Q:769:LEU:HG	1.91	0.51
1:A:922:PHE:N	1:A:1052:ARG:HH11	2.09	0.51
4:D:63:LYS:HD3	7:G:103:PRO:HA	1.92	0.51
17:R:581:ALA:O	17:R:585:ASN:ND2	2.43	0.51
24:Z:568:VAL:HG13	24:Z:570:VAL:HG13	1.91	0.51
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.39	0.51
7:G:118:GLU:HG2	7:G:129:LYS:O	2.11	0.51
24:Z:206:THR:OG1	24:Z:207:ASP:N	2.43	0.51
24:Z:232:GLN:HE21	24:Z:252:GLN:HB2	1.75	0.51
24:Z:454:HIS:HE2	24:Z:463:PHE:HE2	1.58	0.51
1:A:43:TYR:HB3	1:A:45:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ASP:O	1:A:697:LYS:N	2.39	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.92	0.51
13:M:1443:LEU:HD13	13:M:1473:LEU:HD22	1.92	0.51
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.45	0.51
13:M:1473:LEU:HD11	13:M:1484:ILE:HD12	1.92	0.51
14:N:34:DC:H2"	14:N:35:DA:H8	1.76	0.51
24:Z:470:LYS:HD2	24:Z:472:PHE:CZ	2.46	0.51
24:Z:745:VAL:HG11	24:Z:750:LEU:HD21	1.92	0.51
2:B:851:ASP:HB2	12:L:15:MET:HG2	1.91	0.51
2:B:997:GLY:HA2	20:V:131:MET:HG2	1.91	0.51
4:D:123:GLU:OE1	4:D:123:GLU:N	2.44	0.51
16:Q:513:PHE:HB2	21:W:213:TYR:HE1	1.75	0.51
22:X:248:ASN:OD1	22:X:249:ILE:HG13	2.10	0.51
24:Z:478:VAL:HG22	24:Z:490:GLY:O	2.11	0.51
1:A:927:GLU:HG3	1:A:943:LEU:HD11	1.92	0.51
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.11	0.51
2:B:1007:ASN:N	2:B:1007:ASN:OD1	2.42	0.51
16:Q:744:ARG:HG2	16:Q:748:PRO:HA	1.93	0.51
17:R:417:LEU:N	17:R:420:THR:O	2.40	0.51
20:V:193:HIS:H	20:V:197:PRO:HA	1.73	0.51
21:W:17:ASP:HB2	21:W:41:ASP:HB3	1.93	0.51
21:W:22:VAL:HG23	21:W:37:THR:HG22	1.92	0.51
1:A:428:ASP:OD1	1:A:430:ARG:NH1	2.44	0.51
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.50	0.51
5:E:84:ILE:HG12	5:E:114:ALA:HA	1.92	0.51
16:Q:530:TYR:HD2	16:Q:533:CYS:HB2	1.76	0.51
16:Q:682:ASP:OD1	16:Q:683:VAL:N	2.43	0.51
18:T:36:DC:C2	18:T:37:DC:C5	2.99	0.51
23:Y:45:ASN:HD21	23:Y:48:MET:HB2	1.75	0.51
24:Z:478:VAL:O	24:Z:489:THR:HG23	2.11	0.51
1:A:120:ASP:O	1:A:122:ASN:ND2	2.44	0.51
1:A:419:ILE:HD12	1:A:440:LEU:HD23	1.92	0.51
1:A:1474:LEU:HB2	6:F:105:ILE:HG12	1.93	0.51
2:B:624:PRO:HA	2:B:663:GLU:O	2.09	0.51
7:G:46:ILE:HD11	7:G:77:PHE:CB	2.40	0.51
16:Q:244:ASN:HD22	20:V:69:GLN:HA	1.76	0.51
17:R:493:GLU:O	17:R:496:VAL:HG22	2.11	0.51
21:W:110:TRP:H	21:W:123:THR:HG23	1.76	0.51
24:Z:312:ASP:O	24:Z:315:ARG:HG2	2.11	0.51
1:A:44:PRO:HG2	1:A:285:LYS:HD3	1.93	0.51
1:A:725:LEU:HD23	1:A:733:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.93	0.51
1:A:1423:ASP:OD2	1:A:1423:ASP:N	2.38	0.51
16:Q:815:ARG:O	16:Q:818:SER:OG	2.25	0.51
17:R:454:LYS:NZ	17:R:458:ALA:HB2	2.26	0.51
21:W:44:VAL:HB	21:W:60:LEU:HB2	1.93	0.51
21:W:231:HIS:ND1	21:W:251:SER:HB3	2.26	0.51
22:X:252:ILE:HG13	22:X:253:LEU:N	2.26	0.51
23:Y:40:LEU:HD21	23:Y:52:CYS:SG	2.51	0.51
1:A:410:ASN:HD22	1:A:430:ARG:HD2	1.76	0.50
1:A:1288:ILE:HA	1:A:1291:ASN:ND2	2.27	0.50
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.29	0.50
2:B:56:GLN:HG2	2:B:91:ILE:HG22	1.92	0.50
5:E:21:CYS:O	5:E:26:TYR:HB2	2.11	0.50
7:G:91:GLN:HA	7:G:139:GLN:NE2	2.26	0.50
16:Q:93:TYR:HB3	16:Q:113:ALA:HB2	1.93	0.50
17:R:564:ASN:ND2	20:V:136:TYR:C	2.64	0.50
19:U:373:LEU:HD23	19:U:375:PHE:H	1.76	0.50
21:W:159:ASP:OD2	21:W:161:LYS:HE3	2.11	0.50
21:W:295:ASP:OD2	21:W:297:GLU:HB2	2.11	0.50
24:Z:436:LEU:HB3	24:Z:454:HIS:CE1	2.45	0.50
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.93	0.50
16:Q:106:LYS:O	16:Q:110:ILE:HG12	2.12	0.50
16:Q:880:GLN:HB2	16:Q:884:LYS:HZ3	1.75	0.50
21:W:116:PRO:HD3	21:W:156:TYR:HB3	1.92	0.50
24:Z:215:VAL:HG12	24:Z:227:VAL:HG23	1.94	0.50
1:A:202:TRP:HE3	1:A:212:LYS:HB2	1.76	0.50
1:A:471:GLY:O	1:A:521:VAL:HG23	2.12	0.50
1:A:1177:TYR:CE1	1:A:1210:TRP:HB3	2.46	0.50
1:A:1302:GLU:C	1:A:1304:ILE:H	2.15	0.50
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.75	0.50
13:M:1398:LEU:HD23	13:M:1400:ILE:HG23	1.93	0.50
13:M:1494:PHE:HE2	13:M:1504:VAL:HG12	1.75	0.50
23:Y:63:MET:SD	23:Y:72:SER:HB2	2.51	0.50
1:A:140:ARG:O	1:A:144:VAL:HG13	2.11	0.50
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.76	0.50
1:A:1180:ASN:CG	1:A:1182:GLN:HE21	2.14	0.50
2:B:130:LYS:HB3	2:B:142:THR:HG23	1.94	0.50
4:D:61:PHE:O	4:D:65:LEU:HG	2.11	0.50
16:Q:38:HIS:CE1	16:Q:73:LEU:HD22	2.47	0.50
16:Q:164:PRO:HA	16:Q:167:LEU:HB2	1.93	0.50
16:Q:310:TYR:CE2	16:Q:342:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:635:ILE:O	16:Q:639:VAL:HG22	2.11	0.50
17:R:441:PHE:HA	24:Z:776:PRO:O	2.11	0.50
4:D:33:LEU:HB2	4:D:36:GLU:HB2	1.93	0.50
14:N:39:DA:C6	14:N:40:DG:C6	3.00	0.50
15:P:39:A:H2'	15:P:40:A:C8	2.47	0.50
16:Q:163:ILE:HB	16:Q:164:PRO:HD3	1.94	0.50
16:Q:841:LEU:HD23	16:Q:844:LYS:HD3	1.93	0.50
17:R:404:GLU:O	17:R:428:LEU:HA	2.11	0.50
24:Z:440:ILE:HA	24:Z:450:ILE:HD11	1.94	0.50
1:A:123:ASN:HD22	1:A:125:LYS:HD3	1.75	0.50
1:A:738:GLU:OE2	1:A:797:ARG:NH1	2.45	0.50
2:B:169:ARG:NH2	20:V:139:THR:O	2.43	0.50
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.45	0.50
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.10	0.50
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.75	0.50
5:E:47:LYS:O	5:E:53:PRO:HD2	2.11	0.50
5:E:64:HIS:HB2	5:E:70:ASP:OD1	2.12	0.50
15:P:38:G:N3	15:P:39:A:C8	2.80	0.50
18:T:37:DC:H2''	18:T:38:DG:C8	2.46	0.50
1:A:324:GLY:O	1:A:325:LEU:HD22	2.12	0.50
1:A:1147:SER:OG	1:A:1351:ASP:OD1	2.29	0.50
16:Q:166:LEU:HA	16:Q:169:LYS:NZ	2.26	0.50
16:Q:837:GLU:O	16:Q:840:GLU:HG3	2.11	0.50
17:R:414:VAL:HG22	17:R:423:ASN:HB3	1.94	0.50
1:A:651:SER:O	1:A:655:ILE:HG12	2.11	0.50
13:M:1347:MET:HB2	13:M:1372:LYS:HE3	1.94	0.50
16:Q:288:VAL:HG13	16:Q:289:GLN:HG3	1.93	0.50
24:Z:444:ASP:HB3	24:Z:448:ILE:HA	1.93	0.50
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.93	0.49
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.76	0.49
7:G:46:ILE:HD11	7:G:77:PHE:HB3	1.94	0.49
14:N:39:DA:H2'	14:N:40:DG:C8	2.47	0.49
16:Q:163:ILE:O	16:Q:166:LEU:HG	2.12	0.49
21:W:258:VAL:O	21:W:267:VAL:HG22	2.11	0.49
1:A:833:PRO:HB2	2:B:677:MET:SD	2.52	0.49
2:B:649:ASN:OD1	2:B:649:ASN:N	2.46	0.49
2:B:728:MET:SD	2:B:942:LYS:HB3	2.52	0.49
3:C:86:ARG:NH1	24:Z:716:PRO:O	2.45	0.49
4:D:133:ASP:O	4:D:137:LYS:HG2	2.12	0.49
5:E:177:ASP:O	5:E:181:ARG:HG3	2.11	0.49
16:Q:524:LEU:HD11	16:Q:537:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:735:GLU:OE1	16:Q:738:GLN:HB2	2.13	0.49
17:R:403:ALA:HB3	17:R:428:LEU:HD13	1.93	0.49
21:W:65:LEU:HG	21:W:85:ASP:HB3	1.94	0.49
22:X:233:THR:HG22	22:X:236:THR:HG23	1.94	0.49
24:Z:529:ASP:HB3	24:Z:553:LEU:HD23	1.94	0.49
1:A:290:LEU:HD13	1:A:306:ASP:CG	2.33	0.49
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.93	0.49
2:B:218:THR:HG22	2:B:236:TRP:HD1	1.77	0.49
10:J:22:LEU:HD22	17:R:563:ILE:HG21	1.94	0.49
16:Q:743:ALA:O	16:Q:746:VAL:HG22	2.12	0.49
16:Q:829:ALA:HA	16:Q:832:ARG:HD2	1.94	0.49
1:A:742:ASN:O	1:A:746:ASN:ND2	2.45	0.49
2:B:237:VAL:HG11	2:B:369:VAL:HG22	1.94	0.49
20:V:126:LYS:HE3	20:V:126:LYS:HA	1.94	0.49
24:Z:470:LYS:HB3	24:Z:472:PHE:HE2	1.78	0.49
24:Z:588:ASP:HB3	24:Z:594:ILE:HG13	1.95	0.49
24:Z:735:GLU:HG3	24:Z:735:GLU:O	2.13	0.49
1:A:316:THR:HA	1:A:319:ASP:O	2.11	0.49
1:A:428:ASP:OD1	1:A:430:ARG:HG3	2.11	0.49
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.47	0.49
1:A:1295:ASP:OD2	1:A:1295:ASP:N	2.46	0.49
4:D:44:ARG:HA	4:D:47:GLN:OE1	2.12	0.49
16:Q:183:LEU:O	16:Q:187:LYS:HG2	2.13	0.49
17:R:363:ARG:HE	17:R:446:GLU:HG2	1.78	0.49
17:R:410:GLU:HA	17:R:424:LYS:HA	1.93	0.49
17:R:416:GLN:HE21	17:R:421:ARG:CZ	2.26	0.49
17:R:471:GLU:O	17:R:474:LYS:HG3	2.13	0.49
2:B:537:GLN:HG3	2:B:538:PRO:HD2	1.93	0.49
2:B:626:LEU:HD13	2:B:698:ILE:HG12	1.94	0.49
14:N:35:DA:H2''	14:N:36:DG:H8	1.75	0.49
16:Q:68:ARG:NE	16:Q:89:LEU:HD12	2.27	0.49
19:U:443:TRP:HE1	19:U:449:SER:HG	1.58	0.49
21:W:228:LEU:HD11	21:W:259:TRP:CZ3	2.48	0.49
1:A:587:THR:HG22	1:A:588:GLY:N	2.27	0.49
7:G:151:ARG:HG3	24:Z:477:HIS:NE2	2.26	0.49
13:M:1374:SER:HB2	13:M:1377:ILE:HD13	1.93	0.49
13:M:1485:GLU:OE1	13:M:1497:ARG:NE	2.34	0.49
16:Q:750:ASP:HB3	16:Q:753:LEU:HG	1.93	0.49
21:W:108:ASP:HB3	21:W:125:THR:HG23	1.95	0.49
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.43	0.49
2:B:130:LYS:NZ	2:B:429:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.48	0.49
7:G:110:ARG:HD2	7:G:113:ILE:HB	1.95	0.49
12:L:16:ILE:HG13	12:L:26:ASN:O	2.13	0.49
17:R:416:GLN:HG2	17:R:421:ARG:HB3	1.95	0.49
19:U:453:GLY:HA2	20:V:185:ASP:OD2	2.12	0.49
22:X:242:GLY:O	22:X:243:LYS:HE2	2.13	0.49
24:Z:257:ILE:O	24:Z:260:MET:HG2	2.13	0.49
1:A:54:LEU:O	1:A:61:ARG:NH2	2.45	0.49
1:A:496:PHE:HB2	2:B:791:GLU:O	2.12	0.49
1:A:963:ARG:O	1:A:967:ARG:HG3	2.13	0.49
1:A:1000:LEU:O	1:A:1059:ARG:NH1	2.45	0.49
2:B:22:TRP:CZ2	2:B:679:PRO:HG3	2.48	0.49
2:B:824:ASP:O	2:B:872:THR:HG23	2.13	0.49
13:M:783:GLY:N	13:M:797:ALA:O	2.46	0.49
17:R:358:GLU:HA	17:R:361:ARG:NE	2.27	0.49
17:R:389:ILE:O	17:R:400:TYR:HD1	1.95	0.49
24:Z:199:LYS:HG2	24:Z:210:LEU:HD21	1.93	0.49
24:Z:426:VAL:HG21	24:Z:468:LEU:HD13	1.95	0.49
1:A:926:ASN:O	1:A:930:LEU:HG	2.13	0.49
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.63	0.49
2:B:792:ASP:CG	2:B:975:ARG:HH22	2.16	0.49
14:N:37:DG:N2	18:T:12:DC:C2	2.77	0.49
16:Q:128:GLN:HA	16:Q:158:GLN:NE2	2.26	0.49
16:Q:129:ASN:OD1	16:Q:132:LEU:HD13	2.12	0.49
17:R:416:GLN:HA	17:R:421:ARG:HA	1.94	0.49
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	1.95	0.48
2:B:431:LEU:HD23	2:B:431:LEU:H	1.77	0.48
2:B:679:PRO:HG2	2:B:680:ASP:H	1.78	0.48
2:B:816:GLU:OE2	2:B:869:LYS:HE3	2.13	0.48
2:B:1120:ASN:HD22	2:B:1145:GLN:HB3	1.77	0.48
4:D:108:ALA:N	4:D:128:GLN:OE1	2.46	0.48
16:Q:764:LEU:HD22	16:Q:785:GLU:OE1	2.12	0.48
17:R:563:ILE:O	17:R:566:ARG:HG2	2.13	0.48
21:W:35:VAL:O	21:W:47:TRP:N	2.44	0.48
21:W:231:HIS:ND1	21:W:235:VAL:HG22	2.26	0.48
1:A:84:HIS:H	1:A:84:HIS:CD2	2.31	0.48
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.28	0.48
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.95	0.48
2:B:92:TYR:HD1	19:U:506:ALA:HB3	1.79	0.48
2:B:420:GLN:C	2:B:422:PHE:H	2.17	0.48
2:B:910:THR:OG1	2:B:911:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:THR:HG23	7:G:99:THR:HA	1.95	0.48
8:H:11:ASP:OD1	8:H:11:ASP:N	2.46	0.48
8:H:36:LYS:CE	16:Q:709:ARG:HH12	2.26	0.48
9:I:96:PHE:HA	9:I:111:TYR:O	2.13	0.48
16:Q:663:PHE:HB3	16:Q:690:ILE:HG23	1.95	0.48
21:W:204:LEU:HD22	21:W:216:ILE:HG22	1.95	0.48
23:Y:33:CYS:SG	23:Y:36:CYS:N	2.85	0.48
1:A:1359:SER:O	1:A:1359:SER:OG	2.16	0.48
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.14	0.48
8:H:13:LYS:HG3	8:H:31:GLU:HG2	1.95	0.48
14:N:4:DT:OP2	14:N:4:DT:H71	2.13	0.48
16:Q:188:LYS:HB3	16:Q:191:ARG:NH1	2.29	0.48
16:Q:236:VAL:O	16:Q:240:VAL:HG23	2.13	0.48
16:Q:454:LEU:HB3	16:Q:477:SER:OG	2.13	0.48
16:Q:855:LYS:O	16:Q:858:LYS:HG3	2.13	0.48
23:Y:56:SER:HA	24:Z:271:ALA:HA	1.96	0.48
24:Z:436:LEU:HD13	24:Z:454:HIS:CD2	2.49	0.48
24:Z:746:ASP:OD1	24:Z:747:ARG:N	2.46	0.48
2:B:299:GLU:HA	2:B:302:LYS:HD3	1.95	0.48
3:C:74:THR:HG23	3:C:128:ILE:O	2.14	0.48
5:E:114:ALA:O	5:E:117:SER:OG	2.23	0.48
16:Q:80:LYS:O	16:Q:84:THR:HG23	2.13	0.48
16:Q:268:ASN:HB3	16:Q:271:VAL:HG12	1.95	0.48
16:Q:854:GLN:HB2	16:Q:855:LYS:NZ	2.28	0.48
19:U:522:THR:O	19:U:524:LYS:N	2.46	0.48
20:V:97:ASN:ND2	20:V:98:VAL:O	2.46	0.48
21:W:89:ARG:HA	21:W:101:SER:HA	1.94	0.48
1:A:111:CYS:SG	1:A:114:CYS:HB2	2.54	0.48
1:A:330:GLN:C	1:A:332:SER:H	2.17	0.48
1:A:733:LEU:HB2	9:I:106:ASP:HB2	1.96	0.48
17:R:576:GLU:O	17:R:580:VAL:HG13	2.14	0.48
24:Z:548:GLY:CA	24:Z:562:ASN:HA	2.44	0.48
24:Z:615:ARG:HB2	24:Z:616:HIS:CD2	2.49	0.48
4:D:76:ASN:O	4:D:79:THR:OG1	2.31	0.48
7:G:49:THR:OG1	7:G:50:THR:N	2.47	0.48
15:P:40:A:C2	18:T:32:DT:N3	2.81	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:NZ	2.29	0.48
24:Z:342:ALA:HB1	24:Z:346:ARG:NH2	2.28	0.48
1:A:86:GLY:C	1:A:255:VAL:HG12	2.34	0.48
1:A:606:HIS:CG	1:A:607:SER:N	2.82	0.48
1:A:922:PHE:N	1:A:1052:ARG:HD2	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:THR:HG23	1:A:1214:VAL:HG22	1.94	0.48
1:A:1218:ARG:HH22	1:A:1253:GLU:HA	1.77	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:HE3	1.94	0.48
16:Q:346:GLY:HA2	16:Q:349:GLN:HE21	1.79	0.48
16:Q:423:GLU:OE1	22:X:231:TRP:NE1	2.43	0.48
16:Q:568:TRP:CE2	16:Q:592:LEU:HD13	2.49	0.48
17:R:366:ARG:HH22	24:Z:773:SER:H	1.62	0.48
18:T:7:DA:H2"	18:T:8:DG:C8	2.48	0.48
21:W:76:LEU:HG	21:W:78:ILE:HG23	1.95	0.48
21:W:130:VAL:HG22	21:W:151:ILE:HG13	1.95	0.48
24:Z:206:THR:HG23	24:Z:208:THR:H	1.79	0.48
2:B:425:ARG:HH21	2:B:427:LYS:HD3	1.78	0.48
16:Q:542:ARG:NH2	16:Q:574:LEU:HA	2.28	0.48
17:R:359:LEU:HD22	17:R:452:PHE:CE1	2.48	0.48
17:R:370:GLU:HA	17:R:373:CYS:SG	2.54	0.48
21:W:46:VAL:HG11	21:W:58:TRP:HD1	1.78	0.48
21:W:89:ARG:HG2	21:W:101:SER:OG	2.13	0.48
21:W:110:TRP:CD2	21:W:150:PHE:HZ	2.32	0.48
24:Z:310:ARG:CZ	24:Z:337:GLN:HB2	2.44	0.48
24:Z:366:TYR:HB2	24:Z:374:LYS:HA	1.95	0.48
1:A:104:MET:CE	1:A:193:ARG:HD2	2.44	0.48
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.48
1:A:1129:ASN:O	1:A:1131:SER:N	2.47	0.48
1:A:1263:ASN:N	1:A:1263:ASN:OD1	2.47	0.48
2:B:355:ASP:OD2	2:B:356:PHE:N	2.46	0.48
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.48
14:N:12:DG:C4	14:N:13:DG:C8	3.02	0.48
16:Q:153:HIS:HA	16:Q:169:LYS:HE3	1.96	0.48
16:Q:568:TRP:CZ2	16:Q:591:ILE:HB	2.48	0.48
16:Q:645:LYS:HD2	22:X:242:GLY:O	2.14	0.48
16:Q:835:ASP:O	16:Q:839:ARG:HG3	2.14	0.48
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.96	0.48
1:A:557:ARG:O	1:A:561:MET:HG3	2.14	0.48
1:A:1162:GLU:HG2	1:A:1163:HIS:N	2.29	0.48
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.95	0.48
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.49	0.48
7:G:38:CYS:SG	7:G:39:THR:N	2.87	0.48
7:G:82:GLY:N	7:G:147:ILE:O	2.34	0.48
7:G:101:ILE:N	7:G:104:MET:O	2.43	0.48
8:H:15:ILE:O	8:H:16:ASP:C	2.51	0.48
8:H:106:THR:OG1	8:H:107:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:232:VAL:O	16:Q:236:VAL:HG22	2.13	0.48
16:Q:390:ASP:HB2	16:Q:392:GLU:OE1	2.14	0.48
16:Q:578:LYS:HB2	16:Q:580:GLU:HG3	1.94	0.48
16:Q:682:ASP:OD1	16:Q:683:VAL:HG13	2.14	0.48
16:Q:844:LYS:O	16:Q:848:GLU:HG3	2.14	0.48
17:R:359:LEU:HD11	17:R:386:PHE:CE2	2.49	0.48
19:U:443:TRP:HA	20:V:201:PRO:HA	1.95	0.48
21:W:237:ASN:ND2	21:W:279:GLY:HA2	2.21	0.48
21:W:248:VAL:HG13	21:W:282:TYR:OH	2.14	0.48
21:W:254:LYS:HB3	21:W:273:HIS:O	2.14	0.48
24:Z:426:VAL:HG13	24:Z:440:ILE:HD11	1.95	0.48
1:A:495:ASP:HB3	1:A:499:ASP:OD2	2.14	0.47
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.95	0.47
1:A:1245:CYS:O	1:A:1246:ILE:HD13	2.13	0.47
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.14	0.47
3:C:92:GLU:HG2	24:Z:711:ARG:CZ	2.43	0.47
16:Q:39:THR:OG1	16:Q:43:ILE:HD13	2.14	0.47
16:Q:576:LEU:CD2	16:Q:585:GLN:HE22	2.27	0.47
16:Q:850:GLU:O	16:Q:854:GLN:NE2	2.44	0.47
17:R:363:ARG:HA	17:R:386:PHE:O	2.14	0.47
17:R:485:TYR:OH	17:R:489:ASP:OD2	2.32	0.47
1:A:141:LEU:HB2	1:A:236:LEU:O	2.14	0.47
2:B:108:MET:HE2	2:B:113:ALA:HB2	1.96	0.47
2:B:166:LEU:HG	2:B:170:ASP:HB2	1.96	0.47
2:B:320:PHE:O	2:B:323:SER:OG	2.31	0.47
2:B:719:SER:OG	2:B:720:PRO:HD3	2.13	0.47
2:B:768:ARG:HG3	2:B:771:GLU:OE2	2.15	0.47
7:G:109:SER:HB2	24:Z:503:PHE:CE2	2.48	0.47
16:Q:128:GLN:NE2	20:V:86:LEU:HD13	2.26	0.47
16:Q:336:ALA:HB1	16:Q:339:SER:OG	2.14	0.47
16:Q:358:GLU:O	16:Q:361:SER:OG	2.32	0.47
16:Q:689:HIS:HA	16:Q:692:VAL:HG12	1.96	0.47
16:Q:753:LEU:O	16:Q:757:VAL:HG13	2.14	0.47
1:A:46:THR:HB	1:A:58:MET:HB2	1.96	0.47
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.95	0.47
1:A:1177:TYR:HD2	9:I:28:GLU:OE1	1.97	0.47
2:B:44:LEU:HD23	2:B:155:MET:CE	2.44	0.47
5:E:2:ASP:OD2	5:E:3:ASP:N	2.47	0.47
10:J:64:PRO:HG2	10:J:65:LEU:H	1.78	0.47
21:W:191:MET:HB2	21:W:209:SER:HB3	1.96	0.47
1:A:10:ASP:O	2:B:1130:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.97	0.47
1:A:514:GLU:OE1	2:B:1101:GLN:HB2	2.14	0.47
1:A:527:THR:HG22	1:A:532:ARG:O	2.14	0.47
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.79	0.47
1:A:1060:LEU:HA	1:A:1060:LEU:HD23	1.60	0.47
1:A:1083:PRO:HD2	6:F:58:THR:HG21	1.96	0.47
3:C:2:PRO:HB3	11:K:54:PRO:CD	2.44	0.47
5:E:78:GLU:OE1	5:E:78:GLU:N	2.48	0.47
8:H:45:ILE:HA	8:H:45:ILE:HD12	1.68	0.47
16:Q:143:ASP:N	16:Q:143:ASP:OD1	2.44	0.47
21:W:112:LEU:HB3	21:W:121:LEU:HD11	1.96	0.47
24:Z:626:CYS:HB3	24:Z:629:LEU:HD12	1.95	0.47
2:B:313:GLU:HG2	2:B:316:VAL:HG12	1.95	0.47
2:B:680:ASP:O	2:B:684:GLU:HG2	2.14	0.47
4:D:93:HIS:HB3	4:D:96:GLU:OE1	2.14	0.47
7:G:4:HIS:CG	7:G:73:LYS:HE3	2.50	0.47
16:Q:172:ILE:HG22	16:Q:176:LYS:HZ1	1.79	0.47
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.47
17:R:363:ARG:HG3	17:R:447:PHE:CZ	2.49	0.47
17:R:587:LYS:O	17:R:588:ASN:ND2	2.48	0.47
1:A:199:TYR:CE2	1:A:215:LEU:HD13	2.49	0.47
7:G:119:PHE:HA	7:G:128:TYR:CD1	2.49	0.47
15:P:39:A:H2'	15:P:39:A:N3	2.29	0.47
16:Q:68:ARG:HE	16:Q:86:LEU:HD13	1.80	0.47
1:A:70:ARG:HD2	2:B:1131:ARG:HH12	1.79	0.47
1:A:416:ALA:HA	1:A:448:ARG:HA	1.97	0.47
1:A:513:ALA:O	1:A:517:GLU:HG2	2.14	0.47
1:A:1027:ASP:HB3	1:A:1030:SER:HB3	1.96	0.47
1:A:1177:TYR:CD2	9:I:28:GLU:OE1	2.68	0.47
2:B:170:ASP:N	2:B:170:ASP:OD1	2.43	0.47
2:B:1007:ASN:O	2:B:1011:ILE:HG13	2.14	0.47
14:N:12:DG:C6	14:N:13:DG:C6	3.02	0.47
16:Q:76:ARG:HH11	16:Q:76:ARG:HG3	1.80	0.47
16:Q:366:LYS:HG3	16:Q:369:LYS:HZ3	1.79	0.47
16:Q:721:LEU:HD11	20:V:31:CYS:HA	1.97	0.47
16:Q:737:LYS:HE3	16:Q:760:VAL:HG22	1.96	0.47
21:W:11:GLN:HB3	21:W:298:ILE:HB	1.97	0.47
24:Z:479:LYS:HD3	24:Z:521:CYS:HB2	1.96	0.47
1:A:724:GLU:OE1	1:A:724:GLU:N	2.47	0.47
1:A:951:GLU:HG2	1:A:1007:ILE:HD11	1.97	0.47
1:A:1236:ASN:O	1:A:1240:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.14	0.47
2:B:255:ARG:CD	2:B:307:GLU:HG3	2.44	0.47
2:B:347:MET:HG3	2:B:347:MET:O	2.15	0.47
4:D:62:MET:O	4:D:66:ASN:ND2	2.47	0.47
16:Q:167:LEU:HD21	16:Q:189:ALA:HB2	1.96	0.47
16:Q:373:ASN:HB2	16:Q:376:GLU:HG2	1.96	0.47
16:Q:750:ASP:OD1	16:Q:752:VAL:N	2.48	0.47
19:U:394:TYR:C	20:V:172:ARG:HH21	2.18	0.47
1:A:621:ILE:HG23	1:A:621:ILE:O	2.14	0.47
1:A:831:LEU:HB3	1:A:835:GLU:HG3	1.97	0.47
2:B:84:TYR:HA	2:B:132:VAL:HA	1.97	0.47
4:D:79:THR:O	4:D:82:SER:OG	2.33	0.47
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.96	0.47
15:P:38:G:C2'	15:P:39:A:H8	2.24	0.47
16:Q:347:LEU:HB2	16:Q:363:CYS:SG	2.54	0.47
16:Q:411:ASP:HB3	16:Q:415:TRP:CZ3	2.50	0.47
16:Q:624:LYS:HA	16:Q:627:ARG:HE	1.79	0.47
16:Q:712:TYR:O	16:Q:713:LYS:HG3	2.15	0.47
16:Q:833:LYS:O	16:Q:836:GLU:HG3	2.15	0.47
17:R:573:VAL:O	17:R:576:GLU:HG3	2.15	0.47
21:W:5:TYR:CE1	21:W:303:CYS:HB3	2.50	0.47
24:Z:433:LEU:HD13	24:Z:461:LEU:HD13	1.96	0.47
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.97	0.47
2:B:690:CYS:SG	2:B:693:TYR:CZ	3.08	0.47
2:B:1136:GLU:CB	2:B:1143:LYS:HG2	2.44	0.47
7:G:113:ILE:HG22	7:G:114:PRO:O	2.15	0.47
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.97	0.47
9:I:84:HIS:CD2	9:I:125:GLU:OE1	2.68	0.47
16:Q:7:GLU:OE2	16:Q:18:GLU:HB3	2.14	0.47
16:Q:716:ASN:HB3	16:Q:719:VAL:HG22	1.96	0.47
20:V:96:PRO:HA	20:V:97:ASN:HA	1.57	0.47
24:Z:521:CYS:HB3	24:Z:523:GLU:OE1	2.15	0.47
1:A:71:CYS:HB3	1:A:74:CYS:O	2.15	0.46
1:A:239:GLU:HG3	1:A:240:PRO:HD2	1.96	0.46
1:A:1184:THR:C	1:A:1186:VAL:N	2.64	0.46
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
5:E:3:ASP:OD1	5:E:47:LYS:HD2	2.15	0.46
5:E:82:VAL:HG12	5:E:110:MET:CB	2.45	0.46
8:H:112:LEU:HA	8:H:112:LEU:HD23	1.59	0.46
12:L:16:ILE:HD12	12:L:27:GLU:OE2	2.16	0.46
13:M:848:VAL:O	13:M:883:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:DT:H2''	14:N:43:DG:C8	2.51	0.46
21:W:215:LYS:HG2	21:W:227:THR:HG22	1.97	0.46
23:Y:22:VAL:HB	23:Y:84:VAL:HG12	1.97	0.46
24:Z:547:VAL:HG12	24:Z:563:MET:SD	2.54	0.46
1:A:866:LYS:HG3	1:A:1432:PHE:CD1	2.49	0.46
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.15	0.46
2:B:425:ARG:NH2	2:B:427:LYS:HD3	2.30	0.46
4:D:48:ASN:HB3	4:D:57:LEU:HD11	1.97	0.46
7:G:5:ILE:O	7:G:73:LYS:HD2	2.15	0.46
13:M:1362:LYS:HD3	13:M:1363:GLY:N	2.31	0.46
16:Q:211:LEU:HB2	16:Q:213:LYS:HZ2	1.80	0.46
16:Q:380:ILE:HB	16:Q:400:HIS:CE1	2.50	0.46
24:Z:571:ARG:H	24:Z:574:ALA:HB3	1.80	0.46
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	1.97	0.46
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.61	0.46
11:K:7:PHE:CD2	11:K:11:LEU:HD12	2.50	0.46
13:M:1447:LEU:HA	13:M:1450:THR:HG22	1.97	0.46
15:P:43:C:H2'	15:P:44:A:O4'	2.16	0.46
16:Q:30:VAL:HA	16:Q:33:ILE:HG12	1.96	0.46
16:Q:830:ARG:HH21	16:Q:834:GLN:HG3	1.79	0.46
17:R:562:TYR:HB3	17:R:566:ARG:HH21	1.80	0.46
24:Z:340:PHE:HD2	24:Z:370:GLY:HA2	1.81	0.46
1:A:93:PRO:HG2	1:A:219:GLU:OE2	2.15	0.46
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.96	0.46
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.97	0.46
2:B:285:LEU:HD23	9:I:16:PHE:CZ	2.51	0.46
2:B:329:GLY:HA3	2:B:334:LYS:HB3	1.97	0.46
3:C:78:ILE:H	3:C:78:ILE:HG12	1.48	0.46
5:E:63:ALA:HB3	16:Q:880:GLN:HE22	1.80	0.46
5:E:153:LYS:O	5:E:157:THR:HG23	2.14	0.46
7:G:82:GLY:HA2	7:G:146:LYS:HE3	1.96	0.46
9:I:29:ASP:CB	9:I:34:ILE:HG13	2.45	0.46
16:Q:637:LYS:O	16:Q:641:ARG:HD3	2.15	0.46
21:W:151:ILE:HG23	21:W:165:SER:OG	2.15	0.46
1:A:1176:TYR:HD1	9:I:51:SER:O	1.99	0.46
1:A:1177:TYR:CE2	1:A:1210:TRP:HE3	2.34	0.46
1:A:1416:ARG:HD2	1:A:1434:GLU:OE2	2.15	0.46
2:B:566:LYS:HA	2:B:576:ILE:HD12	1.97	0.46
2:B:646:ARG:O	2:B:647:GLU:HG2	2.16	0.46
16:Q:386:ALA:HB1	16:Q:394:ARG:HG3	1.97	0.46
16:Q:452:GLU:OE1	16:Q:490:HIS:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:527:HIS:CE1	22:X:220:VAL:HB	2.51	0.46
16:Q:834:GLN:O	16:Q:838:GLU:HG2	2.15	0.46
1:A:609:HIS:HA	1:A:626:THR:HG21	1.98	0.46
1:A:1150:ASP:OD1	1:A:1150:ASP:N	2.48	0.46
1:A:1305:SER:OG	1:A:1306:LYS:N	2.48	0.46
2:B:26:CYS:O	2:B:30:ILE:HG12	2.15	0.46
8:H:67:ASP:OD1	8:H:67:ASP:N	2.46	0.46
9:I:17:CYS:SG	9:I:18:GLN:N	2.89	0.46
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.16	0.46
10:J:26:GLN:HA	17:R:566:ARG:HD2	1.98	0.46
16:Q:41:LEU:HD13	16:Q:75:TYR:HE2	1.81	0.46
16:Q:460:LEU:O	16:Q:464:LEU:HG	2.14	0.46
16:Q:855:LYS:HD3	16:Q:855:LYS:HA	1.59	0.46
17:R:574:GLU:HA	17:R:577:LYS:NZ	2.31	0.46
19:U:443:TRP:NE1	19:U:449:SER:OG	2.47	0.46
21:W:152:LEU:N	21:W:166:GLY:O	2.34	0.46
21:W:252:SER:HA	21:W:276:GLN:HB3	1.98	0.46
24:Z:182:VAL:O	24:Z:224:TYR:HB2	2.14	0.46
1:A:123:ASN:HB3	1:A:125:LYS:HG2	1.98	0.46
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.78	0.46
2:B:133:ILE:HD12	2:B:139:GLN:HB3	1.98	0.46
2:B:548:TRP:CZ2	2:B:586:THR:HG21	2.51	0.46
7:G:111:HIS:ND1	24:Z:494:ARG:HB3	2.31	0.46
8:H:30:CYS:SG	8:H:56:PHE:HZ	2.39	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.16	0.46
16:Q:566:ASP:OD1	22:X:234:ARG:HD3	2.16	0.46
18:T:30:DG:H2'	18:T:31:DT:C6	2.50	0.46
19:U:469:ASN:HA	20:V:222:ARG:HA	1.98	0.46
21:W:46:VAL:CB	21:W:58:TRP:HB2	2.45	0.46
21:W:182:LEU:HD21	21:W:185:THR:OG1	2.16	0.46
21:W:233:SER:HB3	21:W:253:ASP:HB3	1.98	0.46
24:Z:571:ARG:HB2	24:Z:574:ALA:HB2	1.98	0.46
1:A:732:THR:HG23	1:A:735:GLN:OE1	2.14	0.46
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.56	0.46
1:A:1176:TYR:C	1:A:1177:TYR:HD1	2.19	0.46
16:Q:386:ALA:HB2	16:Q:393:LYS:CB	2.46	0.46
16:Q:563:ASP:O	16:Q:565:PRO:HD3	2.15	0.46
16:Q:803:MET:HE1	16:Q:807:LEU:HD11	1.98	0.46
24:Z:182:VAL:HG23	24:Z:225:ILE:HG13	1.98	0.46
24:Z:239:ILE:O	24:Z:242:VAL:HG22	2.15	0.46
24:Z:539:LEU:O	24:Z:578:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:CZ	1:A:220:ARG:NH1	2.84	0.46
5:E:126:ILE:H	5:E:126:ILE:HD12	1.81	0.46
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.98	0.46
8:H:143:LEU:HD12	8:H:143:LEU:HA	1.62	0.46
10:J:25:LEU:HD23	17:R:567:ASN:HD21	1.81	0.46
16:Q:265:ASP:OD1	16:Q:268:ASN:HB2	2.16	0.46
16:Q:289:GLN:O	16:Q:293:LEU:HD23	2.16	0.46
16:Q:872:LYS:O	16:Q:875:LEU:HG	2.16	0.46
18:T:37:DC:H6	18:T:37:DC:H5'	1.81	0.46
18:T:41:DC:H4'	24:Z:283:ARG:NE	2.21	0.46
20:V:88:ASN:O	20:V:90:ASP:N	2.49	0.46
21:W:86:ALA:HB1	21:W:105:GLY:HA2	1.97	0.46
24:Z:705:LEU:HD21	24:Z:747:ARG:HD2	1.96	0.46
1:A:37:THR:O	1:A:37:THR:OG1	2.30	0.46
1:A:117:LEU:HD21	1:A:232:GLU:HG3	1.98	0.46
1:A:347:GLU:HA	1:A:352:GLY:HA3	1.98	0.46
1:A:753:GLY:O	1:A:757:GLN:HG2	2.16	0.46
1:A:1379:GLU:O	1:A:1379:GLU:HG2	2.16	0.46
3:C:60:HIS:HB3	3:C:61:ASP:H	1.33	0.46
16:Q:208:PHE:CD1	16:Q:213:LYS:HD2	2.51	0.46
16:Q:450:PRO:HB2	16:Q:452:GLU:HG2	1.98	0.46
19:U:378:LEU:HD23	19:U:382:LEU:O	2.16	0.46
24:Z:280:ARG:HG3	24:Z:386:VAL:HG13	1.98	0.46
24:Z:294:ASP:HB2	24:Z:306:LYS:HE2	1.98	0.46
24:Z:480:VAL:HG13	24:Z:487:GLY:H	1.81	0.46
1:A:465:HIS:HB3	1:A:1097:GLU:HG3	1.97	0.45
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.74	0.45
1:A:971:PRO:O	1:A:972:THR:OG1	2.26	0.45
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.97	0.45
2:B:236:TRP:HB2	2:B:259:THR:HB	1.98	0.45
2:B:684:GLU:OE2	2:B:684:GLU:HA	2.16	0.45
12:L:52:LEU:HA	12:L:52:LEU:HD12	1.69	0.45
16:Q:620:ARG:NH1	16:Q:659:HIS:O	2.47	0.45
17:R:429:ARG:NE	17:R:431:GLY:O	2.42	0.45
21:W:13:GLN:H	21:W:297:GLU:HG2	1.80	0.45
22:X:253:LEU:O	22:X:256:VAL:HG12	2.16	0.45
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.99	0.45
1:A:124:PRO:HA	1:A:127:LYS:CG	2.45	0.45
1:A:1254:LYS:HD3	1:A:1254:LYS:HA	1.77	0.45
1:A:1298:LEU:HA	1:A:1298:LEU:HD23	1.77	0.45
2:B:121:SER:HA	2:B:153:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ARG:HD3	2:B:307:GLU:HG3	1.98	0.45
2:B:621:ILE:HD13	2:B:621:ILE:HG21	1.66	0.45
2:B:1006:VAL:HG22	20:V:130:TRP:CB	2.45	0.45
4:D:38:HIS:HB2	4:D:68:THR:OG1	2.16	0.45
11:K:71:ILE:HG21	11:K:71:ILE:HD13	1.61	0.45
16:Q:64:LEU:HA	16:Q:64:LEU:HD23	1.82	0.45
17:R:565:GLN:HA	17:R:568:ARG:CZ	2.47	0.45
20:V:38:SER:OG	20:V:39:LEU:N	2.49	0.45
21:W:7:ILE:HA	21:W:301:TYR:HA	1.98	0.45
21:W:233:SER:OG	21:W:252:SER:N	2.44	0.45
23:Y:35:ASN:ND2	23:Y:85:TYR:OH	2.49	0.45
24:Z:470:LYS:HB3	24:Z:472:PHE:CE2	2.51	0.45
1:A:189:PRO:HB2	1:A:201:GLU:H	1.81	0.45
1:A:989:ASN:O	1:A:993:ILE:HG13	2.16	0.45
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.99	0.45
2:B:317:ALA:O	2:B:321:ILE:HD12	2.15	0.45
2:B:681:ASP:OD2	2:B:681:ASP:N	2.50	0.45
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.62	0.45
14:N:12:DG:C4	14:N:13:DG:N7	2.84	0.45
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.17	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.99	0.45
3:C:92:GLU:HG2	24:Z:711:ARG:NH1	2.32	0.45
8:H:70:LEU:HD12	8:H:70:LEU:HA	1.76	0.45
9:I:73:SER:O	9:I:80:ARG:NH2	2.50	0.45
9:I:74:GLN:H	9:I:74:GLN:HG2	1.51	0.45
9:I:91:HIS:CD2	9:I:93:GLU:H	2.35	0.45
16:Q:474:PHE:CB	16:Q:503:LEU:HD13	2.46	0.45
16:Q:591:ILE:HG22	16:Q:592:LEU:HD12	1.97	0.45
23:Y:116:LYS:HD3	23:Y:116:LYS:HA	1.74	0.45
24:Z:469:ARG:NH2	24:Z:497:GLU:O	2.49	0.45
1:A:775:LYS:HD2	2:B:974:SER:HB3	1.97	0.45
2:B:332:LYS:HB3	2:B:332:LYS:HE3	1.57	0.45
2:B:388:TYR:HB2	2:B:504:THR:HG23	1.99	0.45
2:B:395:LEU:HA	2:B:395:LEU:HD23	1.67	0.45
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.48	0.45
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.50	0.45
21:W:235:VAL:HA	21:W:251:SER:HA	1.98	0.45
23:Y:66:PRO:HD3	23:Y:82:PRO:HG3	1.98	0.45
2:B:834:ARG:HH22	2:B:842:HIS:HA	1.80	0.45
14:N:12:DG:N1	18:T:38:DG:N2	2.64	0.45
16:Q:246:LYS:HD2	16:Q:246:LYS:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:620:ARG:HH22	16:Q:660:LYS:HA	1.81	0.45
17:R:388:ARG:HD3	17:R:445:GLN:HB2	1.99	0.45
17:R:570:TRP:CD1	20:V:133:LYS:HD2	2.43	0.45
20:V:103:ALA:O	20:V:107:LEU:HG	2.17	0.45
21:W:29:LYS:HE2	21:W:75:THR:HA	1.99	0.45
22:X:222:ARG:HA	22:X:225:VAL:HG22	1.97	0.45
23:Y:65:SER:O	23:Y:65:SER:OG	2.33	0.45
1:A:111:CYS:HG	1:A:114:CYS:HB2	1.81	0.45
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.47	0.45
1:A:1369:LEU:HD23	1:A:1369:LEU:HA	1.73	0.45
2:B:1134:THR:HG23	2:B:1134:THR:O	2.17	0.45
4:D:74:PHE:CE2	4:D:80:ILE:HG12	2.52	0.45
16:Q:763:ARG:HE	20:V:25:GLU:N	2.14	0.45
17:R:566:ARG:HA	17:R:569:GLU:OE1	2.16	0.45
21:W:56:LEU:HD21	21:W:59:SER:OG	2.16	0.45
24:Z:546:THR:HG22	24:Z:547:VAL:N	2.32	0.45
1:A:291:ARG:HG3	1:A:292:ARG:N	2.32	0.45
1:A:1226:LEU:HA	1:A:1230:GLN:NE2	2.31	0.45
2:B:357:CYS:SG	2:B:360:LYS:NZ	2.85	0.45
2:B:651:TYR:N	19:U:460:TYR:OH	2.49	0.45
2:B:714:PRO:CD	2:B:1001:PRO:HG3	2.47	0.45
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.16	0.45
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.98	0.45
4:D:32:LEU:HD23	4:D:32:LEU:HA	1.83	0.45
12:L:22:CYS:SG	12:L:39:CYS:SG	3.06	0.45
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.90	0.45
16:Q:123:ILE:HG23	16:Q:124:ILE:H	1.82	0.45
16:Q:134:ARG:HA	16:Q:134:ARG:HD2	1.76	0.45
16:Q:170:ALA:HB2	16:Q:185:TYR:HB2	1.99	0.45
17:R:402:VAL:HG23	17:R:451:GLU:HG2	1.98	0.45
20:V:190:ILE:O	20:V:190:ILE:HG13	2.17	0.45
21:W:64:GLN:OE1	21:W:89:ARG:NH2	2.48	0.45
24:Z:243:GLY:O	24:Z:246:ARG:HG2	2.17	0.45
2:B:319:ASN:HD21	2:B:332:LYS:HG2	1.82	0.45
8:H:64:LEU:HD23	8:H:64:LEU:HA	1.79	0.45
16:Q:386:ALA:HB2	16:Q:393:LYS:HB3	1.99	0.45
17:R:356:PRO:HB3	17:R:452:PHE:CB	2.47	0.45
1:A:557:ARG:HG3	1:A:558:GLY:N	2.27	0.45
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.45
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.98	0.45
16:Q:95:GLN:HG3	20:V:85:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:131:LEU:HD12	16:Q:155:VAL:HG22	1.98	0.45
16:Q:133:GLY:HA2	16:Q:136:CYS:SG	2.57	0.45
16:Q:200:VAL:HA	20:V:82:VAL:HG22	1.97	0.45
16:Q:380:ILE:HG21	16:Q:396:ILE:HD12	1.98	0.45
16:Q:568:TRP:CE3	16:Q:592:LEU:HB2	2.51	0.45
16:Q:736:CYS:O	16:Q:739:THR:HG22	2.17	0.45
23:Y:8:LYS:HE2	23:Y:27:GLN:NE2	2.32	0.45
24:Z:272:ASN:ND2	24:Z:384:GLU:HB2	2.32	0.45
24:Z:729:GLU:O	24:Z:747:ARG:NH2	2.50	0.45
1:A:74:CYS:SG	1:A:81:CYS:HB2	2.56	0.44
1:A:902:GLU:O	1:A:978:VAL:HA	2.17	0.44
1:A:1040:LEU:HA	1:A:1040:LEU:HD12	1.75	0.44
1:A:1118:THR:HG21	1:A:1135:LYS:HB2	1.99	0.44
1:A:1184:THR:O	1:A:1184:THR:OG1	2.28	0.44
2:B:655:ASP:O	2:B:659:SER:HB3	2.17	0.44
7:G:4:HIS:CD2	7:G:73:LYS:HE3	2.52	0.44
8:H:111:ARG:HA	8:H:128:ASP:HA	1.99	0.44
15:P:37:G:H2'	15:P:38:G:C8	2.52	0.44
20:V:75:LEU:HD12	20:V:75:LEU:HA	1.82	0.44
21:W:37:THR:HA	21:W:70:VAL:HG21	1.99	0.44
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.73	0.44
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.31	0.44
2:B:67:LEU:HD13	2:B:420:GLN:OE1	2.17	0.44
4:D:93:HIS:CE1	4:D:94:LYS:HG3	2.52	0.44
14:N:44:DG:H2''	14:N:45:DG:C8	2.51	0.44
16:Q:716:ASN:OD1	16:Q:717:THR:N	2.50	0.44
17:R:428:LEU:HB2	17:R:437:PHE:CE2	2.52	0.44
23:Y:19:CYS:SG	23:Y:35:ASN:ND2	2.84	0.44
24:Z:280:ARG:HB2	24:Z:382:ILE:HG23	2.00	0.44
1:A:299:ALA:C	1:A:301:HIS:H	2.20	0.44
2:B:139:GLN:OE1	2:B:139:GLN:N	2.49	0.44
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.99	0.44
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.51	0.44
16:Q:667:ARG:HD3	16:Q:691:TYR:HE1	1.83	0.44
17:R:353:VAL:HG23	17:R:456:LYS:NZ	2.32	0.44
18:T:11:DC:H2''	18:T:12:DC:C6	2.51	0.44
21:W:203:GLN:OE1	21:W:204:LEU:HG	2.17	0.44
21:W:295:ASP:O	21:W:297:GLU:HG3	2.17	0.44
23:Y:76:ARG:HH11	23:Y:109:LYS:HD3	1.83	0.44
24:Z:639:LYS:HB2	24:Z:642:HIS:HB2	1.99	0.44
2:B:92:TYR:N	2:B:92:TYR:CD2	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.78	0.44
3:C:107:CYS:HB3	3:C:154:ARG:O	2.17	0.44
14:N:42:DT:C2	14:N:43:DG:C6	3.06	0.44
16:Q:415:TRP:HA	16:Q:418:LEU:HD12	2.00	0.44
16:Q:868:LYS:HD3	16:Q:868:LYS:HA	1.79	0.44
17:R:353:VAL:HG11	17:R:472:ILE:HD12	1.99	0.44
24:Z:258:LYS:HB3	24:Z:258:LYS:HE2	1.73	0.44
24:Z:614:ILE:HA	24:Z:624:LEU:HA	1.98	0.44
1:A:59:ASP:OD2	1:A:61:ARG:HB2	2.18	0.44
1:A:1124:LEU:HA	1:A:1124:LEU:HD12	1.67	0.44
1:A:1168:LYS:HA	1:A:1168:LYS:HD2	1.89	0.44
2:B:652:SER:N	2:B:655:ASP:OD1	2.38	0.44
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.79	0.44
5:E:97:GLU:OE1	5:E:97:GLU:N	2.50	0.44
5:E:99:ILE:O	5:E:99:ILE:HG13	2.18	0.44
7:G:30:LEU:HD12	7:G:30:LEU:HA	1.72	0.44
16:Q:841:LEU:HA	16:Q:844:LYS:HG2	1.99	0.44
20:V:193:HIS:HB3	20:V:196:LYS:O	2.18	0.44
24:Z:479:LYS:O	24:Z:519:GLN:HG2	2.17	0.44
24:Z:489:THR:HB	24:Z:505:ASP:OD2	2.17	0.44
1:A:602:CYS:SG	1:A:652:LEU:HD13	2.57	0.44
1:A:982:ASN:HD22	1:A:985:ARG:HB2	1.83	0.44
2:B:897:ARG:CB	2:B:900:GLU:HG3	2.48	0.44
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.44
15:P:40:A:H2'	15:P:41:C:H6	1.77	0.44
17:R:366:ARG:HH12	24:Z:775:TPO:HA	1.83	0.44
1:A:249:ILE:HG13	1:A:249:ILE:O	2.16	0.44
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.70	0.44
5:E:37:LEU:HD21	5:E:41:LYS:HZ3	1.82	0.44
14:N:31:DC:H2''	14:N:32:DA:H8	1.80	0.44
16:Q:847:GLN:O	16:Q:851:LEU:HG	2.17	0.44
20:V:127:VAL:HG23	20:V:128:VAL:N	2.32	0.44
21:W:65:LEU:HD12	21:W:84:LEU:C	2.38	0.44
24:Z:242:VAL:HG23	24:Z:245:LEU:HB2	2.00	0.44
1:A:198:LEU:O	1:A:215:LEU:HD12	2.18	0.44
2:B:650:ASN:C	19:U:460:TYR:CE2	2.91	0.44
13:M:540:GLY:HA2	13:M:560:GLU:H	1.83	0.44
16:Q:128:GLN:HA	16:Q:158:GLN:HE22	1.82	0.44
16:Q:750:ASP:OD1	16:Q:753:LEU:N	2.40	0.44
16:Q:870:GLU:HA	16:Q:873:LYS:NZ	2.32	0.44
17:R:455:TRP:O	17:R:459:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:171:ILE:HG23	21:W:187:GLU:HG2	1.99	0.44
21:W:253:ASP:OD1	21:W:253:ASP:N	2.51	0.44
24:Z:499:PHE:HB3	24:Z:512:LYS:HD2	2.00	0.44
1:A:365:THR:HG22	1:A:366:VAL:N	2.31	0.44
1:A:676:ILE:HD12	1:A:676:ILE:HG23	1.76	0.44
1:A:1467:GLY:C	1:A:1469:GLY:H	2.21	0.44
2:B:1151:MET:HE2	2:B:1151:MET:HB2	1.71	0.44
6:F:105:ILE:HG21	6:F:105:ILE:HD13	1.63	0.44
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.80	0.44
14:N:37:DG:C2	18:T:12:DC:N3	2.86	0.44
15:P:39:A:N1	15:P:40:A:C6	2.86	0.44
16:Q:527:HIS:CD2	16:Q:530:TYR:HB2	2.53	0.44
16:Q:677:THR:HG22	16:Q:679:ASP:H	1.83	0.44
20:V:182:THR:HA	20:V:185:ASP:OD2	2.17	0.44
21:W:17:ASP:OD2	21:W:40:LEU:HB3	2.17	0.44
1:A:488:VAL:O	1:A:488:VAL:HG12	2.18	0.43
1:A:812:LYS:HE2	9:I:77:THR:HG23	1.99	0.43
1:A:1484:MET:N	1:A:1484:MET:SD	2.91	0.43
2:B:332:LYS:HZ1	2:B:333:GLU:HB2	1.83	0.43
2:B:556:ILE:HD12	2:B:556:ILE:HA	1.59	0.43
4:D:60:VAL:HG11	7:G:44:PHE:HZ	1.83	0.43
5:E:58:LEU:HD23	5:E:58:LEU:H	1.81	0.43
5:E:61:LEU:HA	5:E:61:LEU:HD12	1.77	0.43
7:G:151:ARG:HH11	24:Z:477:HIS:CD2	2.36	0.43
8:H:11:ASP:HB3	8:H:55:LYS:HG2	2.00	0.43
16:Q:513:PHE:HB2	21:W:213:TYR:CE1	2.53	0.43
16:Q:530:TYR:CE2	16:Q:532:ASP:HB2	2.53	0.43
21:W:191:MET:HG3	21:W:211:ASP:HB3	1.99	0.43
1:A:539:GLN:O	1:A:540:ASP:C	2.56	0.43
2:B:705:GLY:O	2:B:709:SER:HB3	2.18	0.43
4:D:93:HIS:HE1	4:D:94:LYS:HE3	1.83	0.43
7:G:131:MET:SD	7:G:131:MET:N	2.92	0.43
10:J:60:LEU:HD23	10:J:60:LEU:HA	1.79	0.43
13:M:1398:LEU:HD11	13:M:1415:TYR:CD1	2.53	0.43
13:M:1435:CYS:SG	13:M:1442:LYS:HG2	2.58	0.43
16:Q:120:ALA:HB1	16:Q:130:HIS:HE1	1.83	0.43
16:Q:538:GLY:HA2	16:Q:553:TRP:HE3	1.83	0.43
18:T:47:DG:H2''	18:T:48:DG:H5'	1.99	0.43
20:V:106:LYS:HA	20:V:106:LYS:HD2	1.87	0.43
21:W:281:LYS:HD2	21:W:281:LYS:HA	1.80	0.43
24:Z:389:THR:O	24:Z:393:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:593:ASN:HB3	24:Z:595:HIS:CE1	2.54	0.43
1:A:75:ALA:O	2:B:1131:ARG:NH1	2.52	0.43
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.18	0.43
2:B:1173:SER:O	2:B:1173:SER:OG	2.36	0.43
4:D:137:LYS:HA	4:D:137:LYS:HD3	1.83	0.43
9:I:53:ILE:HA	9:I:53:ILE:HD13	1.70	0.43
13:M:1476:TYR:CE2	13:M:1483:ARG:HD3	2.54	0.43
16:Q:218:ARG:HD3	16:Q:238:LEU:HD11	2.00	0.43
16:Q:710:LYS:HB2	16:Q:712:TYR:CE1	2.52	0.43
24:Z:188:GLU:OE1	24:Z:188:GLU:N	2.51	0.43
24:Z:420:PHE:HE1	24:Z:470:LYS:HG2	1.83	0.43
24:Z:464:PRO:HD2	24:Z:467:GLU:HB3	1.99	0.43
1:A:106:VAL:O	1:A:110:VAL:HG22	2.19	0.43
1:A:818:GLU:OE2	17:R:599:CYS:HA	2.18	0.43
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.62	0.43
2:B:83:ARG:HH22	2:B:133:ILE:CG2	2.31	0.43
2:B:399:LEU:HA	2:B:399:LEU:HD23	1.80	0.43
2:B:576:ILE:HD12	2:B:576:ILE:HA	1.79	0.43
5:E:55:ARG:HA	5:E:58:LEU:CD2	2.48	0.43
16:Q:68:ARG:NH1	16:Q:82:GLN:HE22	2.16	0.43
16:Q:503:LEU:HG	16:Q:507:TYR:CE2	2.53	0.43
1:A:413:TYR:OH	1:A:450:MET:O	2.32	0.43
2:B:472:ARG:HA	2:B:472:ARG:HD2	1.92	0.43
2:B:497:LYS:HG3	2:B:498:PRO:CD	2.46	0.43
2:B:553:LEU:HA	2:B:553:LEU:HD12	1.73	0.43
5:E:3:ASP:OD1	5:E:49:SER:OG	2.20	0.43
5:E:27:LEU:HD12	5:E:27:LEU:HA	1.77	0.43
5:E:72:MET:HB2	5:E:72:MET:HE3	1.77	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.19	0.43
16:Q:268:ASN:HD22	16:Q:271:VAL:HG12	1.84	0.43
16:Q:456:ASN:OD1	20:V:48:PHE:HA	2.18	0.43
16:Q:772:GLU:HB3	16:Q:774:SER:OG	2.18	0.43
16:Q:877:GLN:OE1	16:Q:881:TYR:CE1	2.72	0.43
17:R:359:LEU:HD22	17:R:452:PHE:HE1	1.84	0.43
17:R:456:LYS:NZ	17:R:466:LEU:HD13	2.33	0.43
21:W:40:LEU:HA	21:W:66:GLY:HA3	2.01	0.43
21:W:152:LEU:HD12	21:W:167:ALA:O	2.19	0.43
21:W:252:SER:HB3	21:W:276:GLN:OE1	2.18	0.43
24:Z:291:ALA:HB2	24:Z:307:MET:HG2	2.00	0.43
24:Z:502:LEU:HD21	24:Z:511:LEU:HD22	2.00	0.43
24:Z:557:THR:O	24:Z:558:PHE:CD1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:VAL:HG13	2:B:520:VAL:O	2.19	0.43
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.83	0.43
13:M:1037:ILE:H	13:M:1055:GLY:HA2	1.84	0.43
13:M:1341:LYS:HA	13:M:1341:LYS:HD2	1.85	0.43
14:N:10:DG:H2''	14:N:11:DC:C6	2.54	0.43
16:Q:69:ILE:H	16:Q:69:ILE:HD12	1.84	0.43
16:Q:239:ALA:O	16:Q:243:LEU:HG	2.17	0.43
16:Q:464:LEU:HB2	16:Q:466:ASN:HD22	1.84	0.43
16:Q:527:HIS:HD2	16:Q:530:TYR:HB2	1.83	0.43
16:Q:691:TYR:HB3	16:Q:699:SER:OG	2.19	0.43
23:Y:29:GLU:HG3	23:Y:45:ASN:O	2.19	0.43
24:Z:200:PHE:HA	24:Z:210:LEU:HD13	2.00	0.43
24:Z:540:VAL:HB	24:Z:575:VAL:CG2	2.49	0.43
1:A:417:LYS:HE2	1:A:418:TYR:CE2	2.53	0.43
1:A:479:TRP:CD1	1:A:479:TRP:N	2.87	0.43
2:B:472:ARG:HH11	2:B:472:ARG:HD3	1.65	0.43
2:B:679:PRO:HG2	2:B:680:ASP:N	2.33	0.43
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.00	0.43
3:C:94:CYS:SG	3:C:95:PRO:HD2	2.59	0.43
16:Q:762:GLN:O	16:Q:766:THR:HG22	2.18	0.43
1:A:37:THR:HG21	1:A:41:ILE:HD11	2.01	0.43
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.18	0.43
2:B:254:GLN:O	2:B:303:PRO:HB2	2.19	0.43
2:B:577:HIS:CE1	2:B:583:LEU:HD11	2.53	0.43
2:B:625:LEU:HA	2:B:625:LEU:HD23	1.87	0.43
2:B:866:ILE:HG23	2:B:866:ILE:HD12	1.57	0.43
2:B:1142:ASN:ND2	2:B:1145:GLN:HB2	2.27	0.43
7:G:151:ARG:HA	24:Z:477:HIS:CE1	2.54	0.43
8:H:15:ILE:HG23	8:H:16:ASP:N	2.33	0.43
11:K:12:LEU:HD23	11:K:12:LEU:HA	1.86	0.43
16:Q:380:ILE:HD12	16:Q:400:HIS:CE1	2.53	0.43
17:R:454:LYS:HA	17:R:454:LYS:HD2	1.77	0.43
2:B:100:GLU:HA	2:B:105:PRO:HB3	1.99	0.43
2:B:313:GLU:HG3	2:B:315:ASN:H	1.82	0.43
4:D:33:LEU:HD21	4:D:97:LEU:HD23	2.00	0.43
7:G:81:LYS:HG3	7:G:148:VAL:C	2.39	0.43
16:Q:471:LYS:O	16:Q:475:LEU:HD23	2.18	0.43
16:Q:484:GLU:HB2	16:Q:492:TYR:HB3	2.00	0.43
21:W:25:GLY:N	21:W:72:ILE:HD12	2.34	0.43
21:W:84:LEU:HD21	21:W:110:TRP:CZ3	2.53	0.43
21:W:231:HIS:CG	21:W:251:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HA	1:A:201:GLU:O	2.19	0.43
1:A:592:PHE:CD2	1:A:592:PHE:O	2.71	0.43
1:A:770:VAL:HG21	1:A:781:ILE:HD11	2.01	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.43
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.19	0.43
1:A:1551:ALA:O	13:M:1509:ARG:HD2	2.19	0.43
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.54	0.43
7:G:80:PHE:HB2	7:G:83:GLU:CD	2.40	0.43
16:Q:645:LYS:HE3	22:X:243:LYS:NZ	2.33	0.43
16:Q:651:ASN:HB3	20:V:37:ASN:HD21	1.82	0.43
16:Q:651:ASN:ND2	16:Q:682:ASP:OD2	2.52	0.43
16:Q:653:ILE:O	16:Q:656:VAL:HG22	2.19	0.43
17:R:378:PHE:CZ	17:R:382:VAL:HG11	2.54	0.43
18:T:35:DG:N2	18:T:36:DC:O2	2.51	0.43
19:U:459:VAL:HG23	19:U:494:HIS:C	2.39	0.43
24:Z:196:LEU:HD12	24:Z:196:LEU:HA	1.79	0.43
24:Z:478:VAL:O	24:Z:489:THR:HA	2.19	0.43
1:A:1132:LYS:H	1:A:1132:LYS:HG2	1.65	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD12	1.59	0.42
2:B:501:LEU:HD12	2:B:505:LEU:HD12	2.01	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	1.99	0.42
15:P:35:A:H5'	15:P:36:G:OP2	2.18	0.42
16:Q:689:HIS:HB2	20:V:35:TYR:HE1	1.84	0.42
16:Q:725:ARG:NE	20:V:31:CYS:SG	2.92	0.42
16:Q:729:LYS:HB2	16:Q:732:LYS:CD	2.46	0.42
16:Q:750:ASP:OD1	16:Q:753:LEU:HG	2.18	0.42
21:W:9:PHE:CE2	21:W:54:LEU:HB3	2.54	0.42
24:Z:261:THR:O	24:Z:264:LEU:HG	2.18	0.42
24:Z:492:ILE:HA	24:Z:502:LEU:HA	1.99	0.42
24:Z:602:VAL:HG21	24:Z:636:PHE:HE2	1.83	0.42
24:Z:705:LEU:HD12	24:Z:724:VAL:HG11	2.01	0.42
1:A:130:LEU:HD11	1:A:235:VAL:HG13	2.01	0.42
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.52	0.42
1:A:639:ILE:HG21	1:A:639:ILE:HD13	1.81	0.42
1:A:1179:PRO:HA	1:A:1209:PRO:CB	2.49	0.42
1:A:1323:THR:HG22	1:A:1329:LYS:HD2	2.01	0.42
2:B:568:PHE:CE1	2:B:573:TRP:HB2	2.54	0.42
3:C:67:ARG:NH1	10:J:2:ILE:HG23	2.33	0.42
3:C:75:SER:HB3	3:C:79:VAL:HB	2.01	0.42
4:D:22:PHE:HB2	4:D:27:GLU:OE1	2.18	0.42
16:Q:508:GLU:OE2	16:Q:540:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:163:LEU:HB2	21:W:177:ILE:HG23	2.00	0.42
24:Z:439:LYS:O	24:Z:452:PRO:HA	2.19	0.42
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.52	0.42
1:A:1177:TYR:CE2	1:A:1210:TRP:CE3	3.06	0.42
2:B:186:ILE:HG21	2:B:186:ILE:HD13	1.74	0.42
3:C:268:GLN:HG3	3:C:269:SER:N	2.34	0.42
4:D:16:ASP:H	4:D:21:ILE:CG2	2.32	0.42
4:D:122:PHE:HD1	4:D:126:GLU:CD	2.23	0.42
16:Q:182:ALA:O	16:Q:186:TYR:CD2	2.72	0.42
16:Q:365:GLU:HG2	16:Q:369:LYS:NZ	2.34	0.42
16:Q:745:HIS:HB2	21:W:20:TRP:CH2	2.53	0.42
20:V:196:LYS:O	20:V:198:ARG:N	2.49	0.42
21:W:135:VAL:HG23	21:W:136:GLU:HG2	2.01	0.42
21:W:170:GLY:HA2	21:W:193:ILE:HG13	2.01	0.42
24:Z:525:ALA:O	24:Z:552:ARG:NH1	2.49	0.42
1:A:104:MET:HE1	1:A:193:ARG:HD2	2.01	0.42
1:A:338:SER:OG	1:A:341:GLN:HG2	2.20	0.42
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.55	0.42
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.85	0.42
1:A:461:GLN:O	1:A:463:THR:N	2.52	0.42
1:A:1137:PRO:O	1:A:1341:VAL:HG23	2.20	0.42
7:G:127:CYS:SG	7:G:138:GLN:HB3	2.60	0.42
14:N:35:DA:H2''	14:N:36:DG:C8	2.53	0.42
16:Q:611:TRP:HZ2	16:Q:631:ARG:HH11	1.65	0.42
16:Q:880:GLN:HE21	16:Q:884:LYS:CE	2.32	0.42
17:R:578:ALA:HA	20:V:127:VAL:HB	2.01	0.42
1:A:427:ILE:N	1:A:427:ILE:HD12	2.35	0.42
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.85	0.42
1:A:820:ARG:HH11	1:A:820:ARG:HD3	1.66	0.42
1:A:1343:LEU:HD12	1:A:1343:LEU:HA	1.76	0.42
2:B:319:ASN:ND2	2:B:332:LYS:HG2	2.34	0.42
2:B:544:PHE:CE2	2:B:548:TRP:NE1	2.81	0.42
2:B:544:PHE:CZ	2:B:548:TRP:NE1	2.87	0.42
2:B:574:VAL:O	2:B:574:VAL:HG22	2.20	0.42
2:B:841:ARG:HD3	2:B:841:ARG:HA	1.77	0.42
13:M:1408:LEU:HD23	13:M:1408:LEU:H	1.84	0.42
13:M:1490:THR:OG1	13:M:1493:GLY:N	2.53	0.42
14:N:37:DG:C6	18:T:12:DC:N4	2.79	0.42
15:P:37:G:C2'	15:P:38:G:H8	2.33	0.42
16:Q:62:LYS:HA	16:Q:62:LYS:HD3	1.74	0.42
16:Q:240:VAL:HG11	20:V:72:HIS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:598:GLN:HA	16:Q:599:SER:HA	1.76	0.42
16:Q:719:VAL:HG23	16:Q:720:VAL:N	2.35	0.42
17:R:581:ALA:CB	20:V:127:VAL:HG21	2.48	0.42
21:W:11:GLN:HE21	21:W:54:LEU:HD23	1.85	0.42
21:W:288:LYS:HA	21:W:288:LYS:HD3	1.77	0.42
1:A:503:LEU:O	1:A:503:LEU:HD23	2.19	0.42
1:A:909:LEU:O	1:A:910:LYS:HG2	2.20	0.42
1:A:932:ARG:HD3	8:H:106:THR:O	2.19	0.42
1:A:1166:LEU:HA	1:A:1166:LEU:HD23	1.84	0.42
1:A:1401:LEU:O	1:A:1405:MET:HG3	2.19	0.42
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.71	0.42
2:B:428:ASP:OD1	2:B:429:PHE:N	2.52	0.42
2:B:638:ARG:HH21	2:B:639:HIS:CE1	2.38	0.42
2:B:1125:MET:HE3	2:B:1156:LYS:HG2	2.02	0.42
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.42
5:E:96:GLU:OE1	5:E:96:GLU:N	2.52	0.42
7:G:106:CYS:SG	7:G:159:ALA:HB3	2.59	0.42
11:K:101:LEU:HA	11:K:101:LEU:HD12	1.85	0.42
14:N:12:DG:C6	18:T:38:DG:N2	2.87	0.42
14:N:14:DC:OP2	24:Z:186:ILE:HD12	2.19	0.42
16:Q:384:LEU:HD11	16:Q:393:LYS:O	2.20	0.42
16:Q:542:ARG:HD2	16:Q:554:PHE:HE2	1.83	0.42
16:Q:553:TRP:HA	16:Q:556:GLU:OE1	2.19	0.42
17:R:397:LYS:O	24:Z:777:MET:HE3	2.19	0.42
17:R:429:ARG:HB2	17:R:434:GLN:HB3	2.02	0.42
17:R:492:ILE:H	17:R:492:ILE:HD12	1.83	0.42
22:X:250:PHE:HA	22:X:253:LEU:HB3	2.02	0.42
23:Y:18:LEU:HD23	23:Y:18:LEU:HA	1.86	0.42
24:Z:178:ASN:OD1	24:Z:179:LEU:N	2.47	0.42
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.52	0.42
2:B:235:ILE:HD12	2:B:235:ILE:HG23	1.64	0.42
2:B:479:LEU:HD23	2:B:479:LEU:HA	1.79	0.42
2:B:557:SER:O	2:B:559:ALA:N	2.53	0.42
2:B:666:ASP:N	2:B:666:ASP:OD1	2.48	0.42
2:B:1062:ARG:CZ	2:B:1065:GLY:H	2.32	0.42
5:E:27:LEU:HD13	5:E:65:ASN:ND2	2.35	0.42
13:M:1421:SER:OG	13:M:1424:ARG:NH2	2.53	0.42
21:W:228:LEU:HD11	21:W:259:TRP:CE3	2.54	0.42
24:Z:450:ILE:O	24:Z:462:GLU:HA	2.20	0.42
1:A:361:PHE:HA	1:A:388:MET:HE2	2.02	0.42
1:A:362:SER:O	1:A:388:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:THR:OG1	1:A:934:LEU:HG	2.19	0.42
1:A:965:VAL:O	1:A:968:VAL:HG22	2.19	0.42
2:B:355:ASP:N	2:B:355:ASP:OD2	2.52	0.42
3:C:131:THR:HG22	3:C:147:ASP:OD1	2.20	0.42
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.54	0.42
4:D:100:LEU:HD11	4:D:118:LEU:HD21	2.01	0.42
5:E:61:LEU:HD23	16:Q:884:LYS:HG2	2.02	0.42
16:Q:188:LYS:HA	16:Q:191:ARG:HG2	2.01	0.42
16:Q:310:TYR:OH	20:V:67:GLU:OE2	2.36	0.42
16:Q:773:LYS:HE2	16:Q:827:HIS:HE1	1.84	0.42
20:V:49:ILE:HG22	22:X:227:ARG:HG3	2.01	0.42
21:W:83:SER:HB3	21:W:85:ASP:OD1	2.20	0.42
22:X:221:THR:O	22:X:225:VAL:HG22	2.19	0.42
1:A:374:SER:OG	1:A:375:ILE:N	2.53	0.42
1:A:621:ILE:HG21	1:A:621:ILE:HD13	1.78	0.42
1:A:1417:HIS:HA	1:A:1421:ARG:NH1	2.35	0.42
2:B:44:LEU:HD23	2:B:155:MET:HE2	2.01	0.42
2:B:839:GLY:O	2:B:891:ASP:HB2	2.20	0.42
7:G:119:PHE:HA	7:G:128:TYR:CE1	2.54	0.42
8:H:132:LEU:HA	8:H:132:LEU:HD23	1.81	0.42
16:Q:132:LEU:HD11	20:V:85:ASP:HA	2.01	0.42
16:Q:211:LEU:HB2	16:Q:213:LYS:CE	2.49	0.42
16:Q:639:VAL:HA	16:Q:642:ASN:OD1	2.20	0.42
16:Q:652:GLY:O	16:Q:656:VAL:HG13	2.20	0.42
17:R:414:VAL:HA	17:R:423:ASN:HB3	2.02	0.42
17:R:429:ARG:NH2	17:R:431:GLY:O	2.51	0.42
17:R:452:PHE:HD2	17:R:453:MET:CE	2.33	0.42
20:V:47:LYS:HA	20:V:47:LYS:HD3	1.75	0.42
21:W:108:ASP:OD1	21:W:126:HIS:ND1	2.53	0.42
21:W:214:ILE:HD12	21:W:228:LEU:HD23	2.02	0.42
21:W:231:HIS:CE1	21:W:249:SER:HG	2.38	0.42
24:Z:490:GLY:HA3	24:Z:503:PHE:O	2.20	0.42
24:Z:526:SER:OG	24:Z:527:GLY:N	2.53	0.42
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.77	0.42
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.85	0.42
1:A:828:LEU:HD12	1:A:828:LEU:HA	1.85	0.42
2:B:53:MET:HB3	2:B:57:ARG:HH21	1.84	0.42
2:B:583:LEU:O	2:B:587:LEU:HD23	2.20	0.42
2:B:847:LYS:HE3	2:B:864:ASP:OD2	2.20	0.42
3:C:113:ARG:HD2	3:C:113:ARG:HA	1.90	0.42
5:E:64:HIS:ND1	5:E:65:ASN:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASN:N	10:J:16:ASN:OD1	2.24	0.42
12:L:35:ARG:HH21	12:L:40:GLY:HA3	1.83	0.42
15:P:27:A:O2'	15:P:28:A:O5'	2.36	0.42
16:Q:152:PHE:HD1	16:Q:172:ILE:HD11	1.83	0.42
17:R:452:PHE:O	17:R:456:LYS:HG2	2.20	0.42
20:V:121:SER:O	20:V:121:SER:OG	2.37	0.42
21:W:155:ALA:O	21:W:163:LEU:HG	2.20	0.42
24:Z:176:ASP:OD2	24:Z:176:ASP:N	2.53	0.42
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.54	0.41
1:A:636:ILE:HG23	1:A:636:ILE:HD12	1.66	0.41
1:A:832:THR:HG23	1:A:833:PRO:HD2	2.02	0.41
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.41
2:B:309:PHE:CD2	9:I:40:ARG:NE	2.88	0.41
2:B:835:GLU:OE1	2:B:835:GLU:N	2.53	0.41
2:B:1116:VAL:HG11	2:B:1125:MET:HE3	2.02	0.41
5:E:10:LEU:HD23	5:E:10:LEU:HA	1.79	0.41
7:G:111:HIS:CD2	24:Z:501:ILE:HD13	2.54	0.41
9:I:31:GLU:OE1	9:I:31:GLU:N	2.53	0.41
16:Q:707:CYS:SG	16:Q:708:LEU:N	2.93	0.41
16:Q:744:ARG:HG3	16:Q:753:LEU:HD12	2.02	0.41
17:R:563:ILE:HD12	17:R:566:ARG:HD2	2.02	0.41
18:T:6:DC:H1'	18:T:7:DA:C8	2.55	0.41
20:V:51:TYR:CD1	20:V:52:PRO:HD2	2.55	0.41
23:Y:14:ARG:NH1	24:Z:300:GLN:OE1	2.53	0.41
1:A:321:GLU:HG2	1:A:327:ARG:NH2	2.35	0.41
1:A:912:SER:O	1:A:914:LYS:N	2.54	0.41
1:A:1216:LEU:HA	1:A:1216:LEU:HD23	1.86	0.41
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.84	0.41
2:B:544:PHE:O	2:B:547:GLU:N	2.48	0.41
2:B:679:PRO:CG	2:B:680:ASP:N	2.84	0.41
2:B:993:LYS:HD3	20:V:131:MET:SD	2.60	0.41
5:E:37:LEU:O	5:E:41:LYS:HG3	2.20	0.41
5:E:166:ARG:NH1	5:E:168:ASN:HB3	2.35	0.41
7:G:24:ASN:O	7:G:28:GLN:HG2	2.20	0.41
9:I:109:ARG:HD3	9:I:124:THR:CG2	2.46	0.41
16:Q:858:LYS:HA	16:Q:861:GLU:HG3	2.03	0.41
24:Z:199:LYS:HG3	24:Z:203:TYR:HD2	1.84	0.41
1:A:993:ILE:HD13	1:A:993:ILE:HG21	1.81	0.41
1:A:1217:ASP:OD2	1:A:1218:ARG:N	2.53	0.41
2:B:199:LYS:HB3	2:B:199:LYS:HE2	1.87	0.41
2:B:566:LYS:HG2	2:B:576:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:ILE:HG22	2:B:601:VAL:HB	2.01	0.41
2:B:739:ASN:N	2:B:739:ASN:OD1	2.53	0.41
4:D:112:LYS:HE3	4:D:112:LYS:HB2	1.74	0.41
13:M:758:TYR:N	13:M:920:ILE:O	2.49	0.41
16:Q:215:GLU:HG2	16:Q:216:LYS:NZ	2.35	0.41
16:Q:431:LEU:HD23	16:Q:431:LEU:HA	1.83	0.41
16:Q:791:ARG:HH12	21:W:87:HIS:CD2	2.38	0.41
17:R:397:LYS:HA	17:R:397:LYS:HD2	1.85	0.41
17:R:402:VAL:HB	17:R:455:TRP:HB2	2.02	0.41
17:R:485:TYR:HD1	17:R:487:PHE:CE1	2.38	0.41
21:W:25:GLY:HA3	21:W:31:ASN:C	2.40	0.41
1:A:140:ARG:NH2	1:A:234:PHE:O	2.50	0.41
1:A:561:MET:SD	11:K:58:PHE:HA	2.59	0.41
1:A:1165:THR:HG22	1:A:1297:THR:H	1.85	0.41
1:A:1255:LEU:HD12	1:A:1255:LEU:N	2.34	0.41
2:B:105:PRO:HG2	19:U:512:THR:CA	2.37	0.41
3:C:64:ILE:HG23	3:C:64:ILE:HD12	1.70	0.41
3:C:166:LYS:HE2	3:C:166:LYS:HB3	1.74	0.41
4:D:41:LEU:HB3	4:D:65:LEU:CD2	2.50	0.41
4:D:84:ARG:HG3	4:D:97:LEU:HD11	2.02	0.41
6:F:90:LEU:HA	6:F:90:LEU:HD23	1.82	0.41
10:J:49:LEU:HD23	10:J:49:LEU:HA	1.82	0.41
16:Q:345:PHE:O	16:Q:349:GLN:HG2	2.20	0.41
16:Q:537:LEU:HB3	16:Q:553:TRP:CZ3	2.55	0.41
16:Q:572:GLY:O	16:Q:576:LEU:HG	2.20	0.41
16:Q:851:LEU:O	16:Q:855:LYS:HG2	2.21	0.41
21:W:8:LEU:HD13	21:W:288:LYS:HE3	2.01	0.41
22:X:246:SER:HA	22:X:249:ILE:HD12	2.02	0.41
24:Z:439:LYS:H	24:Z:453:LYS:H	1.66	0.41
24:Z:548:GLY:HA3	24:Z:562:ASN:HA	2.01	0.41
24:Z:593:ASN:HB3	24:Z:595:HIS:HE1	1.84	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.41
1:A:618:TYR:HB3	1:A:621:ILE:O	2.21	0.41
1:A:1321:ILE:O	1:A:1328:PHE:O	2.38	0.41
2:B:305:LEU:HD12	2:B:305:LEU:HA	1.74	0.41
3:C:259:LEU:HA	3:C:259:LEU:HD12	1.81	0.41
5:E:39:GLU:O	5:E:43:GLN:HB2	2.20	0.41
10:J:30:THR:HG22	10:J:33:ASP:HB2	2.02	0.41
11:K:109:ILE:HD13	11:K:109:ILE:HA	1.88	0.41
16:Q:202:LEU:HD21	16:Q:233:GLY:HA3	2.02	0.41
16:Q:424:GLN:HB2	22:X:231:TRP:CZ3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:37:DC:C4	18:T:38:DG:C6	3.08	0.41
21:W:84:LEU:HD23	21:W:84:LEU:HA	1.77	0.41
1:A:725:LEU:HD21	1:A:736:THR:HG23	2.02	0.41
2:B:186:ILE:O	2:B:187:ILE:HD13	2.20	0.41
2:B:322:GLY:CA	2:B:339:ALA:HB2	2.50	0.41
2:B:422:PHE:HB3	2:B:429:PHE:CB	2.50	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.01	0.41
2:B:937:SER:OG	2:B:938:ARG:N	2.53	0.41
4:D:110:GLU:O	4:D:114:LEU:HD23	2.21	0.41
5:E:36:THR:OG1	5:E:39:GLU:OE1	2.29	0.41
13:M:623:LYS:O	13:M:627:ASP:N	2.51	0.41
16:Q:285:TYR:HA	16:Q:288:VAL:HG12	2.01	0.41
16:Q:720:VAL:HG21	16:Q:743:ALA:HB2	2.01	0.41
16:Q:733:LEU:HA	16:Q:733:LEU:HD23	1.72	0.41
17:R:507:PRO:HA	17:R:508:ASN:HA	1.49	0.41
21:W:46:VAL:CG2	21:W:58:TRP:HB2	2.51	0.41
24:Z:601:LYS:HG3	24:Z:611:GLU:OE2	2.20	0.41
24:Z:736:LEU:HA	24:Z:736:LEU:HD23	1.79	0.41
1:A:46:THR:OG1	1:A:47:THR:N	2.53	0.41
1:A:626:THR:O	1:A:627:LYS:HB3	2.21	0.41
1:A:849:ASP:HA	1:A:852:VAL:HG22	2.03	0.41
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.28	0.41
2:B:273:PHE:CG	2:B:284:ILE:HG23	2.56	0.41
2:B:312:GLN:OE1	9:I:40:ARG:NH2	2.54	0.41
5:E:111:THR:O	5:E:114:ALA:N	2.52	0.41
7:G:7:LEU:HB2	7:G:72:TYR:CE2	2.55	0.41
13:M:1354:ASP:O	13:M:1372:LYS:HG2	2.20	0.41
13:M:1474:LEU:HD21	13:M:1511:PHE:CE1	2.55	0.41
17:R:440:GLU:HG3	17:R:441:PHE:CE1	2.55	0.41
21:W:27:ASN:ND2	21:W:74:HIS:O	2.53	0.41
24:Z:192:THR:OG1	24:Z:244:ASN:ND2	2.54	0.41
1:A:151:LYS:O	1:A:152:ASN:ND2	2.53	0.41
1:A:954:ARG:HH11	1:A:954:ARG:HD2	1.74	0.41
1:A:1290:SER:O	1:A:1294:THR:HG23	2.21	0.41
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.84	0.41
3:C:34:ILE:HG21	3:C:34:ILE:HD13	1.80	0.41
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.87	0.41
5:E:60:VAL:HG23	5:E:74:VAL:HB	2.03	0.41
5:E:185:ILE:HG21	5:E:185:ILE:HD13	1.67	0.41
7:G:81:LYS:HE2	7:G:149:GLY:HA2	2.03	0.41
8:H:96:VAL:HA	8:H:116:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:235:LEU:HD23	16:Q:261:ALA:HB2	2.02	0.41
16:Q:468:GLY:O	16:Q:472:LYS:HG2	2.20	0.41
16:Q:790:HIS:NE2	16:Q:817:CYS:SG	2.94	0.41
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.69	0.41
1:A:120:ASP:O	1:A:122:ASN:N	2.54	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.78	0.41
1:A:419:ILE:HD13	1:A:419:ILE:HG21	1.70	0.41
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.36	0.41
1:A:461:GLN:O	1:A:461:GLN:NE2	2.53	0.41
1:A:497:ASP:HB3	2:B:792:ASP:HB3	2.01	0.41
1:A:596:ILE:HG21	1:A:596:ILE:HD13	1.76	0.41
1:A:738:GLU:OE1	1:A:797:ARG:HD3	2.21	0.41
1:A:1121:VAL:N	1:A:1122:PRO:CD	2.84	0.41
1:A:1164:THR:O	1:A:1298:LEU:N	2.53	0.41
2:B:19:PRO:C	2:B:21:LEU:N	2.74	0.41
2:B:222:ARG:HH11	2:B:222:ARG:HD3	1.72	0.41
2:B:889:LYS:HB2	2:B:889:LYS:HE2	1.46	0.41
2:B:1010:LYS:HE3	20:V:130:TRP:CH2	2.56	0.41
3:C:246:LEU:HA	3:C:246:LEU:HD23	1.87	0.41
7:G:14:HIS:O	7:G:16:ARG:N	2.54	0.41
7:G:50:THR:HG22	7:G:73:LYS:HB3	2.03	0.41
7:G:92:VAL:H	7:G:139:GLN:HE21	1.68	0.41
11:K:93:ASP:OD1	11:K:94:LEU:N	2.53	0.41
15:P:40:A:C2	15:P:41:C:C4	3.08	0.41
16:Q:258:LEU:HD23	16:Q:258:LEU:HA	1.90	0.41
16:Q:858:LYS:O	16:Q:861:GLU:HG3	2.21	0.41
17:R:388:ARG:HG2	17:R:443:SER:HB2	2.03	0.41
17:R:390:GLY:HA2	17:R:400:TYR:CD1	2.55	0.41
17:R:582:GLU:HA	17:R:585:ASN:HD21	1.85	0.41
21:W:196:LEU:HD13	21:W:205:LEU:HD11	2.01	0.41
21:W:222:ALA:O	21:W:223:ASN:ND2	2.54	0.41
24:Z:389:THR:HG23	24:Z:391:SER:H	1.85	0.41
24:Z:491:LEU:HD23	24:Z:491:LEU:HA	1.83	0.41
24:Z:562:ASN:ND2	24:Z:566:LYS:HG3	2.33	0.41
1:A:33:ARG:H	1:A:33:ARG:HG2	1.69	0.41
1:A:102:LYS:HE2	1:A:138:LYS:NZ	2.36	0.41
1:A:117:LEU:O	1:A:119:VAL:N	2.53	0.41
1:A:455:ILE:HD12	1:A:520:MET:HE1	2.03	0.41
1:A:939:VAL:O	1:A:943:LEU:HD12	2.21	0.41
1:A:1090:LEU:HD23	1:A:1090:LEU:HA	1.79	0.41
2:B:650:ASN:C	19:U:460:TYR:HE2	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:SER:HB2	7:G:125:PRO:HD2	2.03	0.41
8:H:6:PHE:CZ	8:H:37:MET:SD	3.14	0.41
11:K:103:GLU:O	11:K:107:VAL:HG13	2.20	0.41
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.41
16:Q:218:ARG:HH11	16:Q:238:LEU:CD2	2.33	0.41
16:Q:467:LEU:HD12	16:Q:506:LEU:HG	2.02	0.41
16:Q:790:HIS:CD2	16:Q:817:CYS:SG	3.14	0.41
18:T:37:DC:H5'	18:T:37:DC:C6	2.56	0.41
18:T:39:DC:H2''	18:T:40:DT:H72	2.02	0.41
21:W:5:TYR:CD1	21:W:303:CYS:HB3	2.56	0.41
21:W:250:SER:OG	21:W:277:VAL:HG23	2.21	0.41
1:A:217:SER:O	1:A:220:ARG:N	2.53	0.40
1:A:812:LYS:O	1:A:813:ASP:HB2	2.21	0.40
1:A:1177:TYR:HH	1:A:1282:ASP:HA	1.86	0.40
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.48	0.40
1:A:1376:LYS:O	1:A:1380:ARG:HG3	2.21	0.40
1:A:1481:LYS:HA	7:G:20:PRO:HA	2.03	0.40
2:B:123:PRO:HB2	2:B:148:PHE:HE1	1.86	0.40
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.02	0.40
16:Q:18:GLU:N	16:Q:18:GLU:OE1	2.53	0.40
16:Q:274:HIS:HA	16:Q:277:ASN:HD21	1.84	0.40
16:Q:296:PHE:CE1	16:Q:305:GLN:HB2	2.56	0.40
16:Q:398:LYS:HE2	16:Q:421:ILE:HG21	2.03	0.40
24:Z:525:ALA:CB	24:Z:552:ARG:HH22	2.31	0.40
1:A:99:PHE:O	1:A:103:THR:HG23	2.21	0.40
1:A:247:TRP:N	1:A:247:TRP:CD1	2.87	0.40
1:A:539:GLN:C	1:A:541:THR:N	2.74	0.40
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.04	0.40
1:A:1222:THR:C	1:A:1225:LYS:H	2.23	0.40
1:A:1288:ILE:HA	1:A:1291:ASN:HD21	1.86	0.40
2:B:583:LEU:N	2:B:583:LEU:HD12	2.36	0.40
4:D:35:SER:OG	4:D:72:SER:HA	2.21	0.40
7:G:110:ARG:HG2	7:G:119:PHE:CZ	2.56	0.40
7:G:152:VAL:HA	7:G:157:ILE:HA	2.03	0.40
16:Q:238:LEU:HD12	16:Q:238:LEU:HA	1.96	0.40
16:Q:393:LYS:HB3	16:Q:393:LYS:HE3	1.70	0.40
18:T:21:DT:H6	18:T:21:DT:H2'	1.67	0.40
21:W:251:SER:HG	21:W:255:SER:HG	1.68	0.40
24:Z:551:VAL:HG21	24:Z:632:ASN:OD1	2.20	0.40
24:Z:571:ARG:HB2	24:Z:574:ALA:CB	2.51	0.40
1:A:92:LYS:CD	1:A:307:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG21	1:A:1435:THR:HG23	2.03	0.40
1:A:413:TYR:O	1:A:449:HIS:CD2	2.67	0.40
1:A:713:VAL:CG2	1:A:817:PRO:HD3	2.45	0.40
1:A:1150:ASP:OD2	1:A:1153:ARG:HG3	2.21	0.40
1:A:1182:GLN:O	1:A:1192:TRP:CE2	2.73	0.40
1:A:1261:ILE:C	1:A:1262:MET:HE3	2.41	0.40
2:B:157:ARG:NH2	2:B:177:CYS:O	2.54	0.40
2:B:665:ILE:HA	2:B:665:ILE:HD12	1.78	0.40
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.22	0.40
5:E:101:ARG:HA	5:E:126:ILE:O	2.20	0.40
7:G:110:ARG:NH2	7:G:117:MET:O	2.55	0.40
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.79	0.40
11:K:80:ASP:N	11:K:80:ASP:OD1	2.32	0.40
12:L:13:GLN:HA	12:L:14:PRO:HD3	1.88	0.40
14:N:42:DT:H6	14:N:42:DT:H2'	1.71	0.40
16:Q:3:ARG:HB3	16:Q:4:GLY:H	1.67	0.40
16:Q:153:HIS:CE1	16:Q:156:LEU:HD12	2.56	0.40
16:Q:333:THR:HG21	16:Q:347:LEU:HD12	2.02	0.40
16:Q:415:TRP:CZ3	16:Q:440:ILE:HG12	2.57	0.40
17:R:392:GLY:HA2	17:R:397:LYS:O	2.20	0.40
17:R:587:LYS:HE2	17:R:587:LYS:HB2	1.93	0.40
20:V:282:ALA:C	20:V:284:GLU:H	2.25	0.40
21:W:243:ASP:OD2	21:W:243:ASP:N	2.54	0.40
21:W:254:LYS:HG2	21:W:275:ASP:C	2.42	0.40
23:Y:93:LEU:HD23	23:Y:93:LEU:HA	1.87	0.40
24:Z:260:MET:N	24:Z:260:MET:SD	2.94	0.40
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.85	0.40
1:A:135:GLY:O	1:A:137:PRO:HD3	2.21	0.40
1:A:538:VAL:O	1:A:539:GLN:HG2	2.22	0.40
1:A:1182:GLN:C	1:A:1192:TRP:HE1	2.18	0.40
2:B:84:TYR:CB	2:B:132:VAL:HA	2.52	0.40
2:B:95:LYS:HA	2:B:95:LYS:HD2	1.92	0.40
2:B:332:LYS:HD2	2:B:332:LYS:C	2.41	0.40
2:B:388:TYR:H	2:B:504:THR:CG2	2.27	0.40
2:B:620:ARG:HH11	2:B:620:ARG:HD2	1.69	0.40
2:B:791:GLU:O	2:B:792:ASP:HB2	2.21	0.40
5:E:25:GLY:O	5:E:65:ASN:HB2	2.22	0.40
13:M:1429:HIS:CE1	13:M:1460:TYR:HH	2.37	0.40
16:Q:24:LEU:HD11	16:Q:56:LYS:NZ	2.36	0.40
16:Q:95:GLN:OE1	20:V:83:THR:OG1	2.38	0.40
16:Q:689:HIS:HB2	20:V:35:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:14:ALA:CB	21:W:298:ILE:HG13	2.52	0.40
24:Z:200:PHE:HB2	24:Z:210:LEU:HD22	2.02	0.40
24:Z:420:PHE:CE1	24:Z:470:LYS:HG2	2.56	0.40
1:A:29:ASP:O	1:A:33:ARG:HG2	2.21	0.40
1:A:955:GLU:OE1	1:A:1010:VAL:HG22	2.22	0.40
1:A:1163:HIS:CD2	1:A:1297:THR:HG23	2.57	0.40
2:B:50:PHE:HA	2:B:54:SER:HB3	2.02	0.40
2:B:242:ARG:NH2	2:B:252:ILE:HD12	2.37	0.40
9:I:14:ILE:HG23	9:I:23:MET:HG3	2.03	0.40
16:Q:386:ALA:HB1	16:Q:394:ARG:CG	2.51	0.40
16:Q:636:TYR:CE2	16:Q:652:GLY:HA3	2.56	0.40
18:T:1:DG:H2"	18:T:2:DC:C6	2.56	0.40
21:W:172:ILE:O	21:W:186:LEU:N	2.54	0.40
21:W:273:HIS:CE1	21:W:291:SER:HG	2.39	0.40
24:Z:501:ILE:HA	24:Z:511:LEU:O	2.21	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	A	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	22	57
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	19	54
3	C	254/275 (92%)	232 (91%)	19 (8%)	3 (1%)	13	44
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	29	64
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	4	23
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	51	83
16	Q	888/1179 (75%)	836 (94%)	52 (6%)	0	100	100
17	R	240/713 (34%)	225 (94%)	14 (6%)	1 (0%)	34	69
19	U	117/666 (18%)	88 (75%)	21 (18%)	8 (7%)	1	7
20	V	234/531 (44%)	199 (85%)	31 (13%)	4 (2%)	9	36
21	W	298/305 (98%)	268 (90%)	30 (10%)	0	100	100
22	X	41/531 (8%)	41 (100%)	0	0	100	100
23	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
24	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	47	79
All	All	7238/11540 (63%)	6624 (92%)	573 (8%)	41 (1%)	29	59

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE
13	M	1330	PRO
17	R	507	PRO
19	U	506	ALA
19	U	508	HIS
20	V	238	PRO
24	Z	760	GLY
1	A	1435	THR
19	U	481	GLY
19	U	521	LYS
2	B	20	ASP
2	B	142	THR
2	B	1004	ASP
10	J	28	GLU
19	U	463	PRO

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Mol	Chain	Res	Type
19	U	513	LEU
19	U	516	ALA
19	U	523	GLN
20	V	228	GLU
20	V	249	ASP
20	V	291	ASN
1	A	300	ALA
1	A	696	SER
2	B	950	ARG
1	A	495	ASP
1	A	1130	ILE
2	B	679	PRO
2	B	834	ARG
3	C	60	HIS
3	C	92	GLU
2	B	650	ASN
2	B	1001	PRO
1	A	478	PRO
5	E	45	GLY
8	H	17	PRO
10	J	64	PRO
1	A	980	PRO

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	A	1245/1761 (71%)	1226 (98%)	19 (2%)	65 85
2	B	986/1084 (91%)	949 (96%)	37 (4%)	33 66
3	C	235/252 (93%)	228 (97%)	7 (3%)	41 71
4	D	109/126 (86%)	108 (99%)	1 (1%)	78 91
5	E	191/192 (100%)	189 (99%)	2 (1%)	76 90
6	F	68/111 (61%)	67 (98%)	1 (2%)	65 85
7	G	146/153 (95%)	143 (98%)	3 (2%)	53 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	130/131 (99%)	122 (94%)	8 (6%)	18	49
9	I	104/112 (93%)	101 (97%)	3 (3%)	42	72
10	J	55/56 (98%)	54 (98%)	1 (2%)	59	82
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	90
12	L	43/55 (78%)	40 (93%)	3 (7%)	15	45
13	M	154/1524 (10%)	154 (100%)	0	100	100
16	Q	761/1011 (75%)	755 (99%)	6 (1%)	81	92
17	R	168/625 (27%)	166 (99%)	2 (1%)	71	88
19	U	63/590 (11%)	63 (100%)	0	100	100
20	V	144/462 (31%)	141 (98%)	3 (2%)	53	79
21	W	255/260 (98%)	254 (100%)	1 (0%)	91	96
22	X	40/467 (9%)	40 (100%)	0	100	100
23	Y	102/105 (97%)	102 (100%)	0	100	100
24	Z	434/939 (46%)	432 (100%)	2 (0%)	88	94
All	All	5537/10122 (55%)	5437 (98%)	100 (2%)	61	82

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	147	LEU
1	A	251	THR
1	A	301	HIS
1	A	382	ARG
1	A	476	ILE
1	A	539	GLN
1	A	571	ASP
1	A	605	THR
1	A	757	GLN
1	A	761	SER
1	A	819	SER
1	A	884	ASN
1	A	931	ARG
1	A	937	ASP
1	A	1030	SER
1	A	1074	SER
1	A	1210	TRP

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Mol	Chain	Res	Type
1	A	1286	ARG
2	B	20	ASP
2	B	83	ARG
2	B	90	GLN
2	B	92	TYR
2	B	115	LEU
2	B	147	THR
2	B	170	ASP
2	B	180	ASP
2	B	218	THR
2	B	236	TRP
2	B	267	VAL
2	B	331	THR
2	B	332	LYS
2	B	348	LEU
2	B	351	VAL
2	B	354	SER
2	B	359	THR
2	B	386	ASP
2	B	411	LEU
2	B	429	PHE
2	B	453	TRP
2	B	592	ARG
2	B	597	ILE
2	B	610	ARG
2	B	626	LEU
2	B	649	ASN
2	B	650	ASN
2	B	659	SER
2	B	715	ASP
2	B	731	GLN
2	B	738	THR
2	B	743	ARG
2	B	784	SER
2	B	931	ILE
2	B	1118	VAL
2	B	1148	LEU
2	B	1174	VAL
3	C	33	SER
3	C	63	PHE
3	C	74	THR
3	C	75	SER

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Mol	Chain	Res	Type
3	C	76	ASP
3	C	147	ASP
3	C	151	VAL
4	D	94	LYS
5	E	82	VAL
5	E	117	SER
6	F	123	LEU
7	G	21	ASN
7	G	37	THR
7	G	67	LEU
8	H	15	ILE
8	H	67	ASP
8	H	83	SER
8	H	95	LYS
8	H	96	VAL
8	H	113	SER
8	H	116	VAL
8	H	141	VAL
9	I	12	VAL
9	I	15	ARG
9	I	101	SER
10	J	47	ARG
11	K	99	SER
12	L	34	ILE
12	L	39	CYS
12	L	44	MET
16	Q	180	ARG
16	Q	191	ARG
16	Q	697	TYR
16	Q	707	CYS
16	Q	820	LEU
16	Q	858	LYS
17	R	422	THR
17	R	474	LYS
20	V	45	ASP
20	V	132	ARG
20	V	181	LYS
21	W	169	ASP
24	Z	176	ASP
24	Z	720	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	96	HIS
1	A	122	ASN
1	A	123	ASN
1	A	152	ASN
1	A	288	ASN
1	A	313	HIS
1	A	449	HIS
1	A	704	ASN
1	A	742	ASN
1	A	780	ASN
1	A	809	HIS
1	A	935	GLN
1	A	982	ASN
1	A	1005	HIS
1	A	1182	GLN
1	A	1230	GLN
2	B	52	GLN
2	B	175	ASN
2	B	319	ASN
2	B	471	ASN
2	B	631	GLN
2	B	649	ASN
2	B	1003	ASN
2	B	1040	GLN
2	B	1120	ASN
2	B	1142	ASN
3	C	60	HIS
3	C	114	HIS
3	C	262	GLN
4	D	34	ASN
4	D	48	ASN
4	D	66	ASN
4	D	76	ASN
4	D	129	GLN
5	E	107	GLN
5	E	168	ASN
7	G	93	ASN
7	G	139	GLN
8	H	131	ASN
9	I	84	HIS
9	I	91	HIS
11	K	49	GLN

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Mol	Chain	Res	Type
13	M	1352	GLN
16	Q	38	HIS
16	Q	40	GLN
16	Q	82	GLN
16	Q	105	ASN
16	Q	128	GLN
16	Q	161	ASN
16	Q	244	ASN
16	Q	268	ASN
16	Q	289	GLN
16	Q	294	HIS
16	Q	298	ASN
16	Q	305	GLN
16	Q	349	GLN
16	Q	359	ASN
16	Q	373	ASN
16	Q	407	GLN
16	Q	466	ASN
16	Q	502	ASN
16	Q	527	HIS
16	Q	561	ASN
16	Q	573	ASN
16	Q	585	GLN
16	Q	616	HIS
16	Q	706	ASN
16	Q	714	HIS
16	Q	877	GLN
16	Q	880	GLN
16	Q	887	ASN
17	R	416	GLN
17	R	432	ASN
17	R	484	ASN
17	R	585	ASN
17	R	588	ASN
20	V	37	ASN
20	V	69	GLN
20	V	72	HIS
20	V	97	ASN
20	V	122	GLN
20	V	193	HIS
21	W	11	GLN
21	W	15	HIS

Continued on next page...

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Mol	Chain	Res	Type
21	W	27	ASN
21	W	98	GLN
21	W	131	ASN
21	W	173	ASN
21	W	223	ASN
21	W	268	HIS
21	W	273	HIS
23	Y	27	GLN
24	Z	232	GLN
24	Z	251	ASN
24	Z	466	GLN
24	Z	519	GLN
24	Z	595	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	7 (35%)	3 (15%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	36	G
15	P	37	G
15	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
24	TPO	Z	775	24	8,10,11	1.54	1 (12%)	10,14,16	1.99	1 (10%)
1	TPO	A	1525	1	8,10,11	1.60	1 (12%)	10,14,16	1.83	1 (10%)
1	SEP	A	1547	1	8,9,10	1.49	1 (12%)	8,12,14	1.39	2 (25%)

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
24	TPO	Z	775	24	-	1/9/11/13	-
1	TPO	A	1525	1	-	4/9/11/13	-
1	SEP	A	1547	1	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.41	1.61	1.50
24	Z	775	TPO	P-O1P	3.34	1.61	1.50
1	A	1547	SEP	P-O1P	3.25	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	775	TPO	P-OG1-CB	-5.85	105.53	123.21
1	A	1525	TPO	P-OG1-CB	-4.96	108.22	123.21
1	A	1547	SEP	P-OG-CB	-2.69	110.89	118.30
1	A	1547	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	2	0
1	A	1525	TPO	1	0
1	A	1547	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
19	U	1
20	V	1
13	M	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	25.86
1	V	299:GLU	C	310:ASN	N	12.74
1	M	1334:ASN	C	1338:ILE	N	5.29
1	B	755:GLN	C	756:LYS	N	1.18
1	B	108:MET	C	109:MET	N	1.17
1	A	999:ARG	C	1000:LEU	N	1.15
1	B	94:SER	C	95:LYS	N	1.07

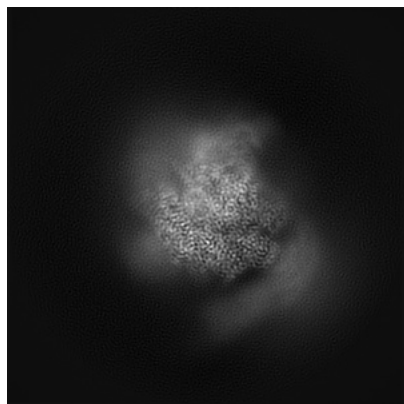
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10480. These allow visual inspection of the internal detail of the map and identification of artifacts.

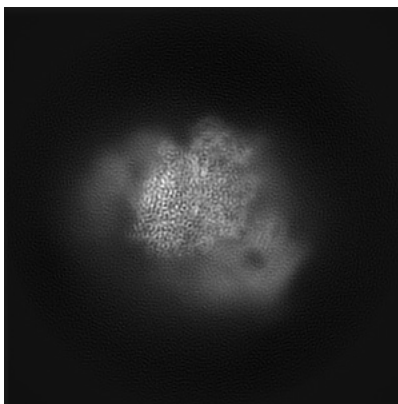
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

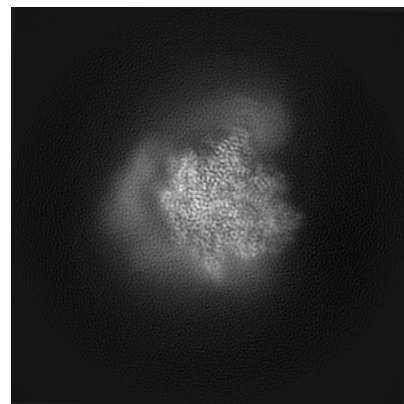
6.1.1 Primary map



X

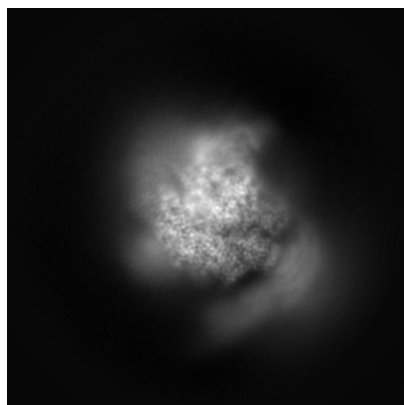


Y

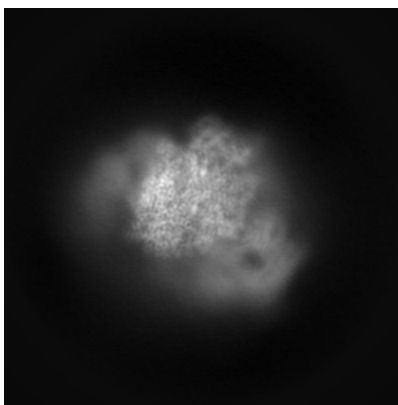


Z

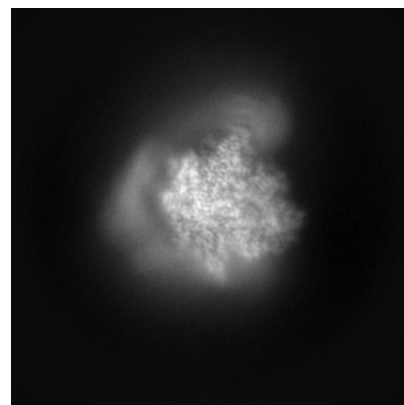
6.1.2 Raw map



X



Y

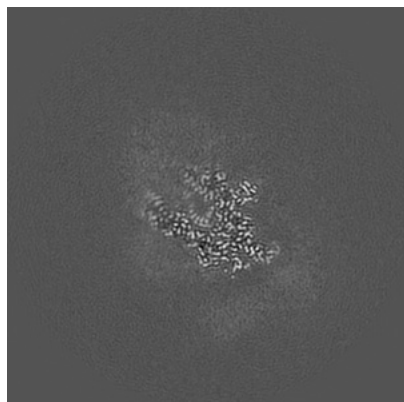


Z

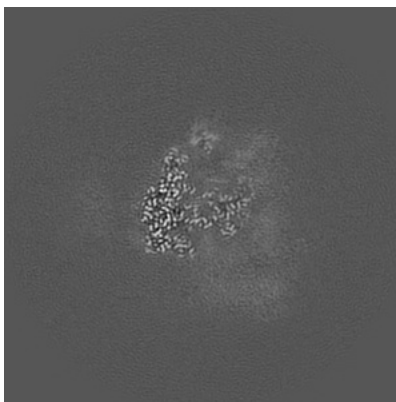
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

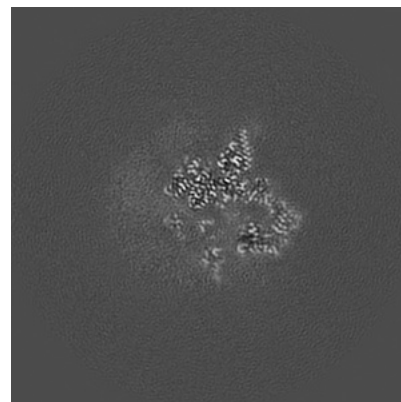
6.2.1 Primary map



X Index: 180

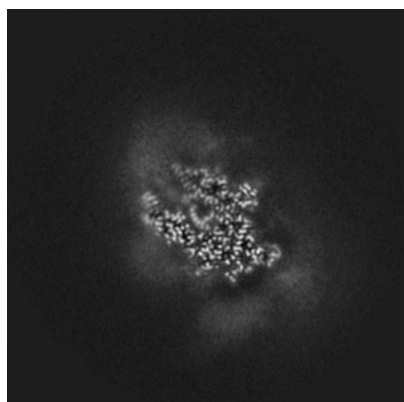


Y Index: 180

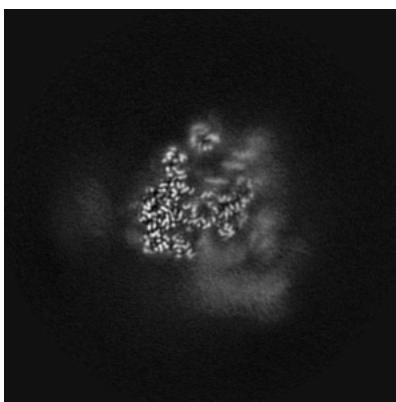


Z Index: 180

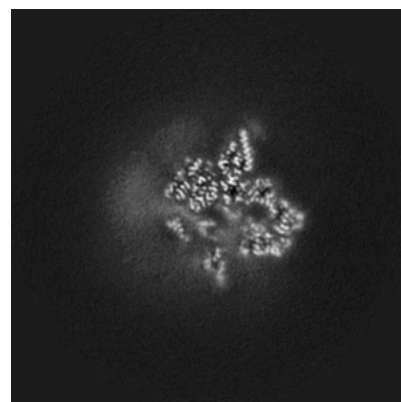
6.2.2 Raw map



X Index: 180



Y Index: 180

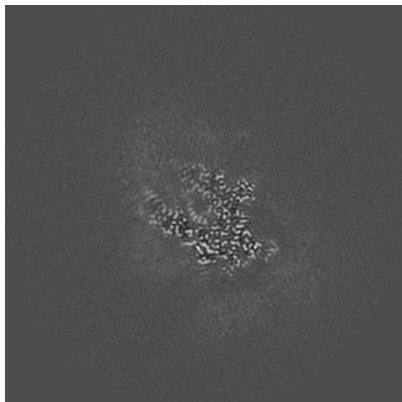


Z Index: 180

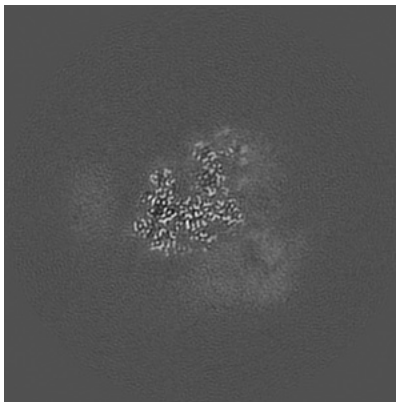
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

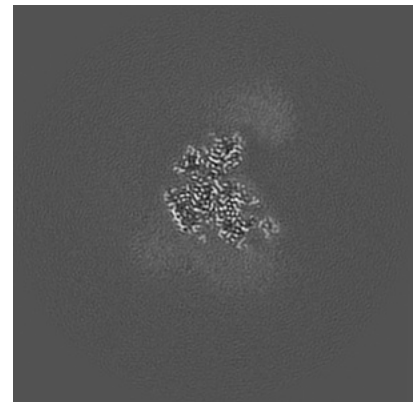
6.3.1 Primary map



X Index: 179

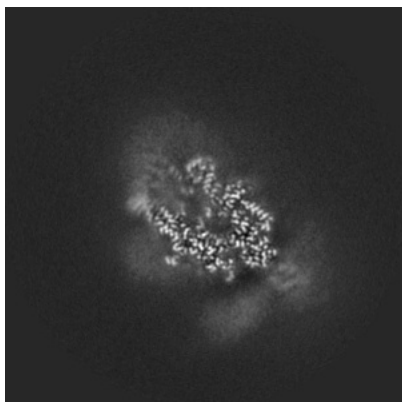


Y Index: 193

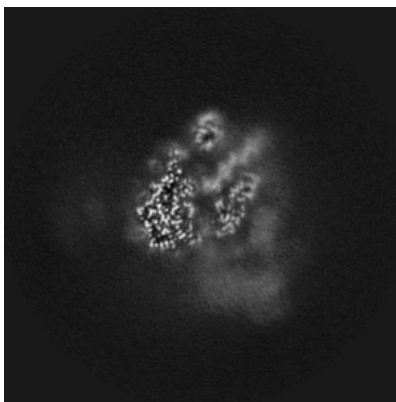


Z Index: 143

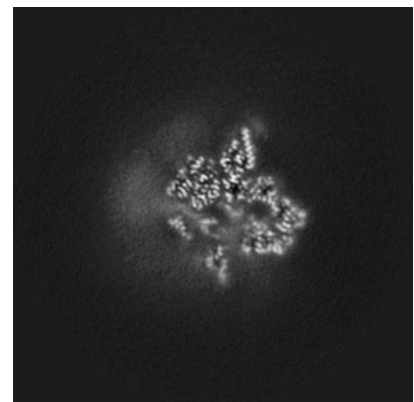
6.3.2 Raw map



X Index: 189



Y Index: 174

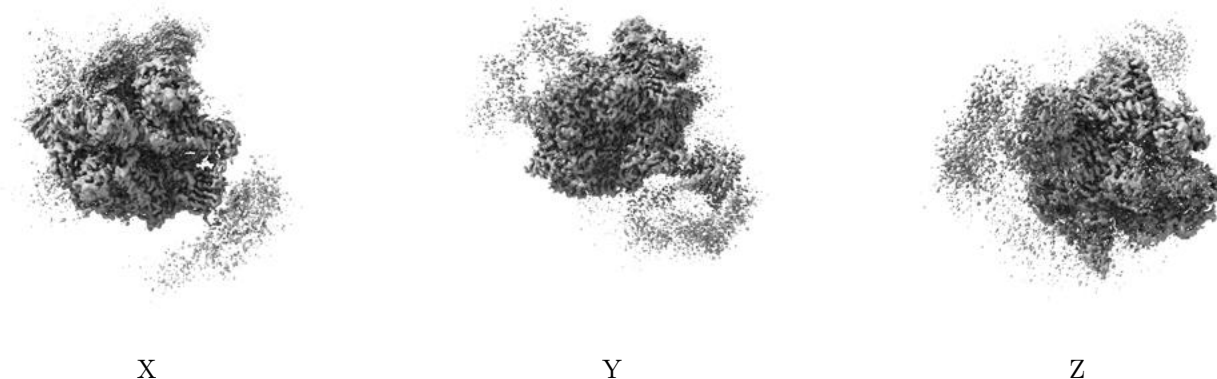


Z Index: 180

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

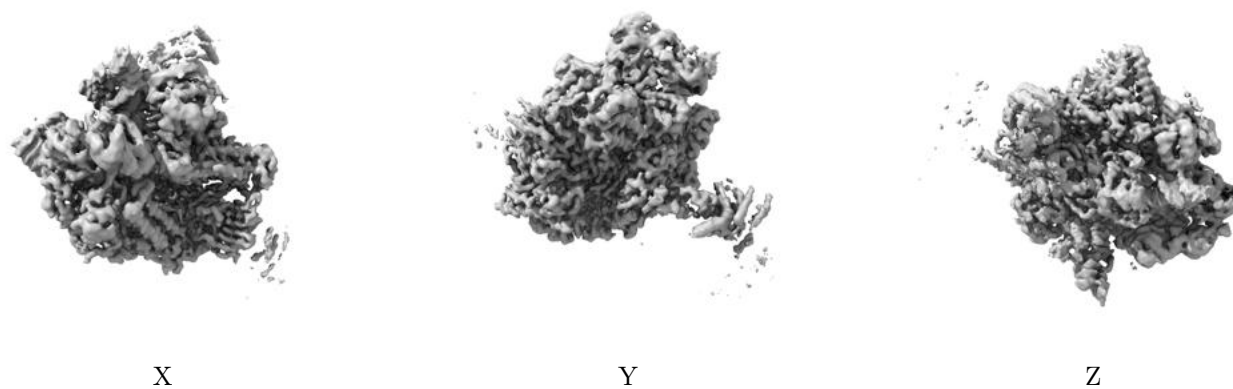
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

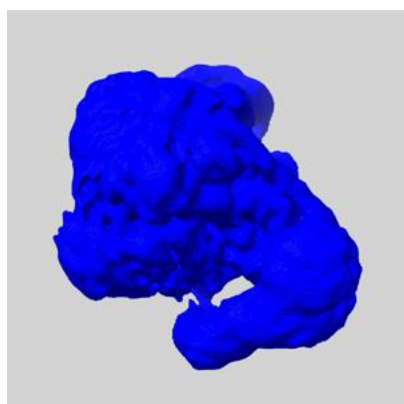
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

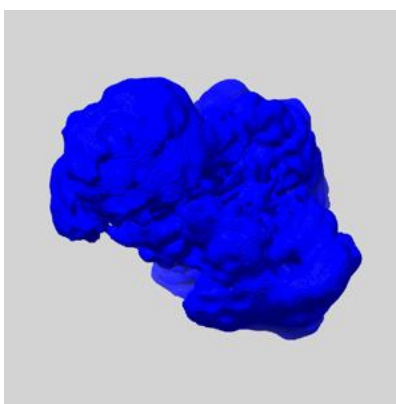
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

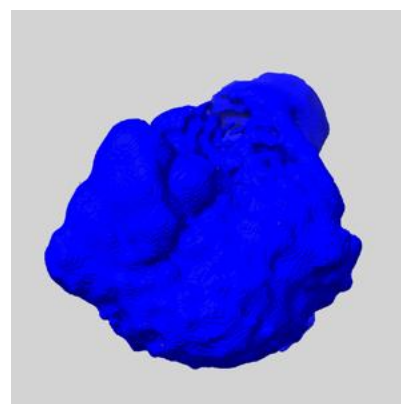
6.5.1 emd_10480_msk_1.map [i](#)



X

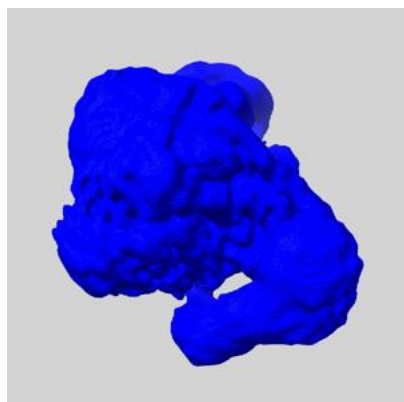


Y

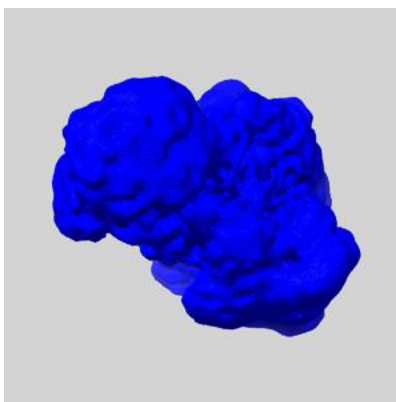


Z

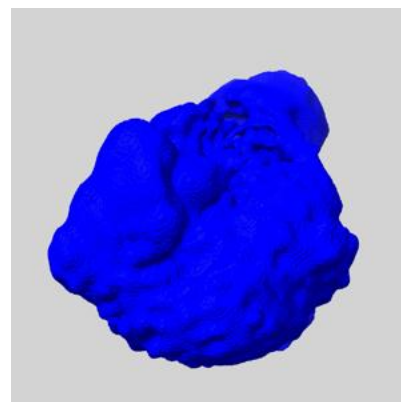
6.5.2 emd_10480_msk_2.map [i](#)



X



Y

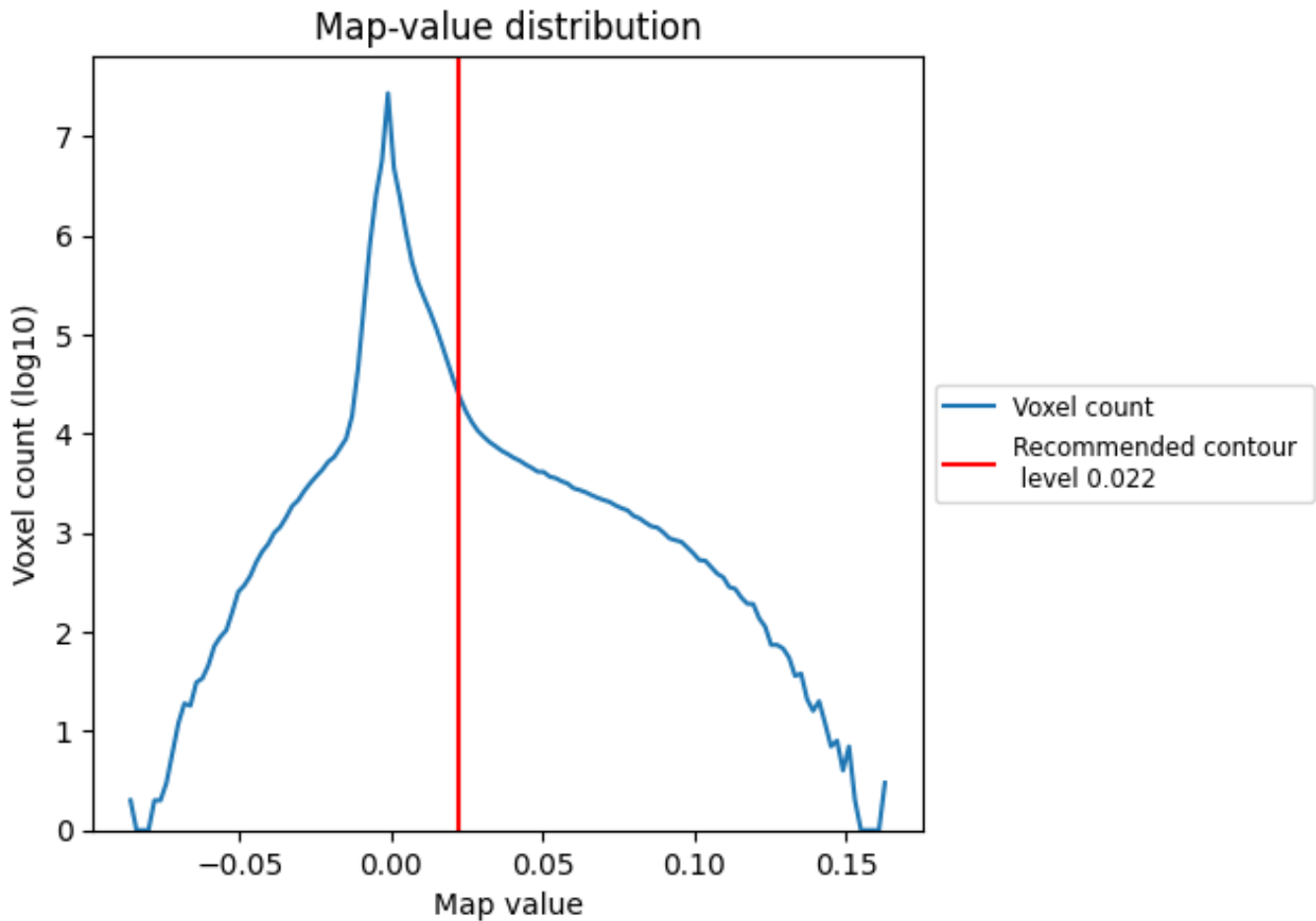


Z

7 Map analysis [i](#)

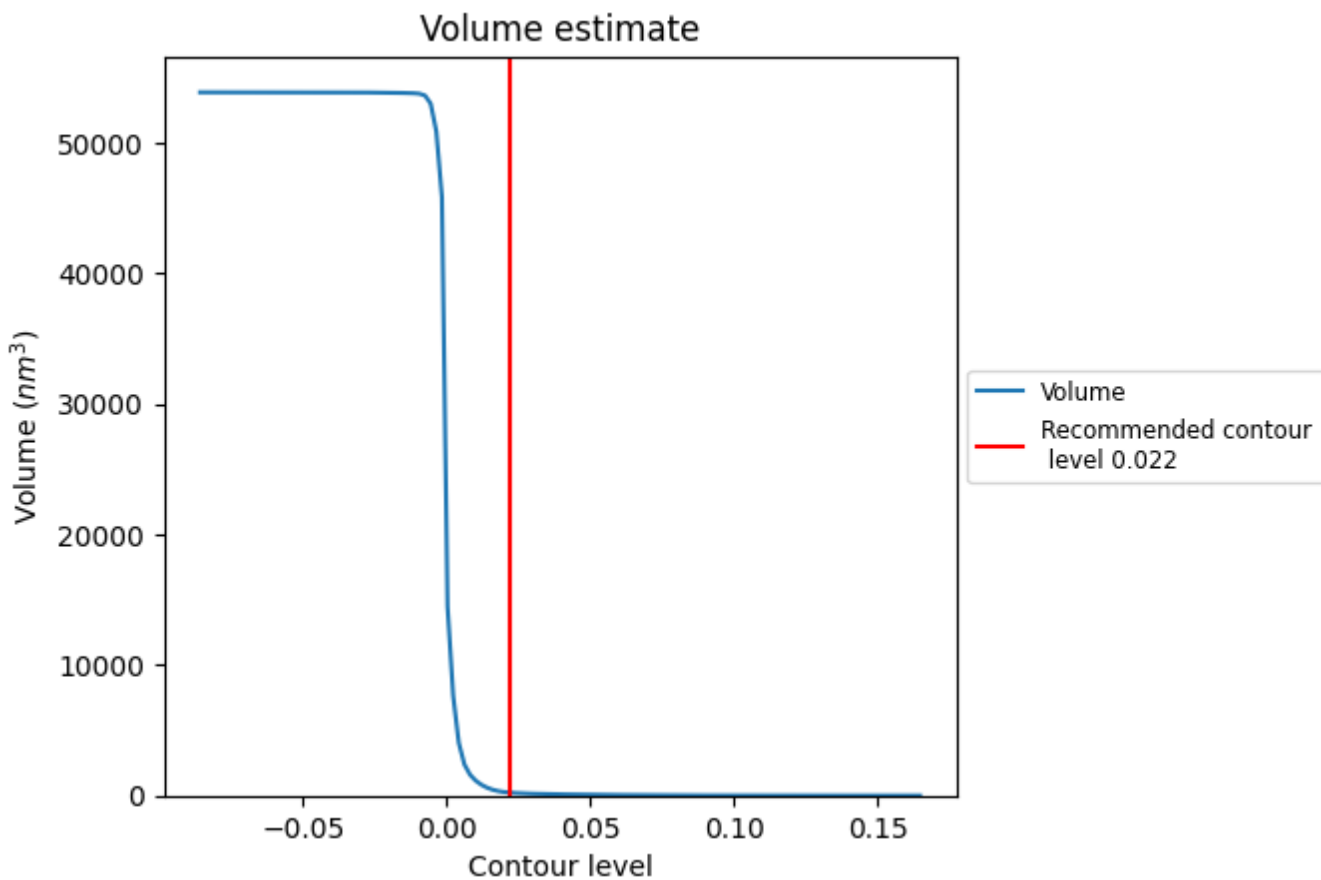
This section contains the results of statistical analysis of the map.

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.

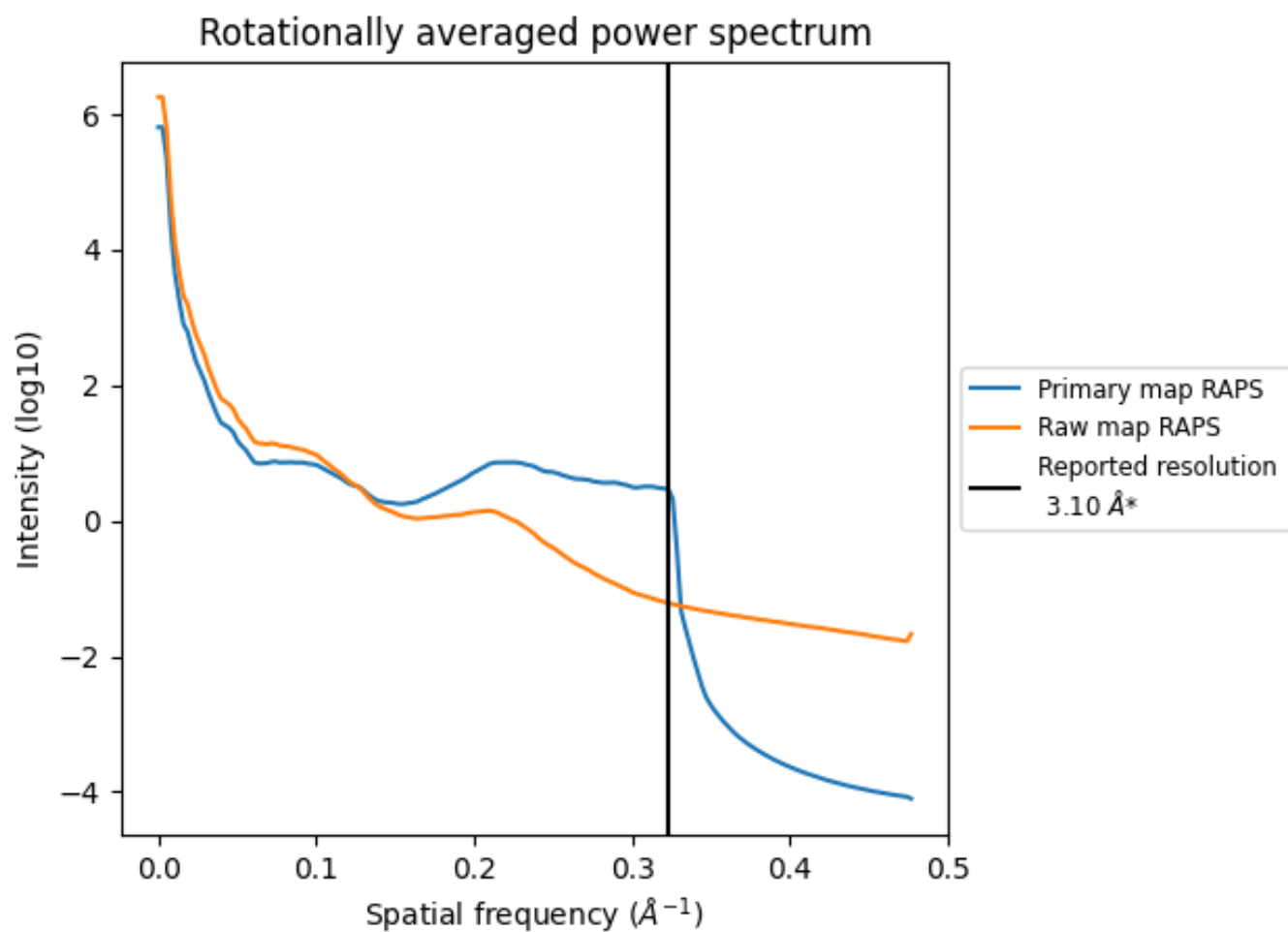
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 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

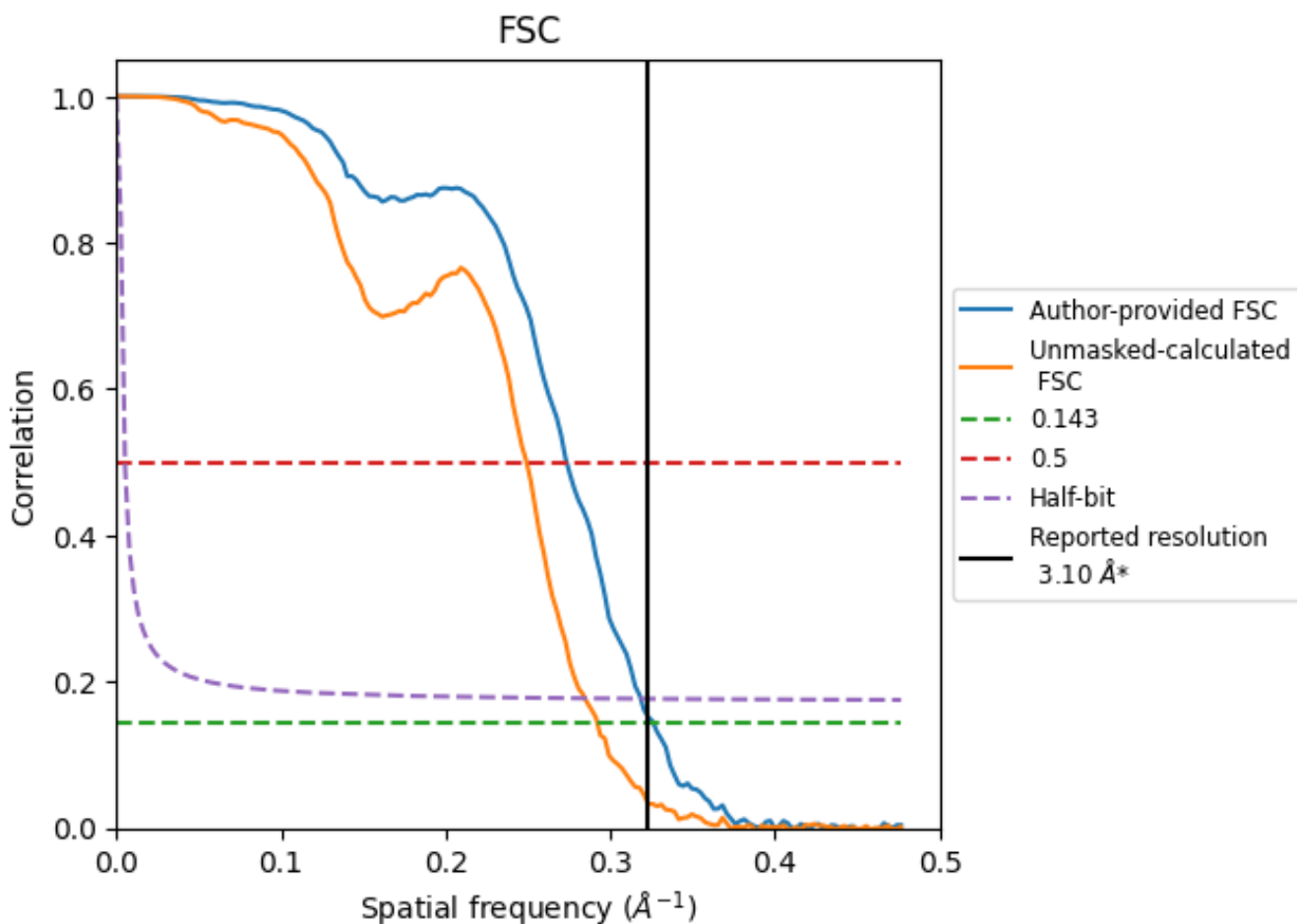


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

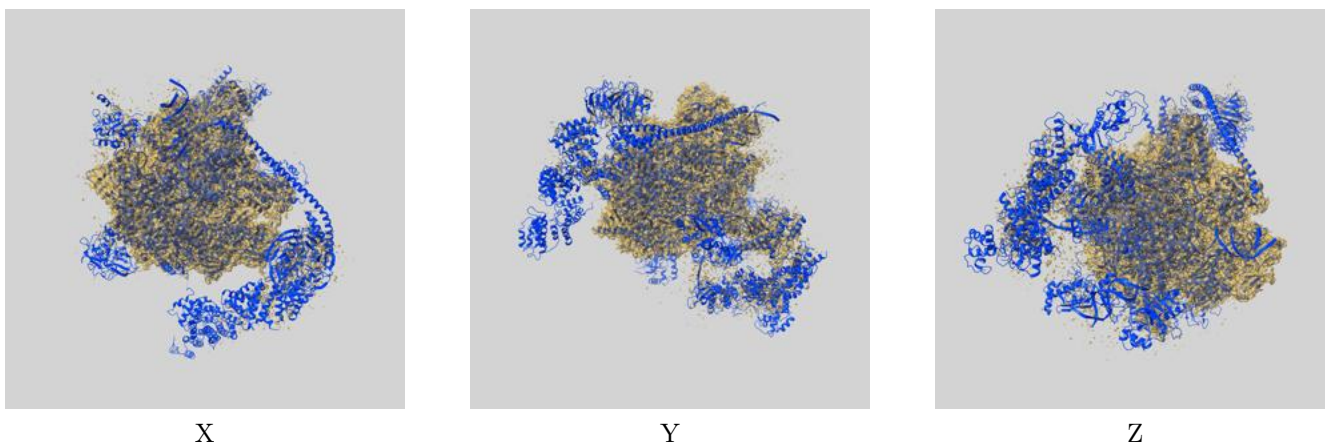
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.66	3.14
Unmasked-calculated*	3.42	4.01	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

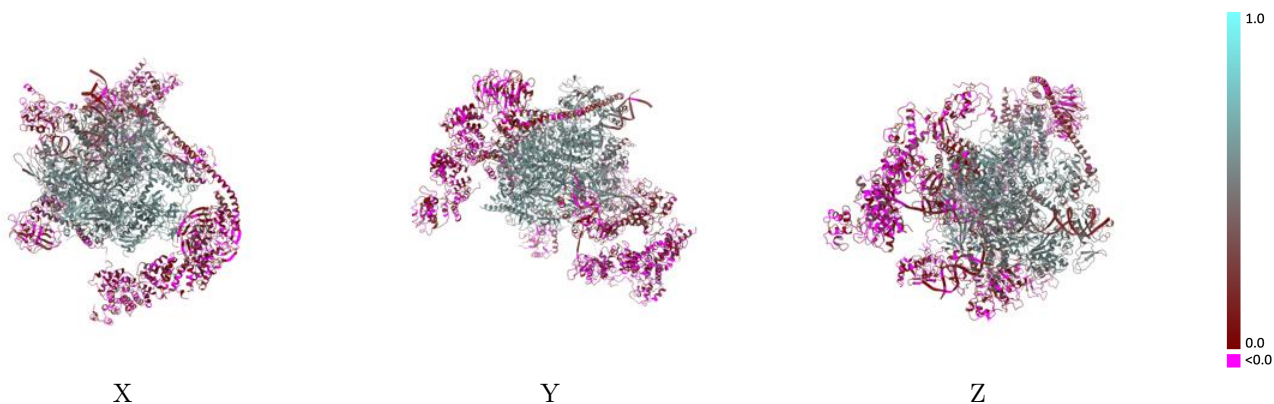
This section contains information regarding the fit between EMDB map EMD-10480 and PDB model 6TED. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



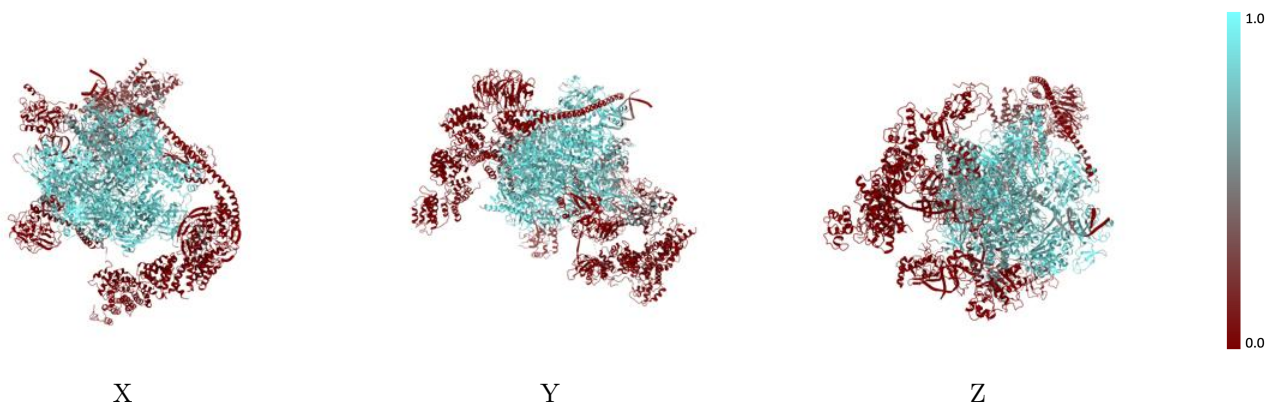
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



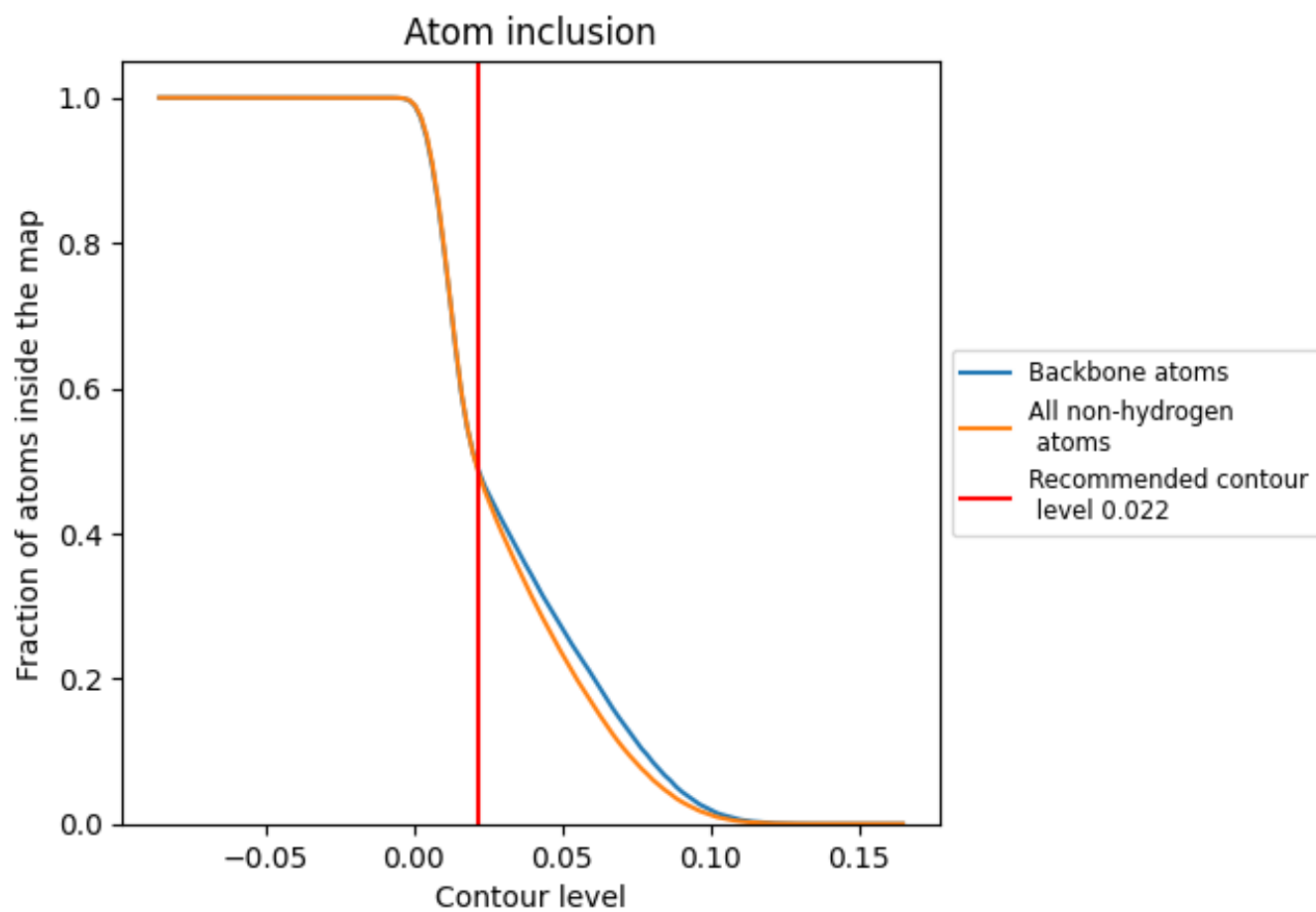
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4806	 0.3380
A	 0.8491	 0.5370
B	 0.8820	 0.5560
C	 0.9108	 0.5800
D	 0.2725	 0.1850
E	 0.8535	 0.5210
F	 0.8962	 0.5740
G	 0.4391	 0.3110
H	 0.8513	 0.5590
I	 0.8472	 0.5110
J	 0.9180	 0.5730
K	 0.9211	 0.5890
L	 0.8480	 0.5090
M	 0.0153	 0.0750
N	 0.3467	 0.2200
P	 0.4248	 0.2780
Q	 0.0282	 0.1020
R	 0.0117	 0.0880
T	 0.5195	 0.3100
U	 0.0548	 0.1140
V	 0.0256	 0.1270
W	 0.0109	 0.0430
X	 0.0235	 0.1060
Y	 0.0056	 0.0770
Z	 0.0993	 0.1660

