



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 09:13 pm GMT

PDB ID : 1H8H
Title : Bovine mitochondrial F1-ATPase crystallised in the presence of 5mm AMPPNP
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2001-02-06
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

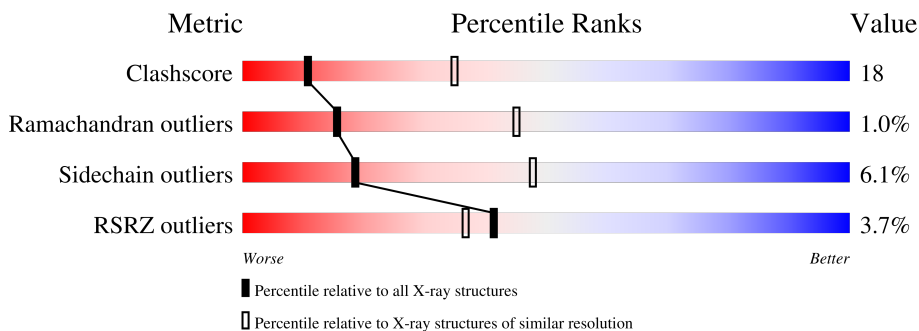
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	 2% 58% 33% 5% 5%
1	B	510	 2% 53% 37% 6% 6%
1	C	510	 % 58% 34% 6% 6%
2	D	482	 2% 60% 34% 6% 6%
2	E	482	 6% 53% 39% 6% 6%
2	F	482	 % 63% 29% 6% 6%

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Mol	Chain	Length	Quality of chain
3	G	272	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (12%), a green segment (26%), a yellow segment (15%), and a grey segment (55%). The percentages are labeled below each segment.</p>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 22941 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	engineered mutation	UNP P19483
B	481	GLY	SER	engineered mutation	UNP P19483
C	481	GLY	SER	engineered mutation	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

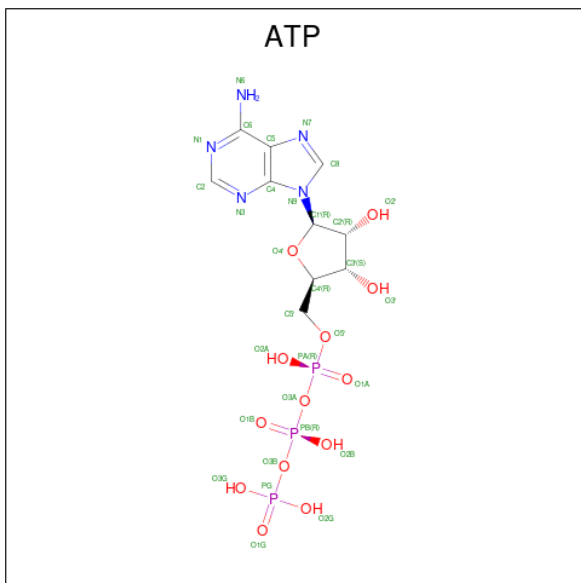
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	43	VAL	ILE	engineered mutation	UNP P05631

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

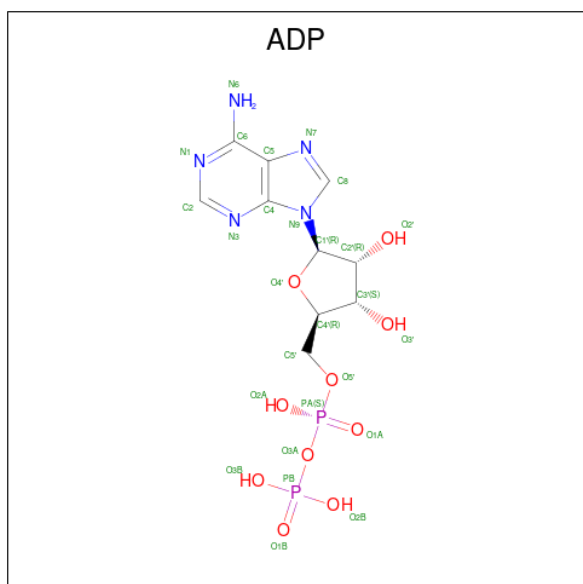
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



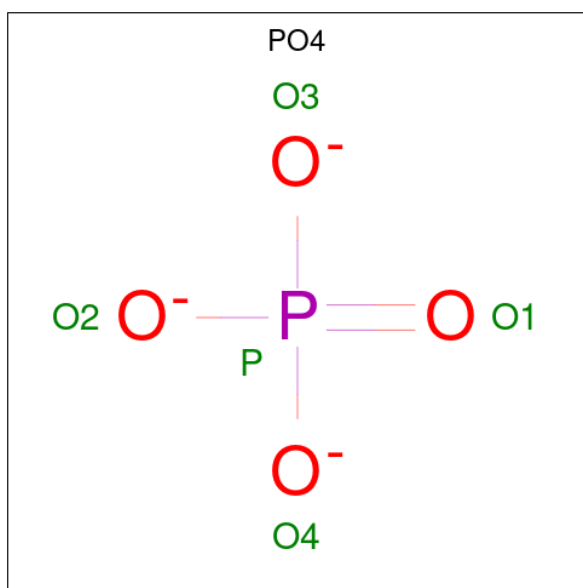
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	O P	0	0
			5	4 1		

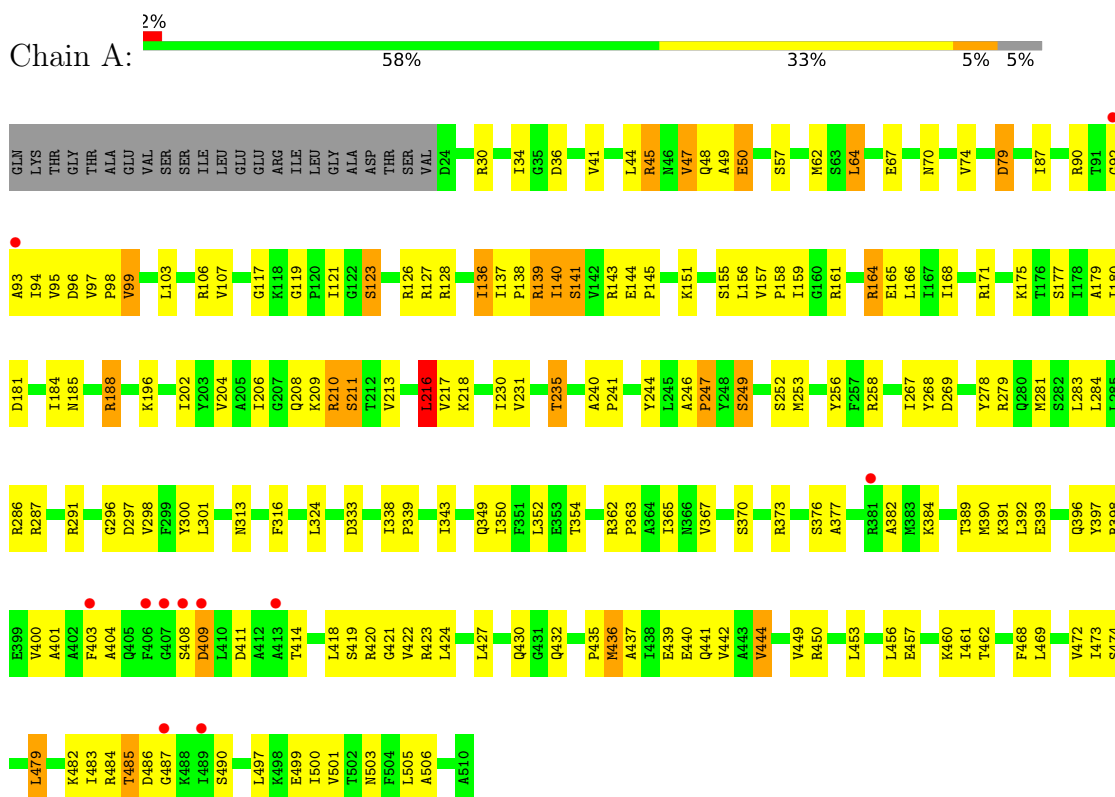
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total	O	0	0
			24	24		
9	B	26	Total	O	0	0
			26	26		
9	C	14	Total	O	0	0
			14	14		
9	D	15	Total	O	0	0
			15	15		
9	E	13	Total	O	0	0
			13	13		
9	F	17	Total	O	0	0
			17	17		
9	G	2	Total	O	0	0
			2	2		

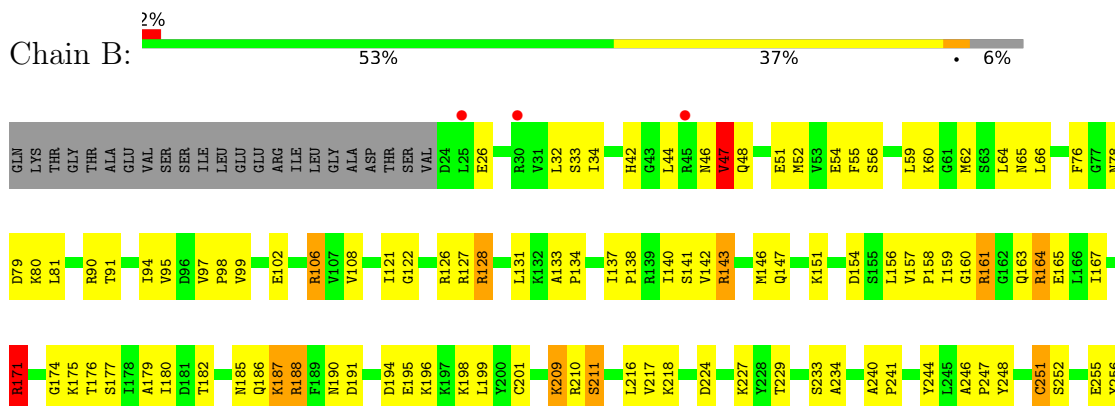
3 Residue-property plots i

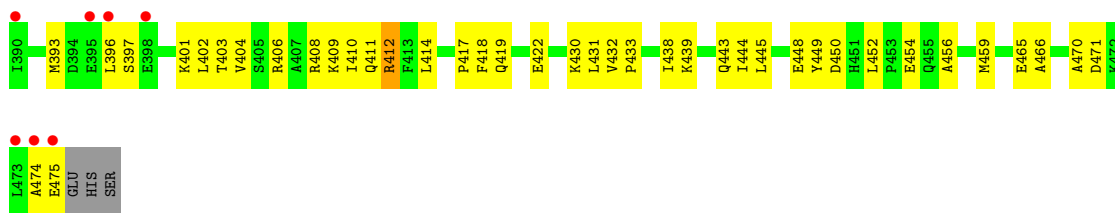
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: BOVINE MITOCHONDRIAL F1-ATPASE

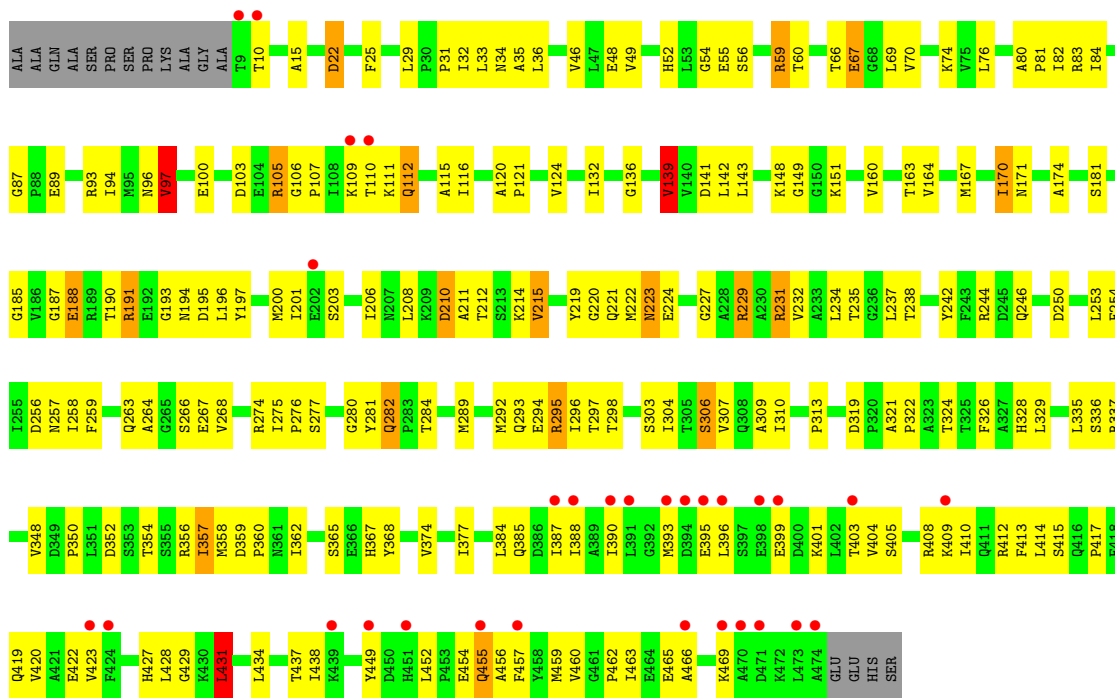


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

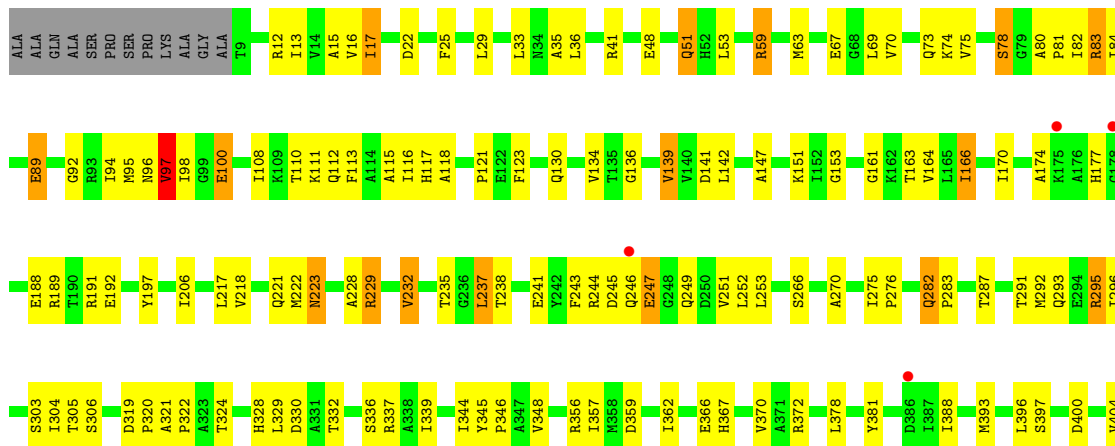


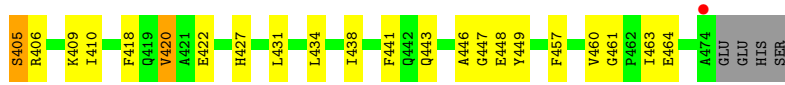


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

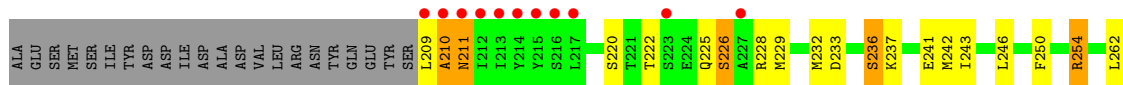
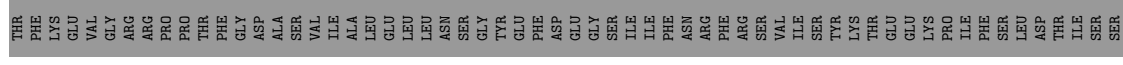
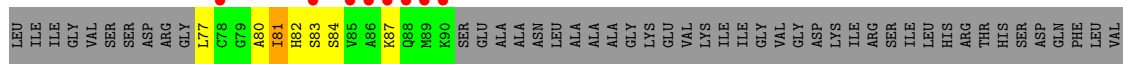
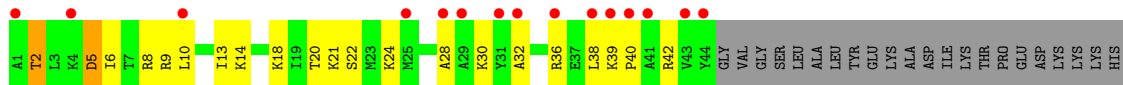


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE





● Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	280.00Å 107.00Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 37.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 96.5 (37.27-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.37 (at 2.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.292 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22941	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, GOL, ADP, PO4, ATP

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	0.54	0/3766	1.23	23/5080 (0.5%)
1	B	0.55	0/3704	1.20	20/4995 (0.4%)
1	C	0.57	0/3799	1.25	21/5126 (0.4%)
2	D	0.56	0/3596	1.23	17/4879 (0.3%)
2	E	0.50	0/3587	1.12	19/4867 (0.4%)
2	F	0.57	0/3587	1.23	21/4867 (0.4%)
3	G	0.44	0/949	0.93	1/1266 (0.1%)
All	All	0.54	0/22988	1.20	122/31080 (0.4%)

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	ARG	NE-CZ-NH2	-12.76	113.92	120.30
2	D	260	ARG	NE-CZ-NH2	12.66	126.63	120.30
2	D	93	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	C	373	ARG	CD-NE-CZ	11.85	140.18	123.60
1	C	139	ARG	NE-CZ-NH1	-11.79	114.40	120.30
2	F	189	ARG	NE-CZ-NH1	-11.43	114.59	120.30
2	D	44	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	291	ARG	NE-CZ-NH1	10.62	125.61	120.30
2	F	189	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	A	106	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	C	423	ARG	NE-CZ-NH2	-9.80	115.40	120.30
2	F	244	ARG	NE-CZ-NH2	-9.69	115.45	120.30
2	F	337	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	B	373	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	216	LEU	CA-CB-CG	9.15	136.34	115.30
1	A	210	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	C	164	ARG	NE-CZ-NH2	-8.96	115.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	NE-CZ-NH2	8.94	124.77	120.30
3	G	254	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	B	126	ARG	NE-CZ-NH1	8.79	124.69	120.30
2	D	44	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	E	274	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	C	373	ARG	NE-CZ-NH2	-8.29	116.15	120.30
2	E	319	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	90	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	126	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	164	ARG	CD-NE-CZ	7.88	134.63	123.60
1	B	304	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	A	291	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	106	ARG	CD-NE-CZ	7.70	134.37	123.60
1	B	373	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	E	231	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	90	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	304	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	D	97	VAL	CB-CA-C	-7.38	97.38	111.40
1	C	423	ARG	CD-NE-CZ	7.28	133.79	123.60
1	B	188	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	A	139	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	C	373	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	F	229	ARG	NE-CZ-NH2	7.07	123.83	120.30
2	E	191	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	279	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	269	ASP	CB-CG-OD1	7.01	124.61	118.30
2	F	191	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	E	83	ARG	CD-NE-CZ	6.98	133.37	123.60
2	F	100	GLU	OE1-CD-OE2	6.89	131.57	123.30
1	B	171	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	D	222	MET	CB-CA-C	-6.83	96.73	110.40
2	F	83	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	90	ARG	NE-CZ-NH2	6.76	123.68	120.30
2	F	41	ARG	CG-CD-NE	6.75	125.98	111.80
1	B	161	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	D	103	ASP	CB-CG-OD1	6.61	124.25	118.30
2	F	244	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	E	139	VAL	CB-CA-C	-6.48	99.08	111.40
1	B	308	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	106	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	D	105	ARG	CD-NE-CZ	6.41	132.57	123.60
2	E	229	ARG	NE-CZ-NH1	-6.37	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	D	139	VAL	CB-CA-C	-6.28	99.47	111.40
1	B	171	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	139	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	B	234	ALA	N-CA-CB	6.22	118.80	110.10
2	D	244	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	349	GLN	CA-CB-CG	6.18	127.01	113.40
2	E	277	SER	N-CA-CB	6.17	119.75	110.50
2	F	59	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	B	126	ARG	CD-NE-CZ	6.13	132.18	123.60
2	F	83	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	287	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	D	412	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	258	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	E	222	MET	CG-SD-CE	6.00	109.80	100.20
2	E	22	ASP	CB-CG-OD1	6.00	123.70	118.30
2	E	244	ARG	CD-NE-CZ	5.97	131.95	123.60
2	D	95	MET	C-N-CA	5.93	136.53	121.70
2	E	359	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	128	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	398	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	C	304	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	C	40	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	D	288	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	286	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	154	ASP	CB-CG-OD2	5.65	123.38	118.30
2	E	59	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	F	381	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	F	139	VAL	CB-CA-C	-5.58	100.81	111.40
2	E	97	VAL	CB-CA-C	-5.52	100.91	111.40
2	D	41	ARG	CD-NE-CZ	5.51	131.31	123.60
1	C	154	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	210	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	139	ARG	NH1-CZ-NH2	5.47	125.42	119.40
2	D	260	ARG	NH1-CZ-NH2	-5.45	113.40	119.40
1	A	92	GLY	C-N-CA	5.42	135.26	121.70
2	D	96	ASN	CB-CA-C	-5.40	99.59	110.40
1	B	244	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	B	371	VAL	CB-CA-C	-5.35	101.23	111.40
1	A	96	ASP	CB-CG-OD1	5.35	123.11	118.30
2	E	105	ARG	NE-CZ-NH1	-5.34	117.63	120.30
2	F	191	ARG	CA-CB-CG	5.34	125.15	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	E	431	LEU	CA-CB-CG	5.32	127.54	115.30
2	E	295	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	B	106	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	300	TYR	CA-CB-CG	5.26	123.39	113.40
1	B	164	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	F	97	VAL	CB-CA-C	-5.24	101.45	111.40
2	F	464	GLU	OE1-CD-OE2	5.21	129.56	123.30
1	C	127	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	F	381	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	450	ARG	NE-CZ-NH2	-5.15	117.73	120.30
2	F	191	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	A	92	GLY	CA-C-N	-5.11	105.95	117.20
1	C	142	VAL	CA-CB-CG1	5.09	118.53	110.90
2	F	295	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	47	VAL	CB-CA-C	-5.06	101.79	111.40
1	C	292	GLU	OE1-CD-OE2	5.05	129.36	123.30
2	E	67	GLU	CA-CB-CG	5.04	124.50	113.40
2	E	195	ASP	CB-CG-OD1	5.03	122.82	118.30
2	F	304	ILE	CB-CA-C	-5.02	101.56	111.60
1	C	47	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3814	134	0
1	B	3656	0	3765	158	0
1	C	3748	0	3844	151	0
2	D	3539	0	3592	127	0
2	E	3530	0	3587	160	0
2	F	3530	0	3587	127	0
3	G	945	0	1019	43	0
4	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	2	0
4	C	31	0	12	5	0
4	F	31	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	B	6	0	8	3	0
7	D	27	0	12	2	0
8	E	5	0	0	1	0
9	A	24	0	0	2	0
9	B	26	0	0	6	0
9	C	14	0	0	0	0
9	D	15	0	0	0	0
9	E	13	0	0	3	0
9	F	17	0	0	3	0
9	G	2	0	0	0	0
All	All	22941	0	23276	845	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 18.

All (845) 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)
1:B:351:PHE:HE2	1:B:353:GLU:HG2	1.26	1.01
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.43	1.00
2:F:12:ARG:HE	2:F:74:LYS:HE2	1.27	1.00
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.48	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.92
2:D:282:GLN:H	2:D:282:GLN:HE21	0.95	0.91
2:E:223:ASN:HD22	2:E:223:ASN:H	1.19	0.91
2:F:252:LEU:HD23	2:F:305:THR:HB	1.53	0.90
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.52	0.90
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.53	0.90
1:B:351:PHE:CE2	1:B:353:GLU:HG2	2.09	0.88
2:F:223:ASN:HD22	2:F:223:ASN:H	1.22	0.88
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.56	0.88
2:F:228:ALA:O	2:F:232:VAL:HG22	1.75	0.87
2:F:164:VAL:HG13	2:F:420:VAL:HG12	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:GLN:H	2:D:282:GLN:NE2	1.73	0.85
2:E:449:TYR:HB3	2:E:452:LEU:HD12	1.57	0.84
2:D:366:GLU:O	2:D:370:VAL:HG23	1.77	0.83
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.59	0.83
1:B:62:MET:HG3	1:B:95:VAL:HG21	1.59	0.82
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.82
1:C:338:ILE:HD12	1:C:338:ILE:H	1.44	0.81
1:C:175:LYS:HE2	4:C:600:ATP:O1B	1.80	0.80
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.63	0.80
1:A:218:LYS:HD2	2:D:128:VAL:HG21	1.64	0.79
1:C:99:VAL:HG13	1:C:253:MET:HA	1.64	0.78
2:E:419:GLN:HA	2:E:429:GLY:HA3	1.64	0.78
1:A:94:ILE:HG12	1:A:95:VAL:H	1.48	0.77
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.67	0.77
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.66	0.77
2:E:223:ASN:H	2:E:223:ASN:ND2	1.83	0.77
2:F:282:GLN:HE21	2:F:282:GLN:N	1.81	0.77
1:A:140:ILE:HD11	1:A:143:ARG:HH22	1.49	0.76
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.67	0.76
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.68	0.75
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.68	0.75
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.69	0.74
2:E:280:GLY:HA2	3:G:262:LEU:HD21	1.69	0.73
1:A:44:LEU:O	1:A:47:VAL:HG22	1.87	0.73
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.71	0.73
2:F:12:ARG:NE	2:F:74:LYS:HE2	2.03	0.72
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.70	0.72
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.70	0.72
1:B:497:LEU:HA	1:B:500:ILE:HD12	1.72	0.72
1:C:404:ALA:C	1:C:406:PHE:H	1.89	0.72
1:A:389:THR:HB	1:A:449:VAL:HG21	1.71	0.72
2:D:80:ALA:HB1	2:D:81:PRO:HD2	1.73	0.71
2:D:282:GLN:HE21	2:D:282:GLN:N	1.81	0.71
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.72	0.71
2:E:224:GLU:O	2:E:229:ARG:NH1	2.23	0.70
1:A:49:ALA:O	1:A:50:GLU:HB2	1.91	0.70
1:A:87:ILE:H	1:A:87:ILE:HD12	1.56	0.70
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.74	0.70
2:D:370:VAL:HG21	2:D:438:ILE:HG23	1.73	0.69
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.74	0.69
2:E:282:GLN:H	2:E:282:GLN:NE2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HB2	1:B:435:PRO:HB2	1.75	0.69
1:C:347:ASP:HA	1:C:373:ARG:HD2	1.73	0.69
1:C:432:GLN:NE2	4:C:600:ATP:H2'	2.07	0.69
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.56	0.69
2:D:346:PRO:HG3	2:D:418:PHE:CZ	2.28	0.68
2:E:282:GLN:H	2:E:282:GLN:HE21	1.40	0.68
1:C:295:PRO:O	1:C:298:VAL:HG23	1.93	0.68
2:F:359:ASP:HB3	2:F:362:ILE:HD12	1.74	0.68
2:E:276:PRO:HD2	3:G:266:ILE:CD1	2.21	0.68
2:F:16:VAL:C	2:F:17:ILE:HD12	2.13	0.68
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.75	0.68
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.74	0.68
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.28	0.68
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.76	0.67
1:B:303:SER:HB2	2:F:222:MET:HB2	1.77	0.67
1:C:472:VAL:HG23	1:C:480:LEU:HD11	1.77	0.67
3:G:2:THR:HG22	3:G:5:ASP:H	1.60	0.67
1:C:355:GLU:O	1:C:359:LYS:HG3	1.95	0.67
2:F:270:ALA:HA	9:F:2012:HOH:O	1.95	0.66
2:D:253:LEU:HD21	2:D:255:ILE:HD11	1.77	0.66
2:E:390:ILE:HG21	3:G:28:ALA:HB3	1.76	0.66
2:D:228:ALA:O	2:D:232:VAL:HG22	1.95	0.66
2:D:242:TYR:CE1	2:D:246:GLN:HG3	2.30	0.66
1:C:400:VAL:HG12	1:C:418:LEU:HD21	1.78	0.66
1:C:423:ARG:HD3	1:C:461:ILE:HD11	1.76	0.66
2:D:163:THR:HA	2:D:166:ILE:HG22	1.76	0.66
1:A:34:ILE:HD11	1:A:79:ASP:HB3	1.76	0.66
2:F:396:LEU:HD13	2:F:400:ASP:HB3	1.78	0.66
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.77	0.65
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.78	0.65
1:A:469:LEU:O	1:A:473:ILE:HG13	1.97	0.65
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.78	0.65
2:F:63:MET:HE3	2:F:97:VAL:HG11	1.77	0.65
1:A:202:ILE:HG12	1:A:230:ILE:HD12	1.77	0.65
2:F:252:LEU:CD2	2:F:305:THR:HB	2.25	0.65
2:F:388:ILE:HD12	2:F:393:MET:HG2	1.78	0.65
1:B:80:LYS:HD3	2:E:33:LEU:HD12	1.77	0.65
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.27	0.65
2:F:405:SER:O	2:F:409:LYS:HG3	1.96	0.65
2:E:223:ASN:HD22	2:E:223:ASN:N	1.94	0.64
2:E:49:VAL:HA	2:E:60:THR:HG22	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.80	0.64
2:E:387:ILE:H	2:E:387:ILE:HD12	1.62	0.64
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.80	0.64
2:F:13:ILE:CD1	2:F:69:LEU:HD13	2.28	0.64
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.78	0.64
1:A:408:SER:O	1:A:409:ASP:HB2	1.98	0.64
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.79	0.64
1:B:185:ASN:HB2	1:B:435:PRO:CB	2.28	0.64
1:C:292:GLU:O	1:C:293:ALA:HB3	1.98	0.63
2:D:96:ASN:HB2	2:D:100:GLU:O	1.99	0.63
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.81	0.63
2:E:32:ILE:O	2:E:33:LEU:HB2	1.97	0.63
1:B:78:ASN:OD1	1:B:80:LYS:HG2	1.99	0.63
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.29	0.63
1:A:196:LYS:H	1:A:196:LYS:HD2	1.64	0.62
2:E:48:GLU:OE2	2:E:231:ARG:NH2	2.30	0.62
1:A:432:GLN:OE1	4:A:600:ATP:H2'	1.99	0.62
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.81	0.62
1:B:171:ARG:HH22	2:E:356:ARG:HH21	1.47	0.62
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.29	0.62
2:F:406:ARG:HH21	2:F:447:GLY:HA3	1.65	0.62
1:B:151:LYS:HG3	1:B:430:GLN:OE1	1.99	0.62
2:F:287:THR:O	2:F:291:THR:HG23	2.00	0.62
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.80	0.62
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.81	0.62
1:C:127:ARG:HH21	1:C:131:LEU:HD12	1.64	0.62
2:E:404:VAL:O	2:E:408:ARG:HG3	2.00	0.62
1:A:188:ARG:NH2	1:A:436:MET:HA	2.14	0.61
2:D:29:LEU:HD12	2:D:30:PRO:HD2	1.82	0.61
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.83	0.61
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.31	0.61
1:C:215:GLN:HG3	2:F:356:ARG:HH12	1.64	0.61
1:B:158:PRO:O	1:B:375:GLY:HA3	2.00	0.61
1:B:486:ASP:C	1:B:488:LYS:H	2.04	0.61
2:D:196:LEU:HG	2:D:200:MET:HE2	1.82	0.61
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.31	0.61
1:C:44:LEU:O	1:C:47:VAL:HG22	2.01	0.61
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.83	0.61
3:G:10:LEU:HD21	3:G:246:LEU:HB2	1.83	0.61
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.83	0.60
2:F:164:VAL:HG13	2:F:420:VAL:CG1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:ILE:HG12	2:E:181:SER:CB	2.32	0.60
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.47	0.60
2:E:96:ASN:HD22	2:E:100:GLU:HB2	1.66	0.60
1:B:134:PRO:HD3	9:B:2012:HOH:O	2.01	0.60
2:E:66:THR:HB	2:E:69:LEU:HD12	1.83	0.60
1:A:278:TYR:HA	1:A:281:MET:HE2	1.84	0.60
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.16	0.60
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.65	0.60
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.60
1:B:420:ARG:HH21	1:B:451:GLY:HA2	1.66	0.60
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.36	0.59
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.82	0.59
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.31	0.59
1:B:453:LEU:HD13	1:B:461:ILE:HG23	1.83	0.59
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.84	0.59
1:B:419:SER:O	1:B:423:ARG:HG2	2.01	0.59
1:C:27:GLU:OE2	1:C:46:ASN:ND2	2.34	0.59
2:D:408:ARG:NH1	2:D:454:GLU:OE1	2.35	0.59
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.83	0.59
1:C:97:VAL:O	1:C:99:VAL:HG23	2.02	0.59
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.84	0.59
1:B:44:LEU:O	1:B:47:VAL:HG22	2.02	0.59
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.84	0.59
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.68	0.59
1:B:350:ILE:CG2	1:B:365:ILE:HG12	2.33	0.59
1:C:404:ALA:C	1:C:406:PHE:N	2.56	0.59
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.85	0.58
1:C:295:PRO:HD2	1:C:298:VAL:CG2	2.33	0.58
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.03	0.58
2:F:151:LYS:HD3	2:F:328:HIS:O	2.03	0.58
1:B:304:ARG:NH2	6:B:701:GOL:O2	2.37	0.58
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.39	0.58
2:D:9:THR:HG22	2:D:27:GLU:OE1	2.03	0.58
3:G:13:ILE:HD13	3:G:242:MET:SD	2.43	0.58
1:B:381:ARG:O	1:B:385:GLN:HG3	2.03	0.58
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.84	0.58
2:F:275:ILE:O	2:F:283:PRO:HG3	2.03	0.58
1:B:486:ASP:C	1:B:488:LYS:N	2.56	0.58
2:D:63:MET:HE3	2:D:97:VAL:HG11	1.84	0.58
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.85	0.58
2:D:419:GLN:O	2:D:422:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.87	0.58
2:D:101:PRO:HD3	2:D:108:ILE:HD12	1.86	0.58
2:D:130:GLN:HE22	2:D:356:ARG:HG2	1.68	0.58
2:D:143:LEU:CD1	2:D:350:PRO:HB3	2.34	0.57
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.86	0.57
1:C:23:VAL:HG12	1:C:23:VAL:O	2.04	0.57
1:C:335:SER:O	2:D:314:ALA:HB1	2.04	0.57
1:C:362:ARG:HA	1:C:363:PRO:C	2.25	0.57
2:E:231:ARG:O	2:E:234:LEU:HB2	2.04	0.57
2:F:94:ILE:HG12	2:F:217:LEU:HD12	1.85	0.57
2:E:352:ASP:O	2:E:354:THR:HG23	2.04	0.57
2:E:422:GLU:HG2	2:E:427:HIS:O	2.03	0.57
2:F:422:GLU:HG2	2:F:427:HIS:O	2.04	0.57
1:B:251:CYS:HB2	1:B:268:TYR:OH	2.04	0.57
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.39	0.57
1:A:99:VAL:HG22	1:A:253:MET:HA	1.87	0.57
2:D:49:VAL:HA	2:D:60:THR:HG22	1.86	0.57
1:A:140:ILE:CD1	1:A:143:ARG:HH22	2.16	0.57
2:F:166:ILE:O	2:F:170:ILE:HG13	2.05	0.57
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.86	0.57
2:E:254:PHE:HA	2:E:307:VAL:O	2.04	0.57
1:A:99:VAL:CG2	1:A:253:MET:HA	2.35	0.57
1:A:389:THR:HG22	1:A:393:GLU:OE2	2.05	0.57
2:F:174:ALA:O	2:F:177:HIS:HB3	2.04	0.57
1:A:497:LEU:O	1:A:501:VAL:HG22	2.04	0.56
1:A:151:LYS:HE2	1:A:427:LEU:O	2.05	0.56
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.87	0.56
2:F:446:ALA:HB3	2:F:448:GLU:HG3	1.87	0.56
1:A:127:ARG:HD3	1:A:252:SER:HB3	1.87	0.56
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.20	0.56
2:F:130:GLN:HB3	2:F:357:ILE:HD12	1.86	0.56
2:F:223:ASN:HD22	2:F:223:ASN:N	1.97	0.56
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.86	0.56
1:B:420:ARG:HH21	1:B:451:GLY:CA	2.19	0.56
1:B:496:LYS:HG2	1:B:500:ILE:HD11	1.88	0.56
1:C:128:ARG:O	1:C:252:SER:OG	2.24	0.56
3:G:38:LEU:HD11	3:G:42:ARG:NH2	2.21	0.56
1:B:187:LYS:NZ	1:B:224:ASP:HB3	2.20	0.56
1:B:383:MET:SD	1:B:387:ALA:HB2	2.45	0.56
1:C:174:GLY:HA2	4:C:600:ATP:PA	2.45	0.56
1:C:295:PRO:HD2	1:C:298:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.40	0.56
1:C:343:ILE:HG22	2:D:158:ALA:HB1	1.87	0.56
1:C:414:THR:O	1:C:418:LEU:HG	2.06	0.56
1:C:452:TYR:OH	1:C:498:LYS:HD2	2.06	0.56
2:D:430:LYS:HD2	2:D:465:GLU:OE2	2.05	0.56
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.20	0.56
2:D:292:MET:CE	2:D:293:GLN:HG2	2.36	0.56
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.71	0.56
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.88	0.56
2:D:63:MET:CE	2:D:97:VAL:HG11	2.37	0.55
1:B:209:LYS:HB3	2:E:294:GLU:OE2	2.06	0.55
2:F:245:ASP:C	2:F:247:GLU:H	2.10	0.55
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.36	0.55
2:D:279:VAL:HG12	2:D:279:VAL:O	2.06	0.55
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.89	0.55
1:A:36:ASP:O	1:A:284:LEU:HD13	2.07	0.55
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.21	0.55
1:B:468:PHE:O	1:B:472:VAL:HG22	2.07	0.55
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.22	0.55
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.41	0.55
1:B:165:GLU:O	1:B:325:PRO:HD2	2.06	0.55
1:C:225:ALA:HA	1:C:228:TYR:CE2	2.42	0.54
2:D:324:THR:HG22	2:D:324:THR:O	2.07	0.54
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.88	0.54
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.72	0.54
3:G:6:ILE:HG21	3:G:250:PHE:HB2	1.90	0.54
1:C:105:GLY:HA2	1:C:226:MET:O	2.07	0.54
1:B:410:LEU:O	1:B:411:ASP:HB3	2.08	0.54
2:F:89:GLU:CD	2:F:89:GLU:H	2.10	0.54
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.89	0.54
2:D:16:VAL:HG13	2:D:21:VAL:HG22	1.89	0.54
2:E:96:ASN:OD1	2:E:97:VAL:HG23	2.08	0.54
1:C:443:ALA:O	1:C:446:TYR:HB3	2.07	0.54
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.88	0.54
1:A:136:ILE:HG13	2:E:194:ASN:HB2	1.89	0.54
1:A:188:ARG:HH22	1:A:436:MET:HA	1.73	0.54
1:B:171:ARG:HB2	1:B:171:ARG:HH11	1.73	0.54
2:D:388:ILE:HG21	2:D:396:LEU:HD11	1.90	0.54
1:B:146:MET:HG3	1:B:322:THR:HG21	1.89	0.53
2:D:363:VAL:HB	2:D:367:HIS:ND1	2.23	0.53
2:E:264:ALA:O	2:E:268:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:393:MET:SD	2:F:404:VAL:HG11	2.48	0.53
1:A:157:VAL:N	1:A:158:PRO:CD	2.71	0.53
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.53
1:A:486:ASP:OD2	1:A:490:SER:HB3	2.08	0.53
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.91	0.53
1:A:48:GLN:HG2	2:E:70:VAL:HG22	1.91	0.53
2:E:390:ILE:HG21	3:G:28:ALA:CB	2.38	0.53
2:E:170:ILE:HD13	2:E:215:VAL:HG21	1.89	0.53
2:E:357:ILE:HB	2:E:362:ILE:HG21	1.90	0.53
2:E:454:GLU:O	2:E:456:ALA:N	2.42	0.53
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.39	0.53
2:D:345:TYR:HA	2:D:346:PRO:C	2.28	0.53
2:F:223:ASN:H	2:F:223:ASN:ND2	2.00	0.53
2:D:277:SER:OG	2:D:278:ALA:N	2.41	0.53
2:D:410:ILE:HD11	2:D:445:LEU:HD23	1.91	0.53
1:B:65:ASN:HD22	2:F:17:ILE:HG23	1.74	0.53
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.90	0.53
2:D:417:PRO:CA	2:D:459:MET:HE1	2.39	0.53
2:E:367:HIS:HA	2:E:438:ILE:HD12	1.91	0.52
2:F:84:ILE:O	2:F:84:ILE:HG13	2.08	0.52
2:D:292:MET:HE2	2:D:293:GLN:HG2	1.92	0.52
3:G:210:ALA:O	3:G:211:ASN:C	2.47	0.52
1:A:188:ARG:HH21	1:A:437:ALA:N	2.07	0.52
1:B:174:GLY:HA2	4:B:600:ATP:PA	2.50	0.52
2:E:282:GLN:HE21	2:E:282:GLN:N	2.07	0.52
2:F:161:GLY:HA3	9:F:2007:HOH:O	2.09	0.52
2:D:151:LYS:HE2	2:D:328:HIS:O	2.10	0.52
2:F:111:LYS:HB2	2:F:112:GLN:OE1	2.10	0.52
1:B:248:TYR:CG	6:B:701:GOL:H12	2.45	0.52
1:C:129:VAL:O	1:C:308:ARG:NH1	2.42	0.52
2:D:196:LEU:HG	2:D:200:MET:CE	2.39	0.52
3:G:20:THR:HG22	3:G:236:SER:HB3	1.92	0.52
1:A:94:ILE:HG21	1:A:128:ARG:NH1	2.24	0.52
1:A:419:SER:O	1:A:423:ARG:HD3	2.10	0.52
1:B:327:ILE:HD11	1:B:342:VAL:HG21	1.92	0.52
1:C:152:ALA:CB	1:C:365:ILE:HD12	2.39	0.52
2:D:93:ARG:NH2	2:D:106:GLY:O	2.26	0.52
1:A:151:LYS:HZ1	1:A:430:GLN:HB2	1.75	0.52
1:C:75:VAL:HG21	1:C:79:ASP:HB3	1.91	0.52
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.09	0.52
1:C:44:LEU:O	2:D:71:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:C:404:ALA:O	1:C:406:PHE:N	2.43	0.51
2:E:84:ILE:HD13	2:E:235:THR:HG23	1.92	0.51
2:E:415:SER:HB2	2:E:459:MET:SD	2.51	0.51
1:A:503:ASN:O	1:A:506:ALA:HB3	2.10	0.51
2:D:186:VAL:HG12	2:D:260:ARG:HB2	1.92	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.73	0.51
1:A:339:PRO:O	1:A:343:ILE:HG13	2.10	0.51
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.76	0.51
1:C:48:GLN:HG2	2:D:70:VAL:CG2	2.39	0.51
2:D:9:THR:HG21	2:D:28:GLY:H	1.74	0.51
2:E:258:ILE:CG2	2:E:310:ILE:HG12	2.40	0.51
1:C:418:LEU:O	1:C:422:VAL:HG23	2.11	0.51
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.92	0.51
1:C:303:SER:HB2	2:D:222:MET:HB3	1.92	0.51
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.91	0.51
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.41	0.51
2:F:357:ILE:O	2:F:359:ASP:N	2.43	0.51
1:A:107:VAL:HG13	1:A:231:VAL:HG12	1.92	0.51
1:C:291:ARG:HD3	1:C:337:TYR:CD1	2.45	0.51
2:D:252:LEU:HD23	2:D:305:THR:HB	1.92	0.51
2:F:247:GLU:HG2	2:F:249:GLN:HG2	1.91	0.51
1:B:62:MET:HG3	1:B:95:VAL:CG2	2.35	0.51
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.45	0.51
1:C:373:ARG:HA	7:D:600:ADP:O3'	2.11	0.51
1:C:479:LEU:HD11	1:C:497:LEU:HG	1.92	0.51
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.38	0.51
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.92	0.51
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.92	0.51
1:C:338:ILE:O	1:C:339:PRO:C	2.47	0.51
2:E:405:SER:O	2:E:409:LYS:HG3	2.10	0.51
2:E:434:LEU:O	2:E:438:ILE:HG12	2.11	0.51
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.46	0.51
1:A:457:GLU:HB3	1:A:460:LYS:HE3	1.92	0.51
1:B:175:LYS:NZ	9:B:2006:HOH:O	2.43	0.50
1:C:74:VAL:HG13	1:C:241:PRO:CG	2.41	0.50
2:F:357:ILE:HG23	2:F:362:ILE:HG21	1.93	0.50
1:A:411:ASP:OD2	1:A:414:THR:HG23	2.12	0.50
2:E:321:ALA:N	2:E:322:PRO:HD2	2.27	0.50
3:G:39:LYS:N	3:G:40:PRO:HD2	2.26	0.50
1:B:157:VAL:O	1:B:159:ILE:HD13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ARG:HD3	4:C:600:ATP:C2	2.46	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.30	0.50
2:F:406:ARG:HH21	2:F:447:GLY:CA	2.24	0.50
1:C:174:GLY:HA2	4:C:600:ATP:O5'	2.12	0.50
2:D:165:LEU:O	2:D:169:LEU:HG	2.11	0.50
2:D:139:VAL:HG12	2:D:143:LEU:HD12	1.93	0.50
3:G:38:LEU:O	3:G:42:ARG:HG3	2.10	0.50
1:C:382:ALA:HA	1:C:385:GLN:OE1	2.12	0.50
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.93	0.50
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.46	0.50
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.93	0.50
1:B:339:PRO:O	1:B:343:ILE:HG13	2.11	0.50
1:B:423:ARG:O	1:B:426:GLU:N	2.44	0.50
2:D:89:GLU:HG2	2:D:110:THR:CG2	2.41	0.50
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.27	0.50
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.93	0.50
1:A:188:ARG:NH2	1:A:436:MET:C	2.66	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.26	0.50
2:E:89:GLU:OE2	2:E:110:THR:HG22	2.11	0.50
2:F:95:MET:HE3	2:F:108:ILE:HD13	1.92	0.50
1:C:110:ALA:HB2	1:C:246:ALA:HB2	1.94	0.49
1:C:127:ARG:NH2	1:C:131:LEU:HD12	2.26	0.49
2:F:164:VAL:HG23	4:F:600:ATP:O1A	2.13	0.49
1:B:479:LEU:CD1	1:B:497:LEU:HD13	2.42	0.49
2:E:393:MET:HG3	2:E:396:LEU:HD11	1.94	0.49
1:B:141:SER:O	1:B:143:ARG:HD2	2.13	0.49
1:B:167:ILE:HG22	1:B:175:LYS:HG2	1.95	0.49
2:D:9:THR:HG22	2:D:27:GLU:HB2	1.95	0.49
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.95	0.49
1:A:151:LYS:NZ	1:A:430:GLN:HB2	2.26	0.49
1:B:106:ARG:NH1	1:B:121:ILE:HD13	2.27	0.49
1:B:400:VAL:HG12	1:B:418:LEU:HD21	1.93	0.49
1:C:438:ILE:O	1:C:442:VAL:HG23	2.12	0.49
2:D:161:GLY:O	2:D:162:LYS:C	2.51	0.49
2:E:116:ILE:HA	2:E:238:THR:OG1	2.12	0.49
1:C:292:GLU:O	1:C:293:ALA:CB	2.61	0.49
2:E:149:GLY:HA2	2:E:304:ILE:O	2.12	0.49
2:F:134:VAL:HA	2:F:141:ASP:OD1	2.13	0.49
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.78	0.49
1:B:361:ILE:HD12	1:B:429:LYS:HE2	1.94	0.49
2:D:314:ALA:O	2:D:315:ASP:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.48	0.49
3:G:28:ALA:HA	3:G:229:MET:SD	2.53	0.49
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.28	0.49
1:B:299:PHE:HB3	9:B:2017:HOH:O	2.11	0.49
2:E:399:GLU:O	2:E:403:THR:HG23	2.12	0.49
2:D:162:LYS:HE3	2:D:311:TYR:HA	1.94	0.49
2:F:221:GLN:NE2	2:F:221:GLN:HA	2.27	0.49
2:F:367:HIS:HA	2:F:438:ILE:HD12	1.93	0.49
1:B:210:ARG:O	1:B:211:SER:C	2.51	0.49
1:C:168:ILE:O	1:C:351:PHE:HA	2.12	0.49
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.94	0.49
2:E:151:LYS:HB2	2:E:328:HIS:O	2.13	0.49
2:E:174:ALA:HB3	2:E:214:LYS:HD3	1.94	0.49
2:F:51:GLN:HG2	2:F:59:ARG:HB3	1.95	0.49
3:G:81:ILE:HG22	3:G:82:HIS:N	2.28	0.49
1:B:98:PRO:O	1:B:99:VAL:HG23	2.13	0.49
1:C:240:ALA:N	1:C:241:PRO:CD	2.75	0.49
1:C:297:ASP:HA	2:D:267:GLU:HG2	1.94	0.49
1:B:59:LEU:HD12	9:B:2001:HOH:O	2.12	0.48
1:B:102:GLU:HG3	1:B:122:GLY:C	2.33	0.48
2:E:151:LYS:HG2	2:E:293:GLN:OE1	2.13	0.48
2:E:257:ASN:HB2	2:E:309:ALA:O	2.13	0.48
2:F:188:GLU:O	2:F:221:GLN:HB3	2.13	0.48
2:F:241:GLU:CD	2:F:295:ARG:HH21	2.16	0.48
2:F:324:THR:O	2:F:324:THR:HG22	2.12	0.48
1:A:188:ARG:NH2	1:A:437:ALA:N	2.60	0.48
1:B:486:ASP:O	1:B:488:LYS:N	2.46	0.48
2:D:417:PRO:HG2	2:D:430:LYS:H	1.78	0.48
2:D:439:LYS:O	2:D:443:GLN:HG3	2.11	0.48
2:D:474:ALA:O	2:D:475:GLU:HB2	2.14	0.48
1:C:100:GLY:HA2	1:C:256:TYR:CE2	2.48	0.48
1:C:213:VAL:O	1:C:216:LEU:HB3	2.13	0.48
2:D:346:PRO:HG3	2:D:418:PHE:HZ	1.74	0.48
2:E:196:LEU:HD23	2:E:219:TYR:OH	2.13	0.48
2:E:221:GLN:N	2:E:224:GLU:OE2	2.44	0.48
1:C:55:PHE:O	1:C:56:SER:C	2.51	0.48
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.36	0.48
2:F:319:ASP:O	2:F:320:PRO:C	2.52	0.48
1:A:87:ILE:HD12	1:A:87:ILE:N	2.27	0.48
1:A:180:ILE:O	1:A:184:ILE:HG12	2.12	0.48
1:A:213:VAL:O	1:A:216:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ILE:HA	2:F:238:THR:OG1	2.13	0.48
1:B:127:ARG:HE	1:B:131:LEU:HD12	1.78	0.48
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.48	0.48
1:C:176:THR:OG1	1:C:269:ASP:OD2	2.32	0.48
1:C:323:ALA:O	1:C:324:LEU:HD23	2.14	0.48
1:A:184:ILE:HB	1:A:435:PRO:HG3	1.95	0.48
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.94	0.48
1:C:76:PHE:HB3	1:C:242:LEU:HD21	1.96	0.48
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.95	0.48
2:F:89:GLU:OE2	2:F:110:THR:HG22	2.14	0.48
3:G:20:THR:HG23	3:G:232:MET:HE3	1.96	0.48
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.79	0.48
3:G:222:THR:O	3:G:226:SER:OG	2.31	0.48
1:A:151:LYS:NZ	1:A:430:GLN:OE1	2.47	0.48
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.46	0.48
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.29	0.48
1:A:479:LEU:O	1:A:479:LEU:HD22	2.14	0.48
1:C:432:GLN:O	1:C:433:TYR:HB2	2.14	0.48
1:C:476:HIS:CD2	1:C:500:ILE:HD11	2.48	0.48
2:F:366:GLU:O	2:F:370:VAL:HG23	2.13	0.48
1:A:175:LYS:HE3	4:A:600:ATP:O1B	2.14	0.47
1:A:240:ALA:N	1:A:241:PRO:CD	2.77	0.47
1:B:80:LYS:HG3	1:B:81:LEU:N	2.29	0.47
1:B:133:ALA:HB1	1:B:134:PRO:HD2	1.96	0.47
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.49	0.47
1:B:441:GLN:O	1:B:445:ILE:HG12	2.14	0.47
1:C:137:ILE:HG21	2:D:104:GLU:OE1	2.14	0.47
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.44	0.47
1:B:361:ILE:CD1	1:B:429:LYS:HE2	2.44	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.44	0.47
1:B:201:CYS:O	1:B:229:THR:HA	2.14	0.47
2:E:449:TYR:CE2	2:E:463:ILE:HG12	2.49	0.47
1:A:97:VAL:HG11	1:A:249:SER:HB3	1.97	0.47
1:A:144:GLU:HB2	1:A:161:ARG:HG3	1.96	0.47
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.43	0.47
1:B:388:GLY:O	1:B:392:LEU:HG	2.13	0.47
2:E:89:GLU:HG3	2:E:109:LYS:O	2.15	0.47
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.15	0.47
2:E:462:PRO:HG2	2:E:465:GLU:HG3	1.96	0.47
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:HA	9:E:2009:HOH:O	2.13	0.47
1:C:52:MET:HE2	1:C:61:GLY:O	2.15	0.47
2:E:10:THR:HG23	2:E:76:LEU:HD23	1.97	0.47
2:E:256:ASP:HA	2:E:257:ASN:HA	1.58	0.47
1:B:210:ARG:NH1	2:E:121:PRO:O	2.45	0.47
1:B:347:ASP:C	1:B:373:ARG:HG3	2.34	0.47
1:C:170:ASP:O	1:C:175:LYS:NZ	2.40	0.47
2:D:92:GLY:HA2	2:D:206:ILE:HG12	1.96	0.47
2:D:411:GLN:O	2:D:414:LEU:HB2	2.13	0.47
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.96	0.47
2:E:455:GLN:O	2:E:469:LYS:HD3	2.15	0.47
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.44	0.47
1:A:180:ILE:O	1:A:181:ASP:C	2.53	0.47
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.79	0.47
1:A:376:SER:O	1:A:377:ALA:C	2.52	0.47
1:B:141:SER:OG	1:B:143:ARG:NH1	2.47	0.47
1:C:40:ARG:NH1	1:C:70:ASN:OD1	2.48	0.47
1:C:186:GLN:HA	1:C:189:PHE:CE2	2.50	0.47
1:C:360:GLY:HA2	1:C:362:ARG:NH1	2.30	0.47
2:D:198:HIS:O	2:D:202:GLU:HG2	2.15	0.47
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.97	0.47
3:G:237:LYS:O	3:G:241:GLU:HG3	2.15	0.47
1:B:55:PHE:O	1:B:56:SER:C	2.53	0.47
2:D:258:ILE:HD11	2:D:292:MET:SD	2.55	0.47
2:D:432:VAL:HA	2:D:433:PRO:HD3	1.83	0.47
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.30	0.47
2:F:243:PHE:HB2	2:F:251:VAL:CG2	2.44	0.47
3:G:32:ALA:O	3:G:36:ARG:HG3	2.15	0.47
1:A:159:ILE:CD1	1:A:165:GLU:HG2	2.45	0.46
1:C:166:LEU:HD13	1:C:342:VAL:CG1	2.46	0.46
1:A:211:SER:N	2:D:126:MET:HE2	2.31	0.46
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.50	0.46
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.96	0.46
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.97	0.46
2:E:259:PHE:HE1	2:E:313:PRO:HG3	1.78	0.46
1:A:103:LEU:HD13	1:A:253:MET:SD	2.56	0.46
1:B:66:LEU:O	2:F:15:ALA:HA	2.15	0.46
1:B:481:GLY:HA2	1:B:484:ARG:CZ	2.45	0.46
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.96	0.46
2:F:118:ALA:O	2:F:295:ARG:HD2	2.15	0.46
2:E:105:ARG:HD3	9:E:2006:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:ILE:HG22	2:E:310:ILE:HG12	1.96	0.46
1:A:439:GLU:CD	1:A:439:GLU:H	2.19	0.46
1:B:186:GLN:HG3	1:B:199:LEU:HD23	1.96	0.46
2:F:95:MET:HG2	2:F:218:VAL:HG22	1.96	0.46
1:A:156:LEU:CD2	1:A:391:LYS:HB2	2.45	0.46
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.98	0.46
2:D:181:SER:O	2:D:215:VAL:HA	2.15	0.46
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.81	0.46
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.45	0.46
1:A:188:ARG:NH2	1:A:436:MET:CA	2.79	0.46
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.46	0.46
1:B:54:GLU:HG3	1:B:91:THR:HG22	1.97	0.46
1:C:162:GLY:HA2	1:C:321:LEU:O	2.16	0.46
3:G:20:THR:HA	3:G:232:MET:HE2	1.97	0.46
1:A:166:LEU:HD21	1:A:168:ILE:HB	1.97	0.46
1:A:479:LEU:O	1:A:483:ILE:HG13	2.16	0.46
1:B:280:GLN:CD	2:E:284:THR:HG22	2.36	0.46
2:D:9:THR:CG2	2:D:27:GLU:HB2	2.45	0.46
1:B:179:ALA:O	1:B:182:THR:HB	2.16	0.46
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.98	0.46
1:C:488:LYS:HG2	1:C:489:ILE:N	2.31	0.46
2:E:422:GLU:OE1	2:E:428:LEU:HA	2.16	0.46
1:A:62:MET:CE	1:A:64:LEU:HD21	2.46	0.46
1:B:151:LYS:HE2	1:B:427:LEU:O	2.15	0.46
1:B:286:ARG:HA	2:E:275:ILE:CD1	2.45	0.46
1:B:300:TYR:HA	1:B:303:SER:OG	2.16	0.46
1:C:45:ARG:NH2	1:C:68:PRO:O	2.49	0.46
1:C:210:ARG:NH1	2:F:121:PRO:O	2.48	0.46
2:E:419:GLN:CA	2:E:429:GLY:HA3	2.42	0.46
2:F:53:LEU:HD21	2:F:59:ARG:HB2	1.97	0.46
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.98	0.46
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.97	0.46
1:A:138:PRO:HB3	1:A:316:PHE:CZ	2.51	0.45
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.46	0.45
1:A:338:ILE:N	1:A:339:PRO:CD	2.78	0.45
1:C:338:ILE:HB	1:C:339:PRO:CD	2.46	0.45
3:G:228:ARG:O	3:G:232:MET:HG2	2.16	0.45
1:B:278:TYR:OH	1:B:297:ASP:OD2	2.30	0.45
1:C:168:ILE:HG23	1:C:351:PHE:HD1	1.80	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.16	0.45
2:D:417:PRO:HA	2:D:459:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:GLN:HA	2:E:246:GLN:HE21	1.82	0.45
2:E:408:ARG:O	2:E:412:ARG:HG3	2.16	0.45
1:A:94:ILE:HG12	1:A:95:VAL:N	2.25	0.45
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.97	0.45
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.47	0.45
2:E:201:ILE:HD13	2:E:208:LEU:CD1	2.45	0.45
1:A:286:ARG:HG2	1:A:286:ARG:NH1	2.31	0.45
1:B:171:ARG:NE	2:E:326:PHE:HB3	2.31	0.45
9:B:2003:HOH:O	2:E:124:VAL:HG13	2.16	0.45
1:C:406:PHE:HE2	2:D:393:MET:HB2	1.81	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.99	0.45
2:F:48:GLU:OE2	2:F:117:HIS:NE2	2.42	0.45
2:D:319:ASP:O	2:D:320:PRO:C	2.54	0.45
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.17	0.45
1:B:147:GLN:OE1	1:B:438:ILE:HD13	2.15	0.45
2:E:142:LEU:HG	2:E:143:LEU:HD23	1.99	0.45
2:E:227:GLY:O	2:E:231:ARG:HG2	2.16	0.45
2:F:163:THR:HG21	2:F:192:GLU:OE1	2.17	0.45
2:F:188:GLU:HA	2:F:222:MET:HE2	1.99	0.45
1:B:159:ILE:HG22	1:B:160:GLY:N	2.31	0.45
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.98	0.45
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.98	0.45
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.98	0.45
1:A:278:TYR:HA	1:A:281:MET:CE	2.46	0.45
1:B:26:GLU:HB3	1:B:46:ASN:HD22	1.81	0.45
2:E:281:TYR:HB3	2:E:282:GLN:HE21	1.82	0.45
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.99	0.45
2:F:139:VAL:HG11	2:F:348:VAL:HB	1.99	0.45
1:C:75:VAL:HG12	1:C:77:GLY:H	1.80	0.45
1:C:161:ARG:NH2	1:C:197:LYS:O	2.44	0.45
2:D:27:GLU:HB2	2:D:28:GLY:H	1.63	0.45
2:E:167:MET:HB2	2:E:167:MET:HE2	1.74	0.45
3:G:20:THR:HG23	3:G:232:MET:CE	2.47	0.45
1:B:352:LEU:HA	1:B:364:ALA:O	2.16	0.44
2:E:25:PHE:O	2:E:56:SER:HB3	2.17	0.44
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.52	0.44
2:E:94:ILE:HD11	2:E:197:TYR:CG	2.52	0.44
2:E:170:ILE:HG13	2:E:254:PHE:HE2	1.82	0.44
1:A:382:ALA:HB2	1:A:487:GLY:O	2.17	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.17	0.44
1:B:280:GLN:NE2	2:E:284:THR:HG22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:HD1	1:B:358:TYR:HD1	1.65	0.44
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.48	0.44
2:E:413:PHE:HB2	2:E:457:PHE:HB3	1.99	0.44
1:B:94:ILE:O	1:B:95:VAL:C	2.56	0.44
1:B:269:ASP:HA	1:B:270:ASP:HA	1.73	0.44
1:C:139:ARG:HH11	1:C:139:ARG:HD3	1.58	0.44
3:G:38:LEU:HD11	3:G:42:ARG:CZ	2.47	0.44
1:A:140:ILE:HG21	1:A:313:ASN:HA	2.00	0.44
1:C:440:GLU:O	1:C:444:VAL:HG13	2.16	0.44
2:D:264:ALA:O	2:D:267:GLU:HB2	2.17	0.44
2:D:402:LEU:HD11	2:D:406:ARG:HH21	1.82	0.44
2:E:289:MET:HG2	2:E:324:THR:HG22	1.98	0.44
2:F:82:ILE:O	2:F:115:ALA:HA	2.18	0.44
2:F:142:LEU:HD22	2:F:441:PHE:CD2	2.53	0.44
2:F:170:ILE:O	2:F:174:ALA:HB3	2.18	0.44
3:G:80:ALA:O	3:G:84:SER:OG	2.32	0.44
1:A:99:VAL:HG13	1:A:256:TYR:CD2	2.53	0.44
1:B:385:GLN:OE1	1:B:488:LYS:HG3	2.18	0.44
1:C:51:GLU:O	1:C:63:SER:HB2	2.17	0.44
1:C:149:GLY:HA3	1:C:435:PRO:HB3	1.99	0.44
2:E:384:LEU:O	2:E:385:GLN:C	2.55	0.44
2:F:253:LEU:O	2:F:306:SER:HA	2.17	0.44
3:G:18:LYS:O	3:G:21:LYS:HB3	2.18	0.44
1:A:240:ALA:N	1:A:241:PRO:HD2	2.33	0.44
1:B:291:ARG:NH2	2:F:319:ASP:HB2	2.32	0.44
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.31	0.44
2:D:381:TYR:CE1	2:D:404:VAL:HG13	2.53	0.44
2:D:402:LEU:O	2:D:406:ARG:HG3	2.18	0.44
2:F:229:ARG:HA	2:F:232:VAL:CG2	2.47	0.44
1:B:393:GLU:HA	1:B:396:GLN:OE1	2.17	0.44
2:E:36:LEU:O	2:E:46:VAL:HA	2.18	0.44
2:E:292:MET:SD	2:E:293:GLN:NE2	2.90	0.44
1:A:208:GLN:O	1:A:235:THR:HG22	2.18	0.44
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.99	0.44
1:B:483:ILE:HD13	1:B:489:ILE:HG12	1.98	0.44
2:E:187:GLY:N	2:E:220:GLY:O	2.51	0.44
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.52	0.44
2:E:276:PRO:CD	3:G:266:ILE:HD11	2.38	0.44
1:B:389:THR:O	1:B:393:GLU:HG3	2.18	0.44
1:B:481:GLY:HA2	1:B:484:ARG:NH1	2.32	0.44
1:C:458:PRO:HA	1:C:461:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:GLU:CD	2:D:89:GLU:H	2.20	0.44
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.44
2:F:460:VAL:HG23	2:F:461:GLY:N	2.33	0.44
3:G:39:LYS:N	3:G:40:PRO:CD	2.81	0.44
1:A:136:ILE:HD11	2:E:193:GLY:HA3	1.99	0.43
1:A:140:ILE:CG1	1:A:143:ARG:HH22	2.30	0.43
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.43
1:C:209:LYS:NZ	2:F:330:ASP:OD1	2.51	0.43
1:C:503:ASN:O	1:C:506:ALA:HB3	2.18	0.43
2:D:406:ARG:O	2:D:410:ILE:HD12	2.18	0.43
2:F:12:ARG:HA	2:F:73:GLN:O	2.18	0.43
2:F:457:PHE:HE1	2:F:463:ILE:HD11	1.84	0.43
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.76	0.43
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.48	0.43
1:C:423:ARG:HG2	1:C:423:ARG:HH11	1.82	0.43
1:C:438:ILE:HG23	1:C:439:GLU:N	2.33	0.43
2:E:163:THR:HG23	8:E:602:PO4:O1	2.18	0.43
3:G:254:ARG:HH11	3:G:254:ARG:HD3	1.58	0.43
1:A:41:VAL:HG11	1:A:44:LEU:HD12	1.99	0.43
1:B:161:ARG:NH1	1:B:198:LYS:O	2.50	0.43
2:D:244:ARG:HG3	2:D:304:ILE:HG13	2.00	0.43
2:D:285:LEU:C	2:D:285:LEU:HD23	2.39	0.43
2:E:120:ALA:O	2:E:121:PRO:C	2.56	0.43
2:E:417:PRO:HD2	2:E:460:VAL:O	2.18	0.43
1:A:209:LYS:HG2	9:A:2010:HOH:O	2.18	0.43
1:C:100:GLY:HA2	1:C:256:TYR:CD2	2.53	0.43
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.49	0.43
1:A:180:ILE:HD11	1:A:216:LEU:HD22	2.01	0.43
2:D:232:VAL:O	2:D:235:THR:N	2.52	0.43
2:E:142:LEU:HB2	2:E:437:THR:CG2	2.48	0.43
2:F:139:VAL:HG23	9:F:2005:HOH:O	2.17	0.43
1:B:48:GLN:HG2	2:F:70:VAL:CG2	2.49	0.43
1:C:99:VAL:HG12	1:C:100:GLY:N	2.34	0.43
2:E:170:ILE:HG13	2:E:254:PHE:CE2	2.53	0.43
2:F:36:LEU:HD13	2:F:75:VAL:HG11	2.00	0.43
2:F:63:MET:CE	2:F:97:VAL:HG11	2.46	0.43
3:G:24:LYS:HD2	3:G:233:ASP:HA	2.00	0.43
1:A:67:GLU:HB2	1:A:70:ASN:O	2.19	0.43
1:A:484:ARG:O	1:A:485:THR:C	2.57	0.43
1:B:444:VAL:CG1	1:B:469:LEU:HD13	2.48	0.43
1:C:30:ARG:NH2	1:C:87:ILE:HD11	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:THR:O	2:D:164:VAL:C	2.55	0.43
2:D:188:GLU:O	2:D:222:MET:HG3	2.19	0.43
2:D:388:ILE:HD13	2:D:396:LEU:HD11	2.01	0.43
2:E:59:ARG:HD2	9:E:2003:HOH:O	2.17	0.43
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.49	0.43
2:E:111:LYS:HB2	2:E:112:GLN:OE1	2.19	0.43
1:A:422:VAL:HG23	1:A:423:ARG:N	2.34	0.43
1:B:146:MET:SD	1:B:146:MET:C	2.97	0.43
1:C:52:MET:HE1	1:C:76:PHE:CD2	2.54	0.43
1:C:130:GLY:O	1:C:131:LEU:C	2.57	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.43
2:D:84:ILE:HB	2:D:85:PRO:CD	2.43	0.43
2:D:256:ASP:HA	2:D:309:ALA:HB3	2.01	0.43
2:E:384:LEU:O	2:E:388:ILE:HG12	2.19	0.43
1:B:164:ARG:HD3	1:B:164:ARG:N	2.34	0.43
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.86	0.43
2:E:393:MET:HG3	2:E:396:LEU:CD1	2.49	0.43
2:F:247:GLU:HB3	2:F:249:GLN:HG2	2.01	0.43
1:B:94:ILE:HG21	1:B:128:ARG:HD3	2.00	0.43
1:B:142:VAL:HG12	1:B:161:ARG:O	2.19	0.43
1:C:361:ILE:O	1:C:364:ALA:HA	2.19	0.43
2:D:456:ALA:HB1	2:D:466:ALA:O	2.18	0.43
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.84	0.43
1:C:30:ARG:HA	1:C:86:ASP:O	2.18	0.42
2:E:263:GLN:O	2:E:267:GLU:HG3	2.18	0.42
1:A:62:MET:HE2	1:A:64:LEU:HD21	2.00	0.42
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.00	0.42
1:A:423:ARG:NH2	1:A:456:LEU:O	2.43	0.42
1:B:176:THR:O	1:B:179:ALA:N	2.52	0.42
2:D:449:TYR:HB3	2:D:452:LEU:HD12	2.01	0.42
2:F:130:GLN:HB3	2:F:357:ILE:HD11	2.01	0.42
1:B:323:ALA:O	1:B:324:LEU:HD23	2.20	0.42
1:C:497:LEU:O	1:C:501:VAL:HG13	2.19	0.42
2:F:94:ILE:HD11	2:F:197:TYR:CG	2.54	0.42
1:A:166:LEU:CD2	1:A:168:ILE:HB	2.50	0.42
1:B:252:SER:O	1:B:255:GLU:N	2.51	0.42
1:C:48:GLN:HA	2:D:69:LEU:O	2.20	0.42
1:C:67:GLU:HB3	1:C:68:PRO:HD2	2.02	0.42
2:E:96:ASN:OD1	2:E:97:VAL:N	2.52	0.42
2:E:112:GLN:NE2	2:E:242:TYR:OH	2.52	0.42
2:E:148:LYS:HE3	2:E:250:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:ARG:NH2	2:F:113:PHE:HB2	2.34	0.42
2:F:147:ALA:HB2	2:F:357:ILE:HG13	2.02	0.42
1:A:117:GLY:C	1:A:119:GLY:H	2.23	0.42
1:A:210:ARG:NH1	2:D:121:PRO:O	2.53	0.42
1:B:160:GLY:O	1:B:163:GLN:HB3	2.19	0.42
1:B:255:GLU:OE2	1:B:258:ARG:NH1	2.48	0.42
2:D:339:ILE:O	2:D:340:ALA:C	2.57	0.42
2:D:409:LYS:NZ	2:D:450:ASP:HA	2.34	0.42
1:B:194:ASP:C	1:B:196:LYS:H	2.22	0.42
1:C:246:ALA:N	1:C:247:PRO:CD	2.83	0.42
2:E:310:ILE:CD1	2:E:329:LEU:HD11	2.49	0.42
2:F:35:ALA:O	2:F:78:SER:HB3	2.20	0.42
1:A:44:LEU:HD22	1:A:47:VAL:HG13	2.00	0.42
1:C:164:ARG:HD2	1:C:306:LEU:O	2.19	0.42
1:C:423:ARG:HH11	1:C:423:ARG:CG	2.33	0.42
2:E:456:ALA:HB1	2:E:466:ALA:O	2.20	0.42
1:B:137:ILE:N	1:B:138:PRO:HD2	2.34	0.42
3:G:14:LYS:HA	3:G:243:ILE:HD11	2.01	0.42
3:G:209:LEU:O	3:G:210:ALA:C	2.58	0.42
1:A:164:ARG:HD3	1:A:164:ARG:N	2.35	0.42
1:B:422:VAL:O	1:B:426:GLU:HG2	2.20	0.42
2:D:9:THR:HA	2:D:27:GLU:OE1	2.20	0.42
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.42
2:F:329:LEU:HD13	2:F:332:THR:HG22	2.02	0.42
1:A:144:GLU:O	1:A:161:ARG:HG3	2.20	0.42
1:A:247:PRO:HB3	1:A:268:TYR:CD1	2.55	0.42
1:B:33:SER:HB2	2:E:52:HIS:O	2.20	0.42
1:B:251:CYS:O	1:B:255:GLU:HG3	2.20	0.42
1:C:74:VAL:CG1	1:C:241:PRO:HB3	2.50	0.42
1:C:151:LYS:NZ	1:C:427:LEU:O	2.44	0.42
2:E:387:ILE:HD12	2:E:387:ILE:N	2.33	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.50	0.42
1:B:351:PHE:HE2	1:B:353:GLU:CG	2.13	0.41
1:C:496:LYS:HD2	1:C:496:LYS:HA	1.94	0.41
2:D:372:ARG:NH1	2:D:375:GLN:OE1	2.52	0.41
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.50	0.41
1:A:352:LEU:HD23	1:A:365:ILE:HA	2.01	0.41
1:C:213:VAL:HG12	2:F:123:PHE:CE1	2.55	0.41
1:C:213:VAL:HG12	2:F:123:PHE:HE1	1.86	0.41
1:C:249:SER:O	1:C:253:MET:HG3	2.20	0.41
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ALA:O	2:D:295:ARG:HD2	2.20	0.41
2:D:160:VAL:CG2	2:D:335:LEU:HB3	2.50	0.41
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.49	0.41
2:E:388:ILE:CD1	2:E:396:LEU:HD11	2.50	0.41
1:A:44:LEU:HB3	1:A:47:VAL:HG22	2.02	0.41
1:B:102:GLU:HG3	1:B:122:GLY:O	2.21	0.41
1:C:362:ARG:NH2	2:F:372:ARG:HD2	2.35	0.41
1:C:446:TYR:O	1:C:447:ALA:C	2.59	0.41
2:E:210:ASP:O	2:E:212:THR:N	2.50	0.41
2:F:12:ARG:HE	2:F:74:LYS:CE	2.14	0.41
3:G:30:LYS:HD2	3:G:225:GLN:OE1	2.20	0.41
1:A:349:GLN:O	1:A:370:SER:HB3	2.20	0.41
1:A:373:ARG:NH2	9:A:2018:HOH:O	2.54	0.41
1:A:437:ALA:O	1:A:441:GLN:HG3	2.20	0.41
1:C:65:ASN:OD1	1:C:287:ARG:NH2	2.46	0.41
2:F:153:GLY:N	2:F:329:LEU:HD22	2.34	0.41
2:E:54:GLY:O	2:E:55:GLU:HB2	2.20	0.41
2:E:160:VAL:CG1	2:E:337:ARG:HG3	2.50	0.41
2:F:16:VAL:O	2:F:17:ILE:HD12	2.21	0.41
1:A:350:ILE:HA	1:A:370:SER:HB3	2.02	0.41
1:A:390:MET:CE	1:A:424:LEU:HD22	2.50	0.41
1:B:54:GLU:HG2	1:B:60:LYS:NZ	2.35	0.41
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.56	0.41
1:A:296:GLY:O	2:E:267:GLU:HB3	2.20	0.41
1:B:52:MET:HE1	1:B:95:VAL:HG13	2.03	0.41
1:B:55:PHE:HD1	1:B:59:LEU:O	2.04	0.41
1:C:434:SER:N	1:C:435:PRO:CD	2.84	0.41
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.56	0.41
2:E:348:VAL:O	2:E:350:PRO:HD3	2.21	0.41
1:A:479:LEU:HA	1:A:482:LYS:HE3	2.02	0.41
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.94	0.41
2:E:170:ILE:HG12	2:E:181:SER:HB2	2.02	0.41
2:F:151:LYS:NZ	2:F:293:GLN:HB3	2.35	0.41
2:F:336:SER:OG	2:F:339:ILE:HG13	2.21	0.41
2:F:378:LEU:HD21	2:F:410:ILE:HG22	2.02	0.41
1:A:139:ARG:CZ	2:E:190:THR:HG21	2.51	0.41
1:A:155:SER:OG	1:A:156:LEU:HG	2.21	0.41
1:B:209:LYS:HG3	9:B:2008:HOH:O	2.21	0.41
1:B:432:GLN:OE1	4:B:600:ATP:H2'	2.20	0.41
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.51	0.41
1:C:209:LYS:HD3	2:F:328:HIS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:LYS:N	7:D:600:ADP:O1B	2.54	0.41
2:E:136:GLY:N	2:E:141:ASP:OD2	2.51	0.41
2:E:253:LEU:O	2:E:306:SER:HA	2.21	0.41
2:E:335:LEU:HD23	2:E:335:LEU:HA	1.82	0.41
2:E:396:LEU:HB2	2:E:401:LYS:HG3	2.03	0.41
2:F:406:ARG:NH2	2:F:447:GLY:HA3	2.33	0.41
3:G:5:ASP:O	3:G:6:ILE:C	2.60	0.41
1:B:453:LEU:CD1	1:B:461:ILE:HG23	2.49	0.41
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.21	0.41
2:E:257:ASN:OD1	2:E:259:PHE:HB3	2.21	0.41
2:E:298:THR:HA	2:E:303:SER:HB2	2.02	0.41
2:E:321:ALA:HB3	2:E:322:PRO:HD3	2.03	0.41
3:G:83:SER:O	3:G:87:LYS:HG3	2.20	0.41
1:B:97:VAL:HB	1:B:98:PRO:HD2	2.03	0.40
1:B:248:TYR:CD1	6:B:701:GOL:H12	2.56	0.40
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.35	0.40
1:B:191:ASP:OD1	1:B:227:LYS:NZ	2.52	0.40
1:B:338:ILE:N	1:B:339:PRO:CD	2.84	0.40
2:E:93:ARG:NH2	2:E:106:GLY:O	2.39	0.40
2:E:94:ILE:HD12	2:E:103:ASP:HB3	2.03	0.40
2:F:370:VAL:HG21	2:F:438:ILE:HG23	2.03	0.40
1:B:62:MET:HB2	1:B:76:PHE:CE2	2.57	0.40
1:B:347:ASP:O	1:B:373:ARG:HG3	2.21	0.40
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.34	0.40
1:C:151:LYS:HG2	1:C:441:GLN:HG2	2.03	0.40
1:C:376:SER:O	1:C:378:ALA:N	2.54	0.40
2:D:83:ARG:HA	2:D:114:ALA:O	2.22	0.40
2:D:163:THR:HA	2:D:166:ILE:CG2	2.49	0.40
2:D:397:SER:O	2:D:401:LYS:HG2	2.21	0.40
2:F:134:VAL:CG2	2:F:434:LEU:HD22	2.51	0.40
2:F:134:VAL:HG13	2:F:141:ASP:OD1	2.21	0.40
2:F:223:ASN:N	2:F:223:ASN:ND2	2.67	0.40
1:A:140:ILE:HD11	1:A:143:ARG:NH2	2.27	0.40
1:B:270:ASP:HB2	1:B:326:VAL:O	2.22	0.40
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.21	0.40
1:C:190:ASN:O	1:C:198:LYS:HE3	2.21	0.40
1:C:419:SER:O	1:C:423:ARG:HG2	2.20	0.40
2:E:84:ILE:HD13	2:E:235:THR:CG2	2.52	0.40
2:F:33:LEU:O	2:F:81:PRO:HB3	2.22	0.40
3:G:5:ASP:O	3:G:8:ARG:N	2.55	0.40
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD12	2:D:283:PRO:HB3	2.04	0.40
1:C:49:ALA:O	1:C:50:GLU:HB2	2.21	0.40
1:C:98:PRO:CG	1:C:112:GLY:HA3	2.51	0.40
1:C:187:LYS:HE3	1:C:224:ASP:HB3	2.02	0.40
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.01	0.40
2:E:35:ALA:HB2	2:E:82:ILE:HG13	2.04	0.40
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.03	0.40
2:E:409:LYS:HD3	2:E:457:PHE:CZ	2.57	0.40
2:F:81:PRO:O	2:F:82:ILE:C	2.59	0.40
3:G:8:ARG:O	3:G:9:ARG:C	2.58	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 X-ray entries followed by that with respect to entries of similar resolution.

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	485/510 (95%)	438 (90%)	38 (8%)	9 (2%)	8	28
1	B	475/510 (93%)	428 (90%)	44 (9%)	3 (1%)	25	58
1	C	490/510 (96%)	446 (91%)	42 (9%)	2 (0%)	34	66
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	25	58
2	E	464/482 (96%)	408 (88%)	50 (11%)	6 (1%)	12	37
2	F	464/482 (96%)	427 (92%)	35 (8%)	2 (0%)	34	66
3	G	116/272 (43%)	103 (89%)	9 (8%)	4 (3%)	3	15
All	All	2959/3248 (91%)	2669 (90%)	261 (9%)	29 (1%)	15	45

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP

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Mol	Chain	Res	Type
1	C	337	TYR
3	G	210	ALA
1	A	93	ALA
1	A	404	ALA
1	B	195	GLU
2	E	211	ALA
2	E	357	ILE
2	E	423	VAL
2	E	455	GLN
2	F	247	GLU
1	A	123	SER
1	A	401	ALA
1	C	405	GLN
2	D	448	GLU
2	F	246	GLN
1	A	485	THR
3	G	5	ASP
3	G	81	ILE
3	G	211	ASN
1	A	141	SER
1	A	333	ASP
1	B	187	LYS
1	B	413	ALA
2	D	247	GLU
1	A	500	ILE
2	D	279	VAL
2	E	107	PRO
2	E	170	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	393/412 (95%)	360 (92%)	33 (8%)	11	31
1	B	388/412 (94%)	364 (94%)	24 (6%)	18	47
1	C	397/412 (96%)	372 (94%)	25 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	377/386 (98%)	358 (95%)	19 (5%)	24	57
2	E	376/386 (97%)	353 (94%)	23 (6%)	18	48
2	F	376/386 (97%)	358 (95%)	18 (5%)	25	58
3	G	102/230 (44%)	97 (95%)	5 (5%)	25	57
All	All	2409/2624 (92%)	2262 (94%)	147 (6%)	18	48

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	45	ARG
1	A	47	VAL
1	A	50	GLU
1	A	57	SER
1	A	64	LEU
1	A	74	VAL
1	A	79	ASP
1	A	99	VAL
1	A	121	ILE
1	A	123	SER
1	A	136	ILE
1	A	140	ILE
1	A	141	SER
1	A	164	ARG
1	A	177	SER
1	A	211	SER
1	A	216	LEU
1	A	217	VAL
1	A	235	THR
1	A	247	PRO
1	A	249	SER
1	A	298	VAL
1	A	354	THR
1	A	420	ARG
1	A	436	MET
1	A	442	VAL
1	A	444	VAL
1	A	462	THR
1	A	474	SER
1	A	479	LEU
1	A	499	GLU

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Mol	Chain	Res	Type
1	A	505	LEU
1	B	47	VAL
1	B	108	VAL
1	B	140	ILE
1	B	143	ARG
1	B	171	ARG
1	B	177	SER
1	B	209	LYS
1	B	211	SER
1	B	217	VAL
1	B	218	LYS
1	B	233	SER
1	B	251	CYS
1	B	298	VAL
1	B	340	THR
1	B	371	VAL
1	B	376	SER
1	B	380	THR
1	B	389	THR
1	B	419	SER
1	B	434	SER
1	B	459	SER
1	B	470	SER
1	B	474	SER
1	B	479	LEU
1	C	47	VAL
1	C	52	MET
1	C	57	SER
1	C	63	SER
1	C	64	LEU
1	C	74	VAL
1	C	123	SER
1	C	131	LEU
1	C	164	ARG
1	C	171	ARG
1	C	189	PHE
1	C	208	GLN
1	C	211	SER
1	C	282	SER
1	C	334	VAL
1	C	349	GLN
1	C	381	ARG

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Mol	Chain	Res	Type
1	C	398	ARG
1	C	416	GLN
1	C	417	LEU
1	C	419	SER
1	C	423	ARG
1	C	474	SER
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	43	THR
2	D	89	GLU
2	D	97	VAL
2	D	112	GLN
2	D	127	SER
2	D	137	ILE
2	D	139	VAL
2	D	172	ASN
2	D	205	VAL
2	D	210	ASP
2	D	232	VAL
2	D	250	ASP
2	D	282	GLN
2	D	303	SER
2	D	335	LEU
2	D	403	THR
2	D	431	LEU
2	D	471	ASP
2	E	67	GLU
2	E	74	LYS
2	E	97	VAL
2	E	112	GLN
2	E	132	ILE
2	E	139	VAL
2	E	164	VAL
2	E	171	ASN
2	E	188	GLU
2	E	191	ARG
2	E	210	ASP
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	266	SER

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Mol	Chain	Res	Type
2	E	282	GLN
2	E	297	THR
2	E	306	SER
2	E	336	SER
2	E	358	MET
2	E	365	SER
2	E	395	GLU
2	E	431	LEU
2	F	17	ILE
2	F	51	GLN
2	F	67	GLU
2	F	78	SER
2	F	89	GLU
2	F	96	ASN
2	F	97	VAL
2	F	166	ILE
2	F	223	ASN
2	F	232	VAL
2	F	237	LEU
2	F	266	SER
2	F	282	GLN
2	F	292	MET
2	F	303	SER
2	F	397	SER
2	F	405	SER
2	F	420	VAL
3	G	2	THR
3	G	77	LEU
3	G	220	SER
3	G	226	SER
3	G	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	A	471	HIS
1	A	475	GLN
1	B	46	ASN
1	B	65	ASN
1	C	260	ASN
1	C	263	HIS

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Mol	Chain	Res	Type
1	C	349	GLN
2	D	39	GLN
2	D	130	GLN
2	D	194	ASN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	E	34	ASN
2	E	223	ASN
2	E	246	GLN
2	E	249	GLN
2	E	282	GLN
2	E	411	GLN
2	E	455	GLN
2	F	51	GLN
2	F	96	ASN
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	F	600	5	26,33,33	0.99	2 (7%)	31,52,52	1.53	4 (12%)
4	ATP	B	600	5	26,33,33	1.11	2 (7%)	31,52,52	1.48	3 (9%)
4	ATP	A	600	5	26,33,33	1.20	4 (15%)	31,52,52	1.88	8 (25%)
8	PO4	E	602	-	4,4,4	0.62	0	6,6,6	0.32	0
7	ADP	D	600	5	24,29,29	1.00	1 (4%)	29,45,45	1.17	4 (13%)
4	ATP	C	600	5	26,33,33	0.98	2 (7%)	31,52,52	1.55	6 (19%)
6	GOL	B	701	-	5,5,5	0.74	0	5,5,5	0.92	0

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
4	ATP	F	600	5	-	0/18/38/38	0/3/3/3
4	ATP	B	600	5	-	0/18/38/38	0/3/3/3
4	ATP	A	600	5	-	1/18/38/38	0/3/3/3
7	ADP	D	600	5	-	0/12/32/32	0/3/3/3
4	ATP	C	600	5	-	0/18/38/38	0/3/3/3
6	GOL	B	701	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ATP	C2-N1	2.83	1.39	1.33
4	A	600	ATP	PG-O3G	-2.65	1.44	1.54
4	B	600	ATP	C2-N1	2.45	1.38	1.33
4	B	600	ATP	PG-O3G	-2.45	1.45	1.54
4	A	600	ATP	O3'-C3'	2.40	1.48	1.43
4	F	600	ATP	PG-O3G	-2.24	1.46	1.54
4	A	600	ATP	PG-O2G	-2.19	1.46	1.54
4	C	600	ATP	PG-O3G	-2.13	1.46	1.54
7	D	600	ADP	C2-N1	2.08	1.37	1.33
4	F	600	ATP	C2-N1	2.01	1.37	1.33
4	C	600	ATP	PA-O2A	-2.01	1.45	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ATP	O3'-C3'-C4'	-4.80	97.17	111.05
4	B	600	ATP	PB-O3B-PG	-4.14	118.63	132.83
4	F	600	ATP	PB-O3B-PG	-4.12	118.70	132.83
4	F	600	ATP	C5-C6-N6	4.11	126.60	120.35
4	F	600	ATP	PA-O3A-PB	-3.91	119.41	132.83
4	A	600	ATP	O3'-C3'-C2'	-3.72	99.80	111.82
4	C	600	ATP	PA-O3A-PB	-3.62	120.41	132.83
4	A	600	ATP	PB-O3B-PG	-3.40	121.16	132.83
4	A	600	ATP	C5-C6-N6	3.39	125.50	120.35
4	B	600	ATP	C4-C5-N7	3.34	112.88	109.40
4	C	600	ATP	PB-O3B-PG	-3.13	122.09	132.83
4	C	600	ATP	C4-C5-N7	3.11	112.64	109.40
4	A	600	ATP	O4'-C1'-C2'	2.89	111.14	106.93
7	D	600	ADP	PA-O3A-PB	-2.84	123.07	132.83
4	B	600	ATP	N6-C6-N1	2.71	124.20	118.57
4	A	600	ATP	O2'-C2'-C3'	-2.70	103.09	111.82
4	A	600	ATP	C2'-C3'-C4'	2.46	107.42	102.64
4	C	600	ATP	N6-C6-N1	2.42	123.59	118.57
7	D	600	ADP	C1'-N9-C4	-2.35	122.50	126.64
4	F	600	ATP	O3G-PG-O2G	2.31	116.47	107.64
4	C	600	ATP	O3'-C3'-C2'	-2.30	104.37	111.82
7	D	600	ADP	N6-C6-N1	2.20	123.14	118.57
7	D	600	ADP	O3B-PB-O1B	2.18	119.20	110.68
4	A	600	ATP	C4-C5-N7	2.10	111.58	109.40
4	C	600	ATP	O2B-PB-O1B	-2.06	102.04	112.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	701	GOL	C1-C2-C3-O3
6	B	701	GOL	O2-C2-C3-O3
4	A	600	ATP	O4'-C4'-C5'-O5'
6	B	701	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 16 short contacts:

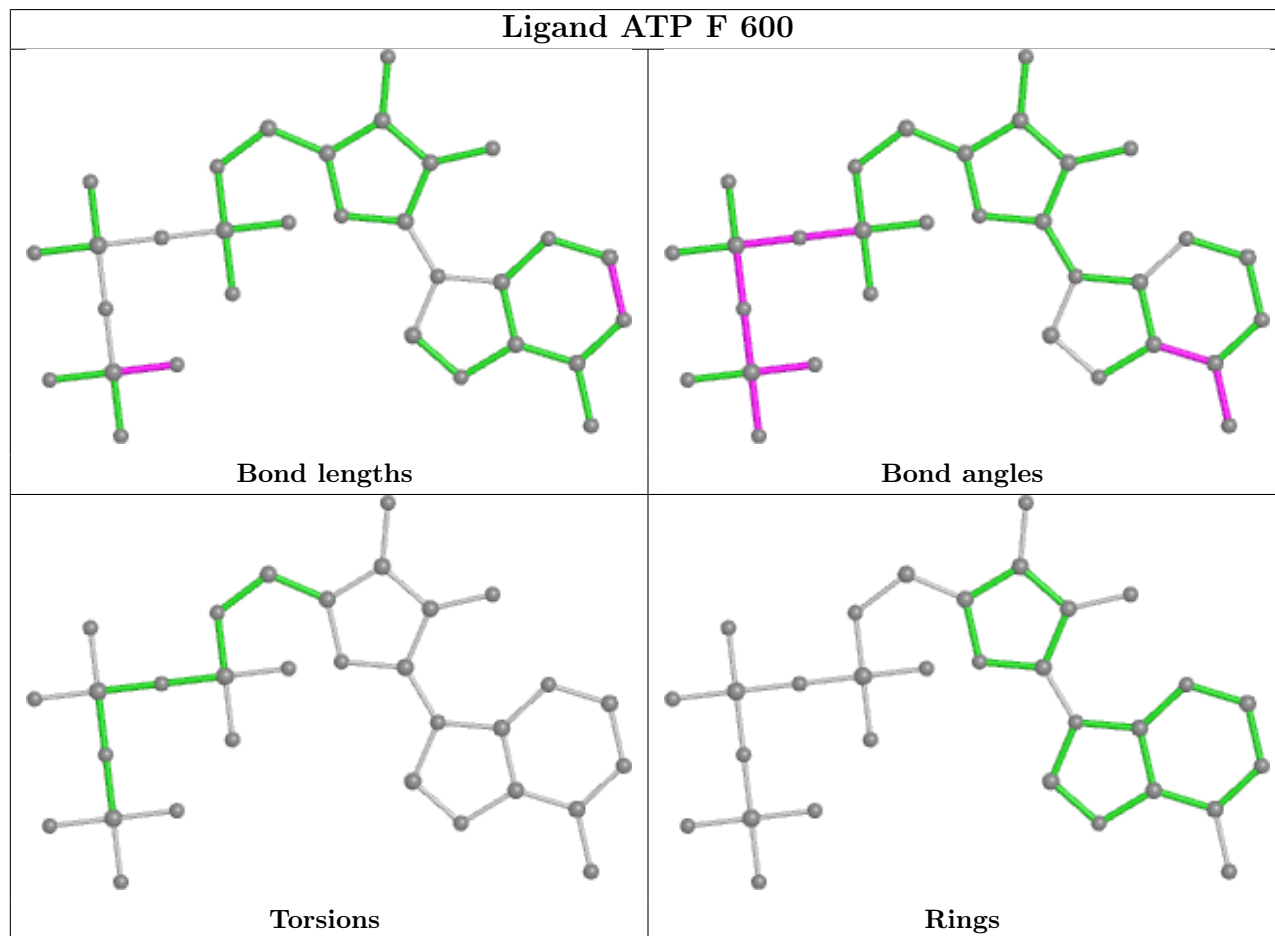
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	600	ATP	1	0

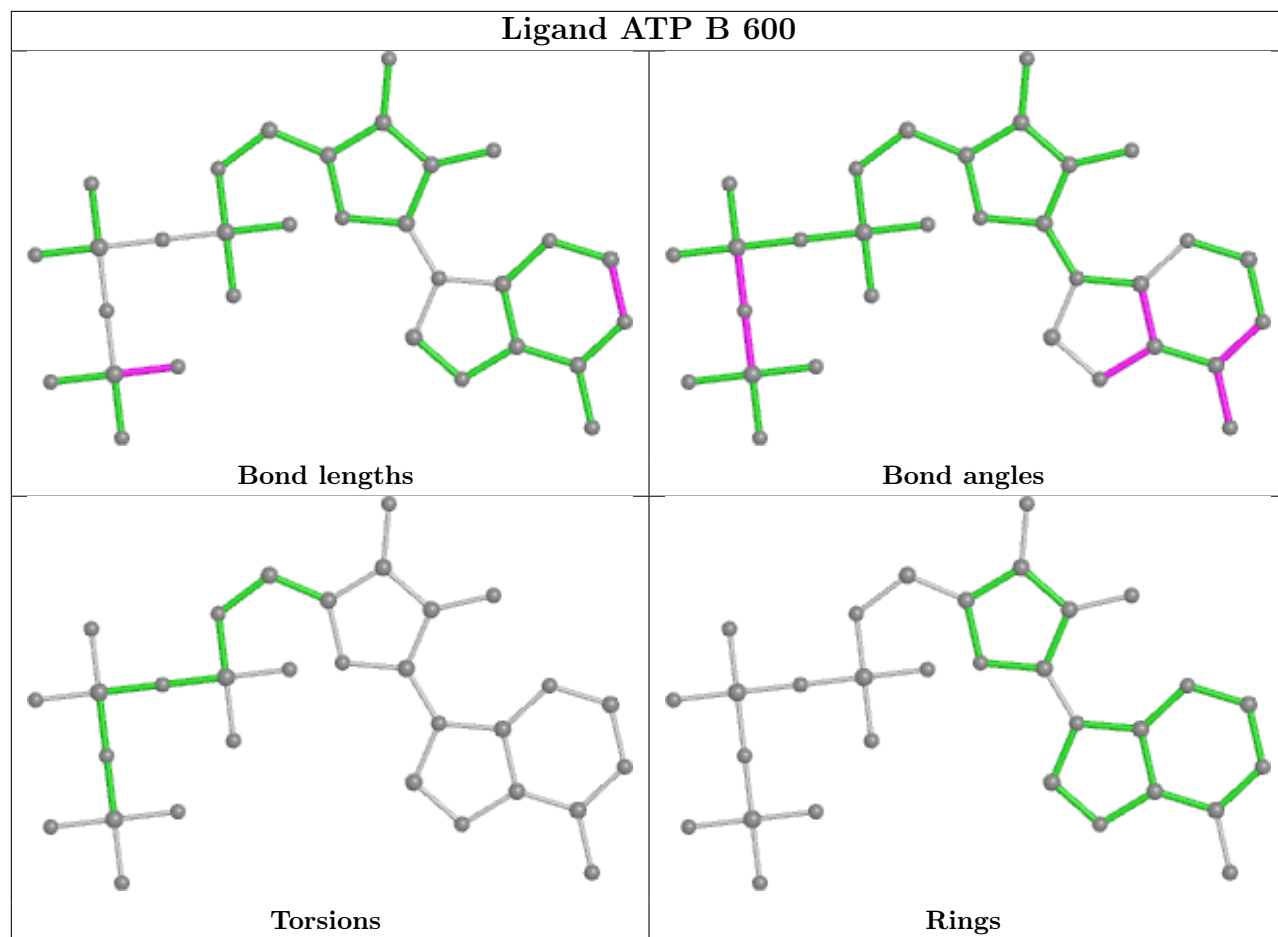
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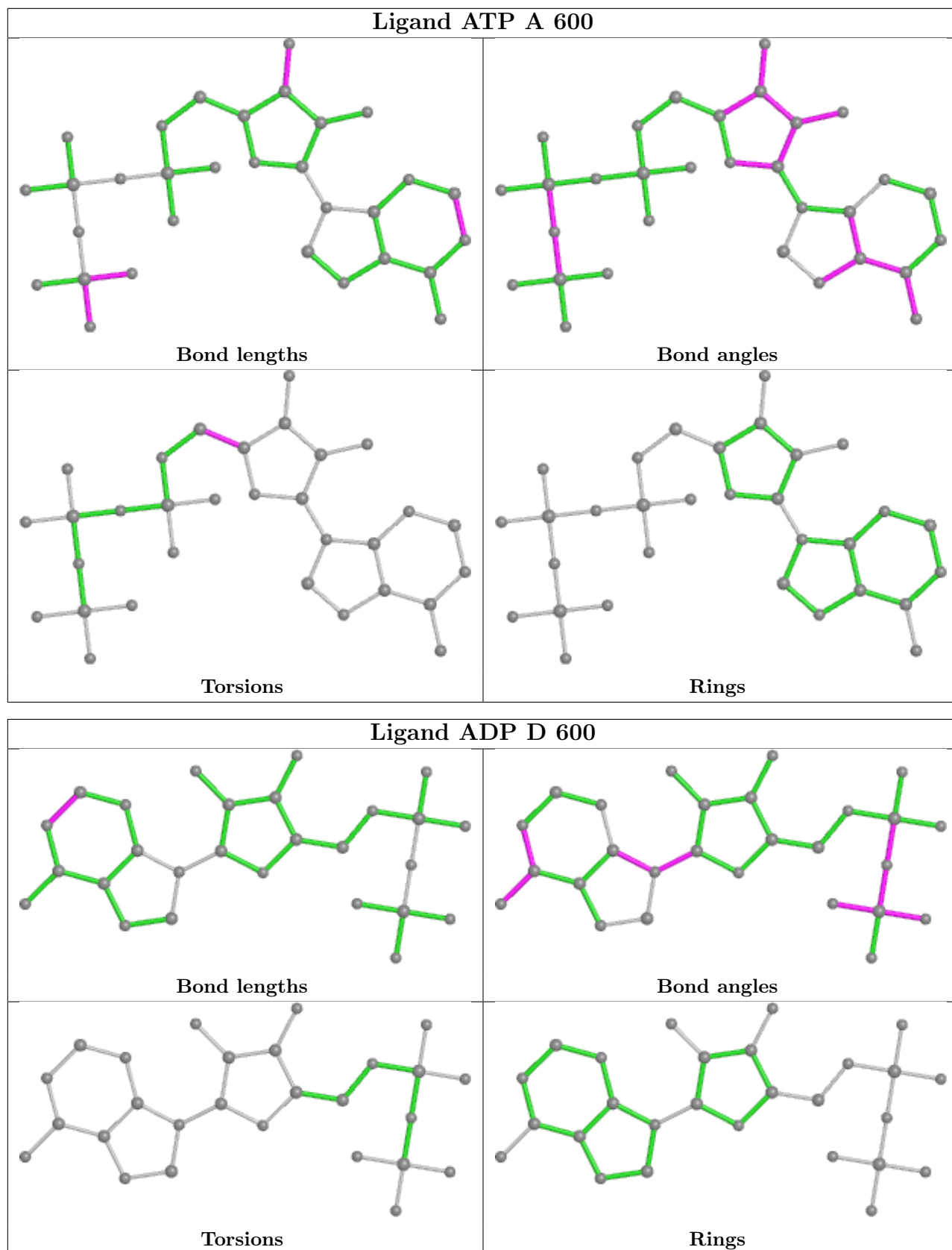
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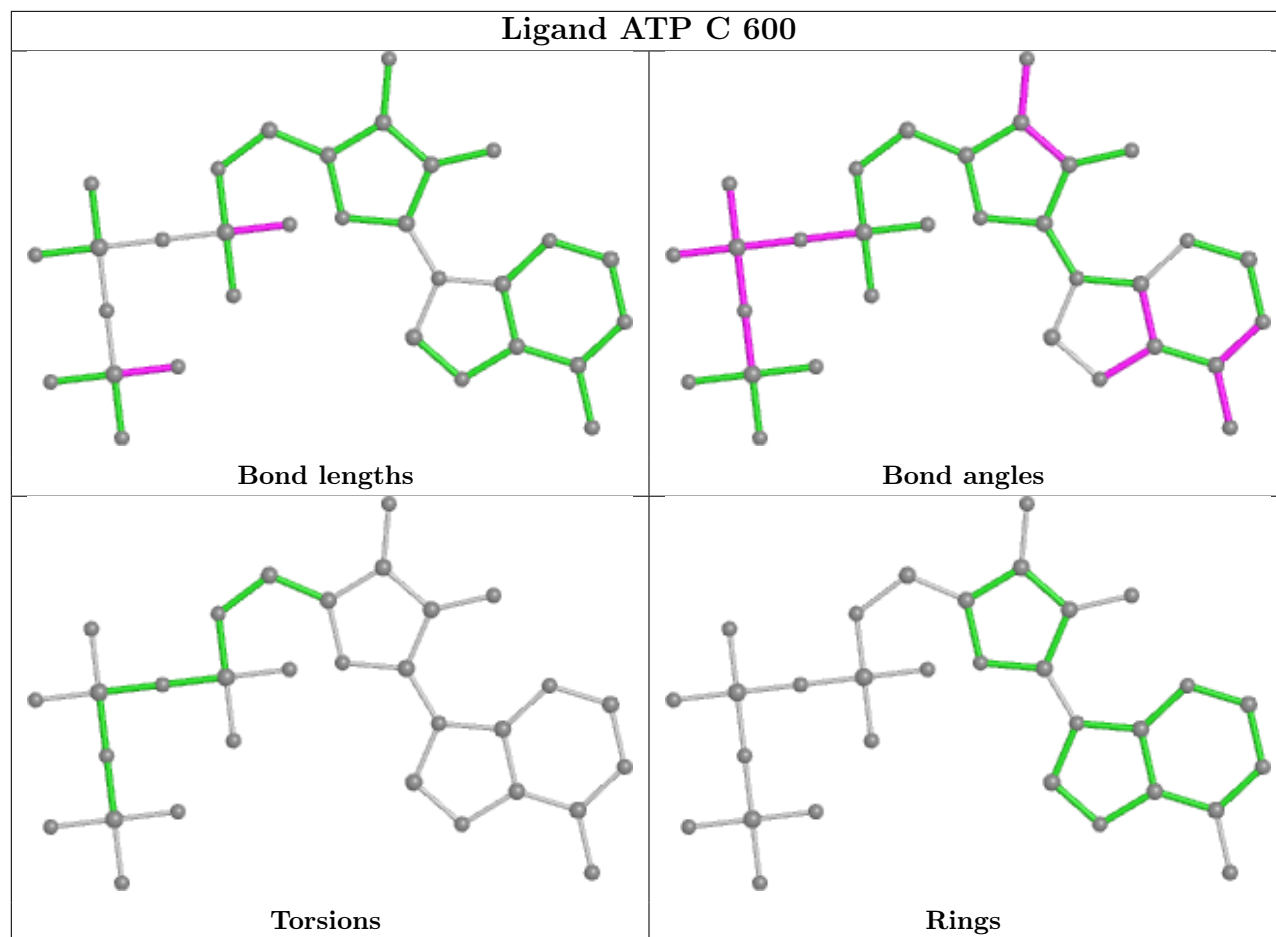
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	ATP	2	0
4	A	600	ATP	2	0
8	E	602	PO4	1	0
7	D	600	ADP	2	0
4	C	600	ATP	5	0
6	B	701	GOL	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	-0.24	11 (2%) 60 58	17, 41, 77, 101	0
1	B	479/510 (93%)	-0.18	12 (2%) 57 55	15, 37, 89, 102	0
1	C	492/510 (96%)	-0.38	7 (1%) 75 75	15, 34, 65, 106	0
2	D	467/482 (96%)	-0.15	12 (2%) 56 52	17, 37, 77, 105	0
2	E	466/482 (96%)	0.11	30 (6%) 19 15	13, 49, 100, 114	0
2	F	466/482 (96%)	-0.31	5 (1%) 80 80	14, 36, 73, 94	0
3	G	122/272 (44%)	1.18	34 (27%) 0 0	17, 70, 100, 104	0
All	All	2979/3248 (91%)	-0.14	111 (3%) 41 37	13, 40, 87, 114	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	390	ILE	6.9
1	C	408	SER	6.5
3	G	209	LEU	6.4
3	G	86	ALA	5.7
2	E	395	GLU	5.1
1	A	408	SER	5.0
2	E	470	ALA	4.7
3	G	28	ALA	4.7
3	G	89	MET	4.6
2	D	473	LEU	4.5
3	G	87	LYS	4.4
3	G	90	LYS	4.4
2	E	388	ILE	4.3
2	E	466	ALA	4.2
1	C	406	PHE	4.2
1	C	407	GLY	3.9
3	G	29	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	395	GLU	3.8
1	A	487	GLY	3.7
2	F	386	ASP	3.7
2	E	394	ASP	3.7
1	A	407	GLY	3.7
2	E	109	LYS	3.7
1	A	406	PHE	3.6
3	G	214	TYR	3.6
2	E	398	GLU	3.5
1	C	409	ASP	3.5
2	E	399	GLU	3.5
2	E	387	ILE	3.4
3	G	38	LEU	3.4
3	G	210	ALA	3.4
3	G	25	MET	3.3
2	E	409	LYS	3.3
2	E	474	ALA	3.3
1	C	412	ALA	3.3
3	G	216	SER	3.3
3	G	85	VAL	3.2
2	F	246	GLN	3.2
3	G	215	TYR	3.2
1	B	510	ALA	3.2
3	G	223	SER	3.1
2	D	475	GLU	3.1
3	G	217	LEU	3.1
1	A	93	ALA	3.0
1	C	410	LEU	3.0
2	D	396	LEU	3.0
3	G	213	ILE	3.0
2	E	473	LEU	3.0
3	G	211	ASN	3.0
2	E	393	MET	3.0
2	E	424	PHE	2.9
2	D	398	GLU	2.9
2	E	391	LEU	2.9
1	B	490	SER	2.9
1	B	45	ARG	2.8
2	E	439	LYS	2.8
2	E	457	PHE	2.8
2	D	28	GLY	2.8
2	F	175	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	405	GLN	2.8
2	E	455	GLN	2.7
3	G	41	ALA	2.7
2	E	396	LEU	2.6
1	A	409	ASP	2.6
3	G	1	ALA	2.6
3	G	39	LYS	2.6
3	G	36	ARG	2.6
2	E	9	THR	2.6
1	B	416	GLN	2.6
3	G	83	SER	2.6
2	D	474	ALA	2.6
2	E	390	ILE	2.5
1	B	410	LEU	2.5
2	D	9	THR	2.5
2	D	27	GLU	2.5
1	B	414	THR	2.5
2	E	451	HIS	2.5
2	E	469	LYS	2.5
2	D	246	GLN	2.5
3	G	40	PRO	2.5
2	E	471	ASP	2.4
3	G	44	TYR	2.4
1	B	412	ALA	2.4
1	B	489	ILE	2.4
1	A	381	ARG	2.4
3	G	43	VAL	2.3
3	G	88	GLN	2.3
3	G	78	CYS	2.3
3	G	212	ILE	2.3
3	G	32	ALA	2.3
2	E	110	THR	2.3
2	E	202	GLU	2.3
1	A	413	ALA	2.3
2	E	449	TYR	2.2
3	G	10	LEU	2.2
3	G	4	LYS	2.2
1	B	413	ALA	2.2
2	D	248	GLY	2.2
2	F	178	GLY	2.2
3	G	227	ALA	2.1
2	E	403	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	ARG	2.1
2	E	423	VAL	2.1
2	E	10	THR	2.1
1	B	482	LYS	2.1
3	G	31	TYR	2.1
2	F	474	ALA	2.1
1	B	25	LEU	2.0
1	A	489	ILE	2.0
1	A	403	PHE	2.0
1	A	92	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

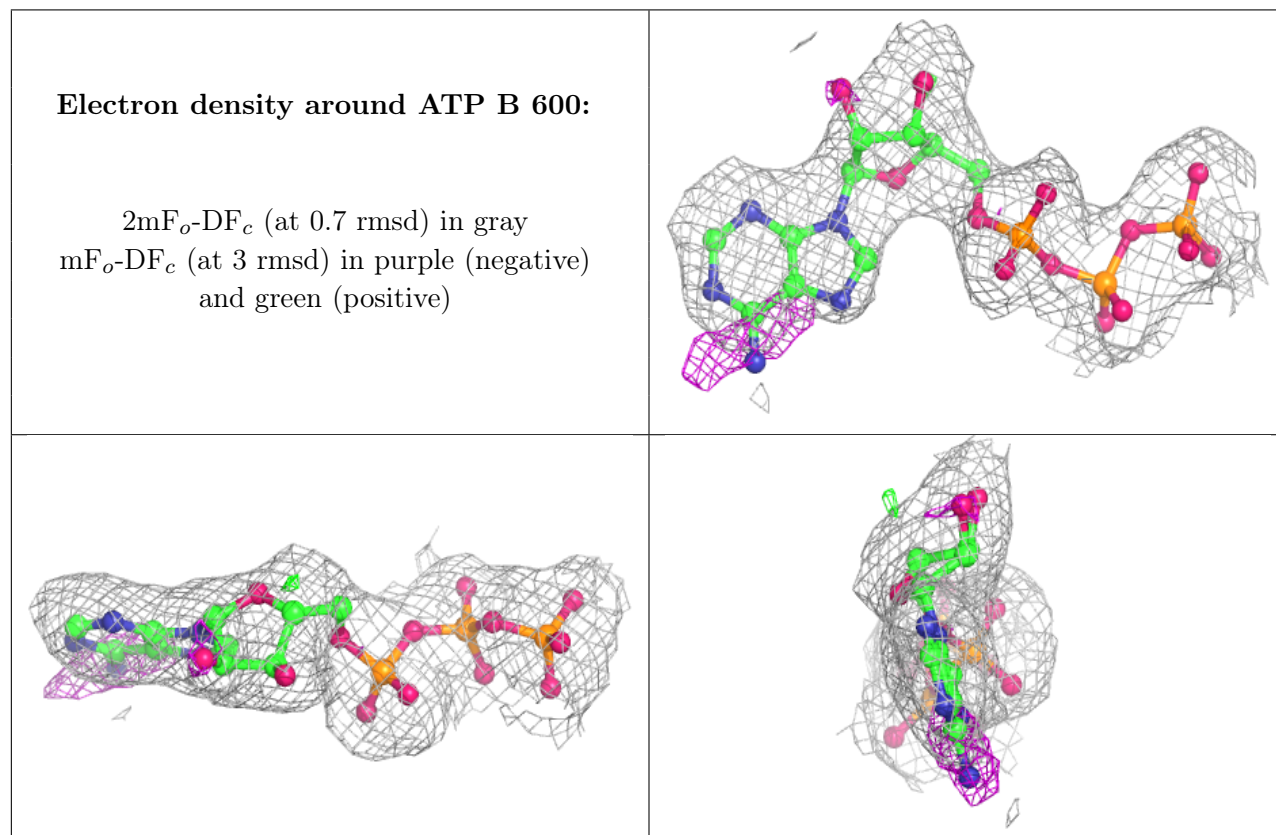
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

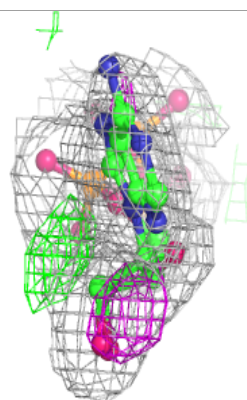
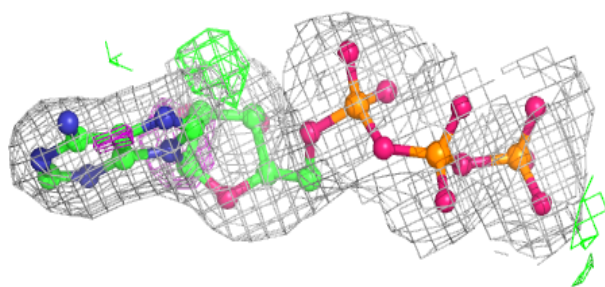
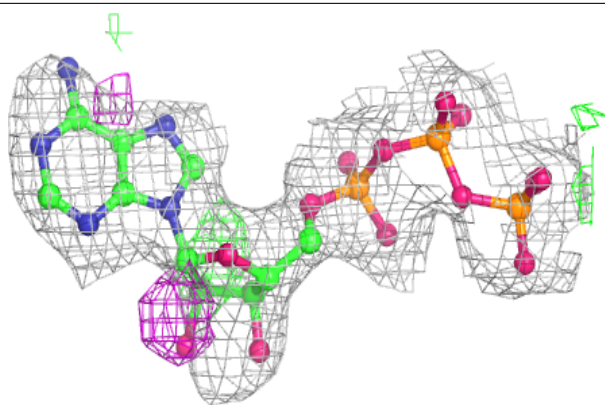
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	F	601	1/1	0.86	0.42	34,34,34,34	0
5	MG	D	601	1/1	0.87	0.52	38,38,38,38	0
5	MG	C	601	1/1	0.89	0.20	23,23,23,23	0
5	MG	A	601	1/1	0.90	0.22	30,30,30,30	0
8	PO4	E	602	5/5	0.93	0.15	80,80,81,81	0
4	ATP	B	600	31/31	0.94	0.16	21,28,32,38	0
4	ATP	A	600	31/31	0.95	0.16	13,25,31,38	0
5	MG	B	601	1/1	0.95	0.21	29,29,29,29	0
6	GOL	B	701	6/6	0.95	0.22	39,40,41,43	0
4	ATP	C	600	31/31	0.95	0.14	3,19,25,29	0
7	ADP	D	600	27/27	0.97	0.12	8,19,26,28	0
4	ATP	F	600	31/31	0.97	0.13	4,21,27,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

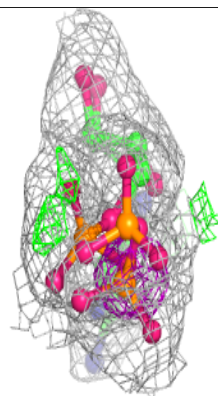
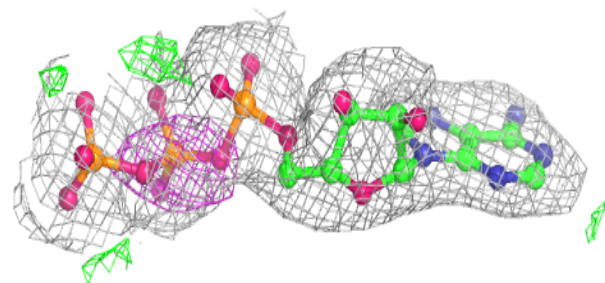
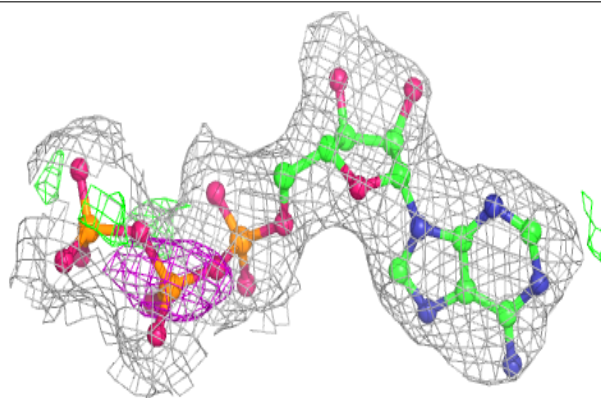


Electron density around ATP A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

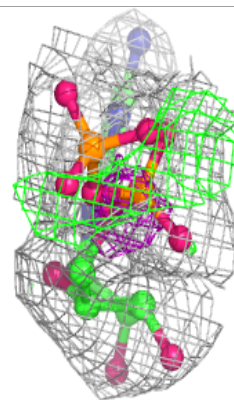
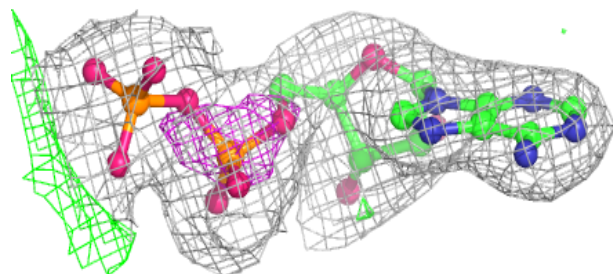
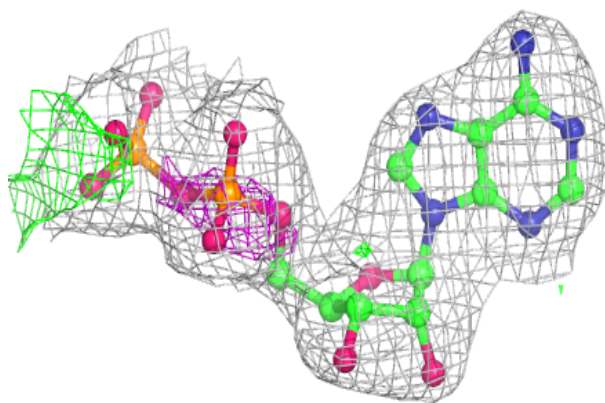
**Electron density around ATP C 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

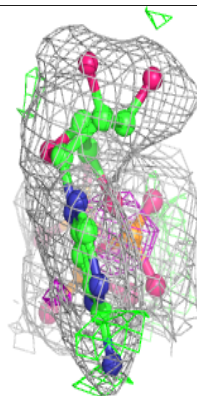
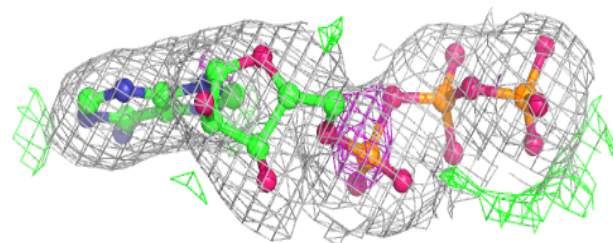
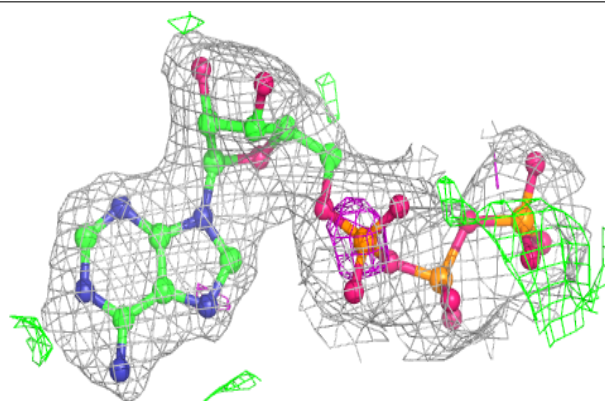


Electron density around ADP D 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP F 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.