



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:38 AM UTC

PDB ID : 9IO5 / pdb_00009io5
EMDB ID : EMD-60718
Title : Cryo-EM structure of G1-ATPase dimer from Mycoplasma mobile gliding machinery
Authors : Toyonaga, T.; Kato, T.; Kawamoto, A.; Miyata, T.; Kawakami, K.; Fujita, J.; Hamaguchi, T.; Namba, K.; Miyata, M.
Deposited on : 2024-07-08
Resolution : 3.20 Å(reported)

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:

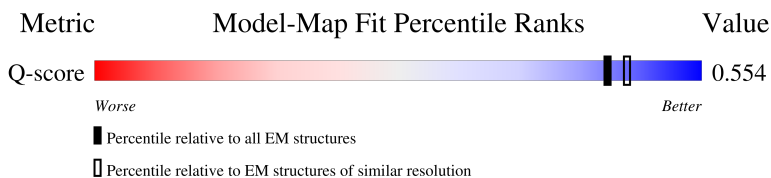
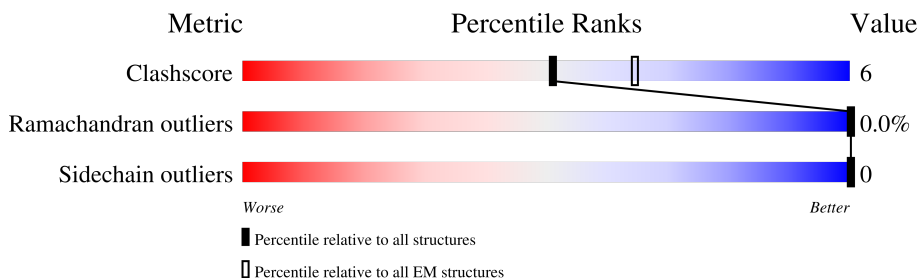
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



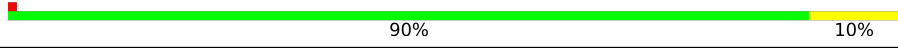
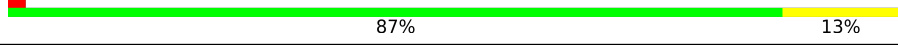
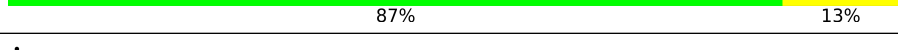
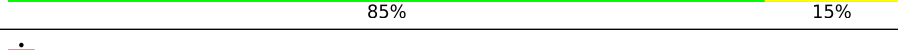
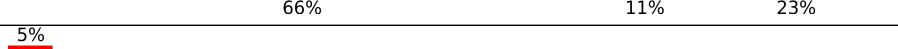
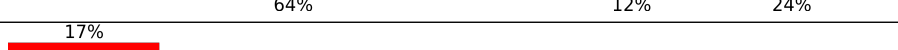
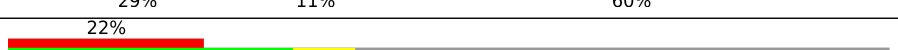
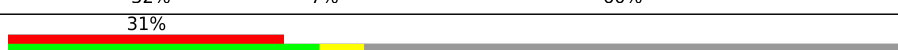
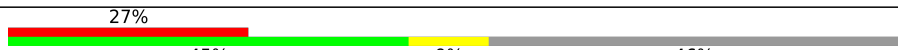
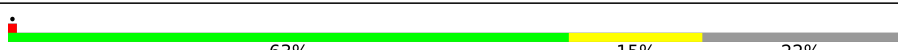
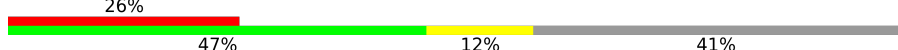
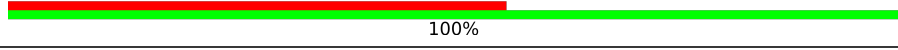
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	784	
1	B	784	
1	C	784	
1	H	784	

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Mol	Chain	Length	Quality of chain
1	I	784	
1	J	784	
2	D	528	
2	E	528	
2	F	528	
2	K	528	
2	L	528	
2	M	528	
3	G	336	
3	N	336	
4	O	511	
4	P	511	
4	Q	511	
5	R	293	
5	S	293	
5	T	293	
5	U	293	
5	V	293	
5	W	293	
6	X	112	
7	Y	13	
8	Z	9	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 69678 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 G1-ATPase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	498	Total	C	N	O	S	0	0
			3899	2508	647	737	7		
1	B	570	Total	C	N	O	S	0	0
			4470	2886	736	840	8		
1	C	561	Total	C	N	O	S	0	0
			4403	2839	730	826	8		
1	H	499	Total	C	N	O	S	0	0
			3896	2506	646	737	7		
1	I	571	Total	C	N	O	S	0	0
			4466	2884	735	839	8		
1	J	597	Total	C	N	O	S	0	0
			4690	3023	777	882	8		

- Molecule 2 is a protein called G1-ATPase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	528	Total	C	N	O	S	0	0
			4147	2680	686	774	7		
2	E	528	Total	C	N	O	S	0	0
			4111	2657	679	768	7		
2	F	528	Total	C	N	O	S	0	0
			4137	2674	685	771	7		
2	K	528	Total	C	N	O	S	0	0
			4147	2680	686	774	7		
2	L	528	Total	C	N	O	S	0	0
			4125	2667	681	770	7		
2	M	528	Total	C	N	O	S	0	0
			4118	2662	683	766	7		

- Molecule 3 is a protein called G1-ATPase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	260	Total	C	N	O	S	0	0
			2153	1382	373	396	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	256	Total	C	N	O	S	0	0
			2119	1359	366	392	2		

- Molecule 4 is a protein called Phosphoglycerate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	204	Total	C	N	O	S	0	0
			1377	889	230	256	2		
4	P	203	Total	C	N	O	S	0	0
			1314	838	227	247	2		
4	Q	203	Total	C	N	O	S	0	0
			1232	778	219	233	2		

- Molecule 5 is a protein called G1-ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	220	Total	C	N	O	S	0	0
			1778	1154	286	336	2		
5	S	158	Total	C	N	O	S	0	0
			984	622	178	183	1		
5	T	229	Total	C	N	O	S	0	0
			1854	1208	294	349	3		
5	U	226	Total	C	N	O	S	0	0
			1832	1188	294	348	2		
5	V	172	Total	C	N	O	S	0	0
			1263	818	211	232	2		
5	W	226	Total	C	N	O	S	0	0
			1818	1184	289	342	3		

- Molecule 6 is a protein called G1-ATPase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	X	109	Total	C	N	O	0	0
			913	590	156	167		

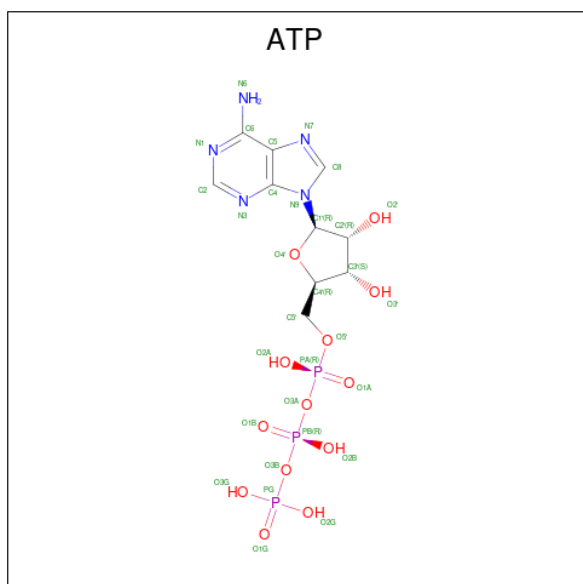
- Molecule 7 is a protein called UNKNOWN HELIX.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Y	13	Total	C	N	O	0	0
			65	39	13	13		

- Molecule 8 is a protein called UNKNOWN HELIX.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Z	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

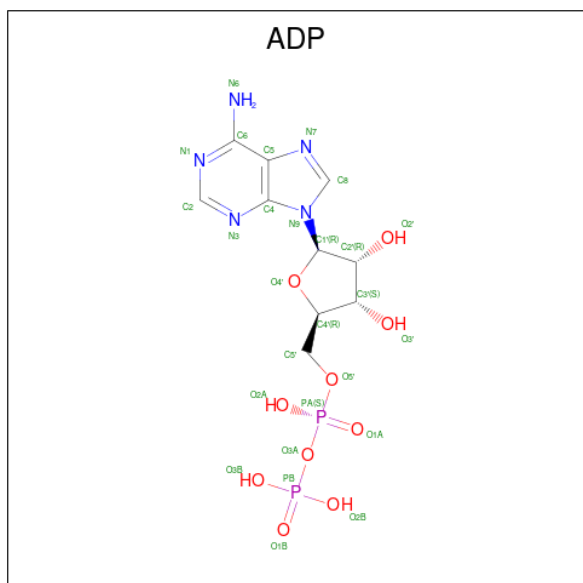


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	
10	I	1	Total	Mg	0
			1	1	
10	K	1	Total	Mg	0
			1	1	
10	L	1	Total	Mg	0
			1	1	
10	M	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



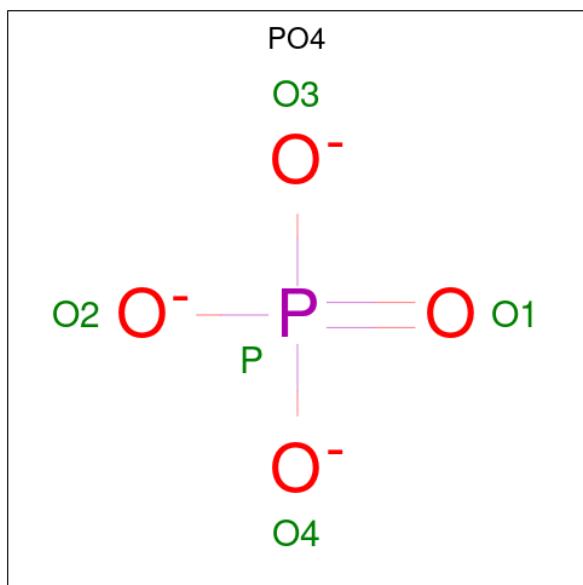
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
11	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

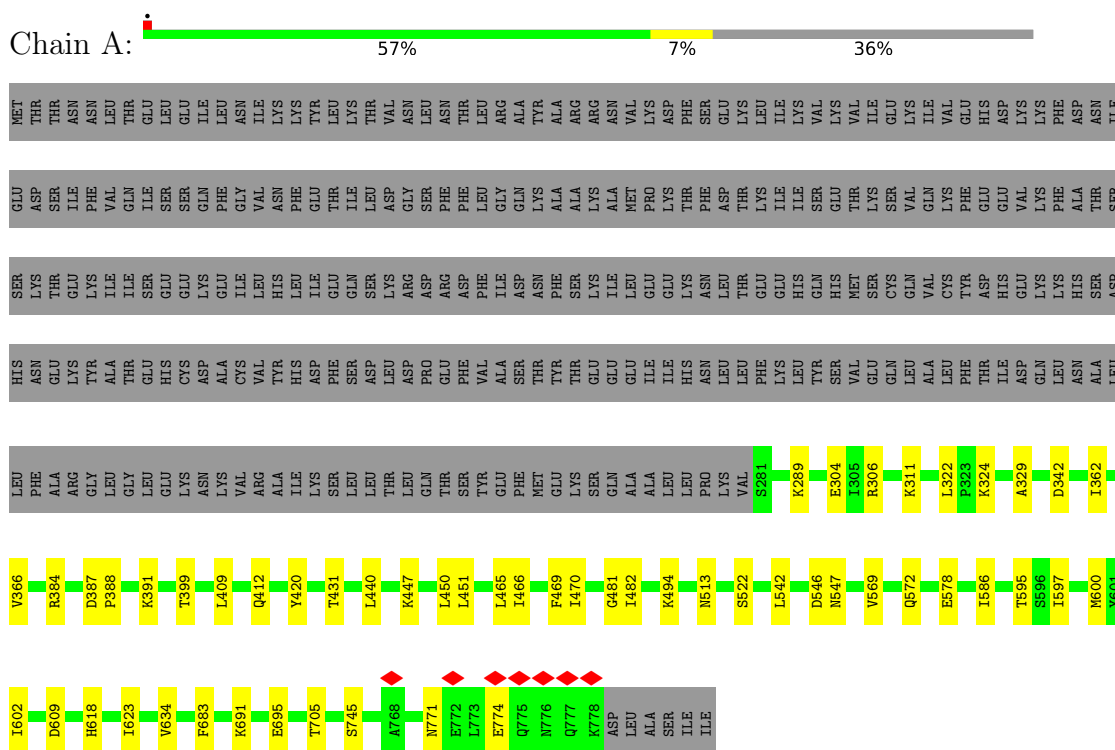


Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	O	P	0
			5	4	1	
12	I	1	Total	O	P	0
			5	4	1	

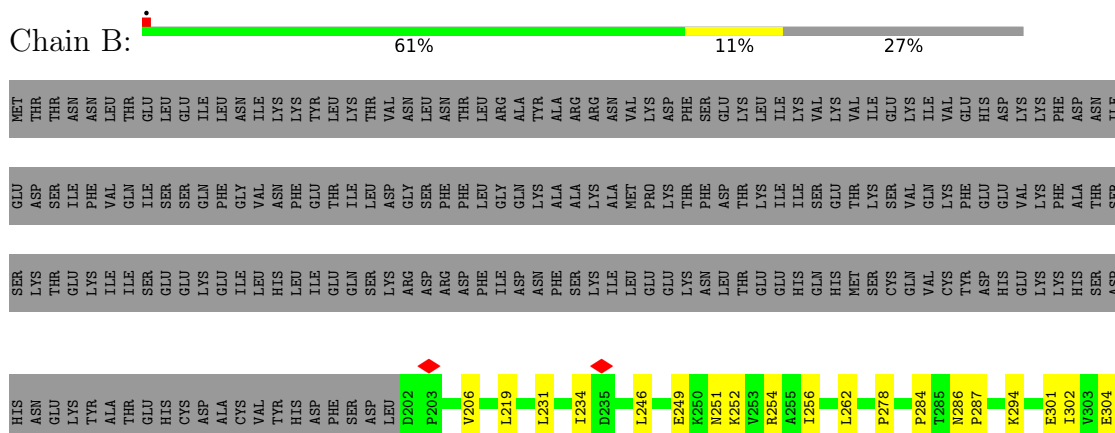
3 Residue-property plots

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.

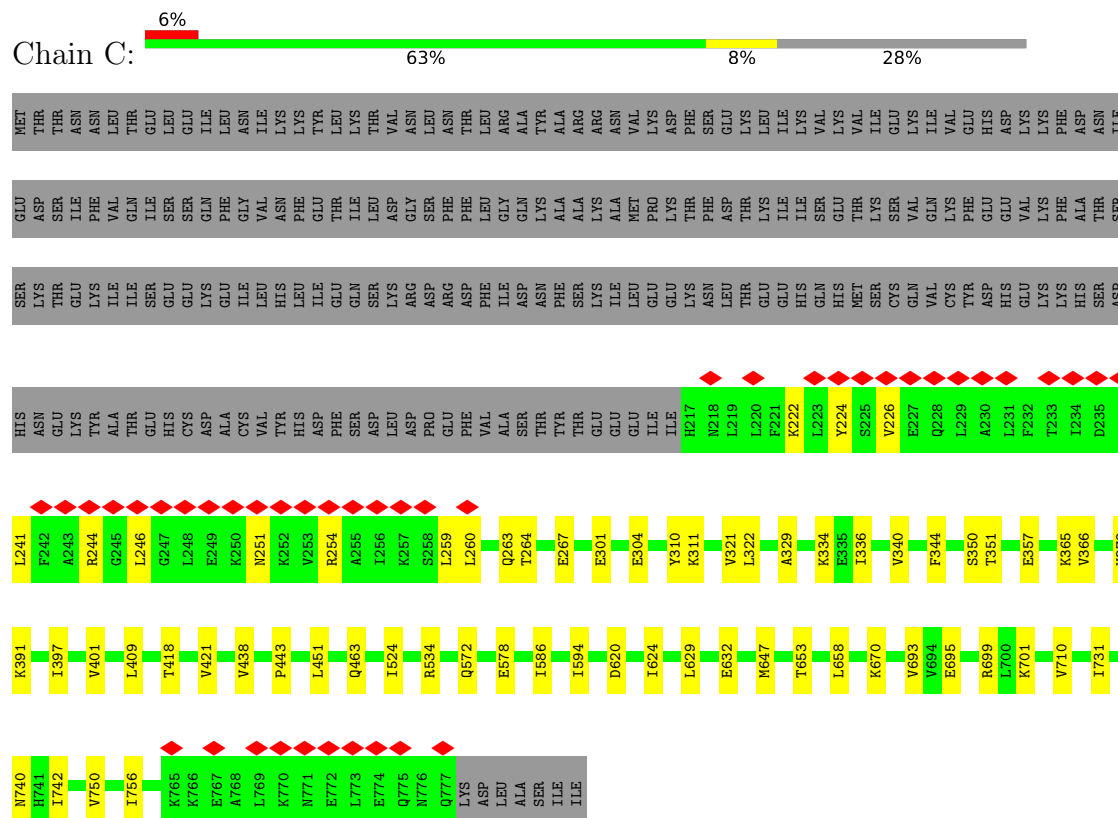
• Molecule 1: G1-ATPase subunit beta



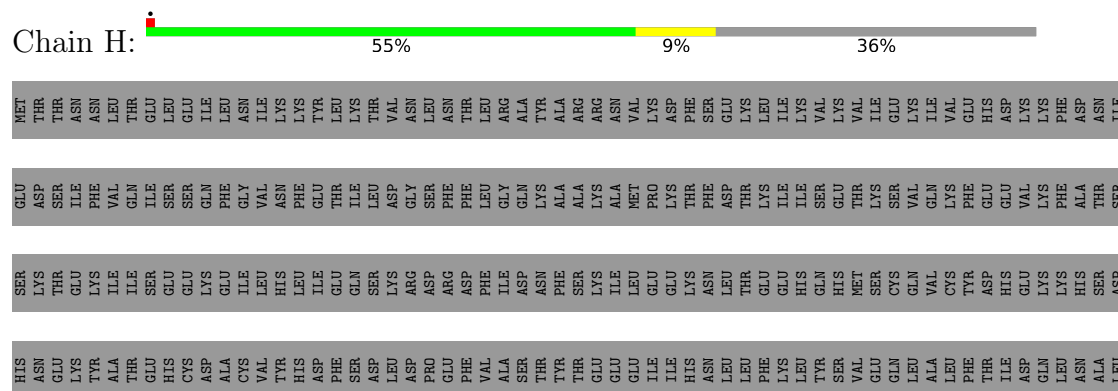
• Molecule 1: G1-ATPase subunit beta

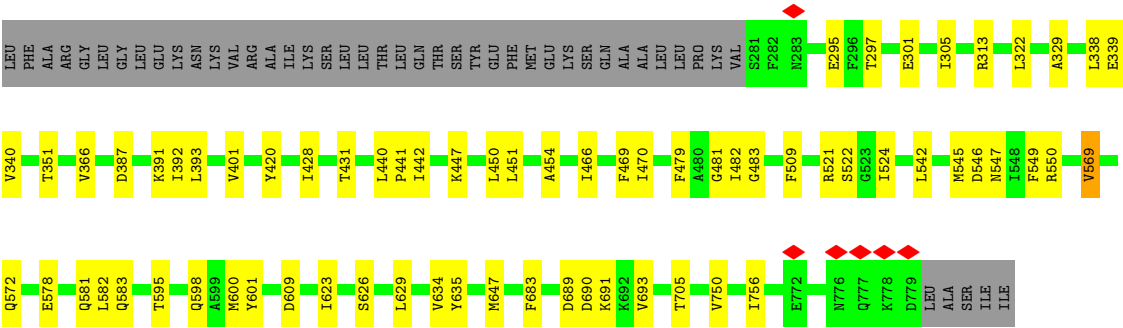


- Molecule 1: G1-ATPase subunit beta

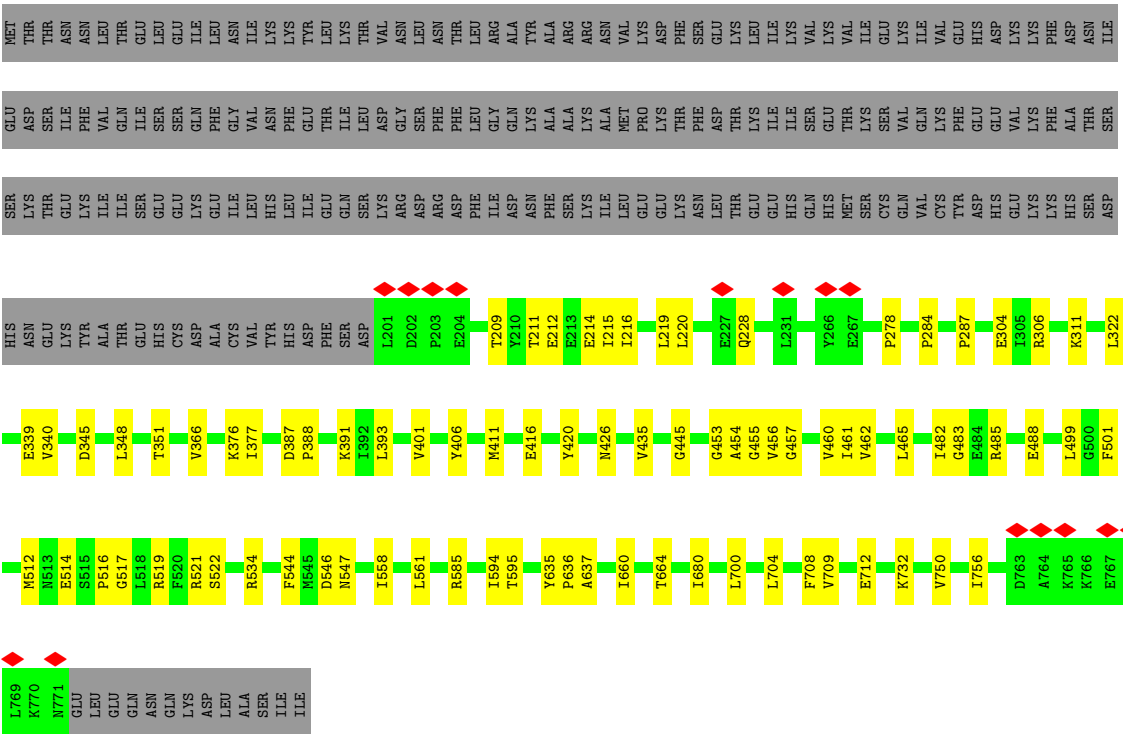


- Molecule 1: G1-ATPase subunit beta

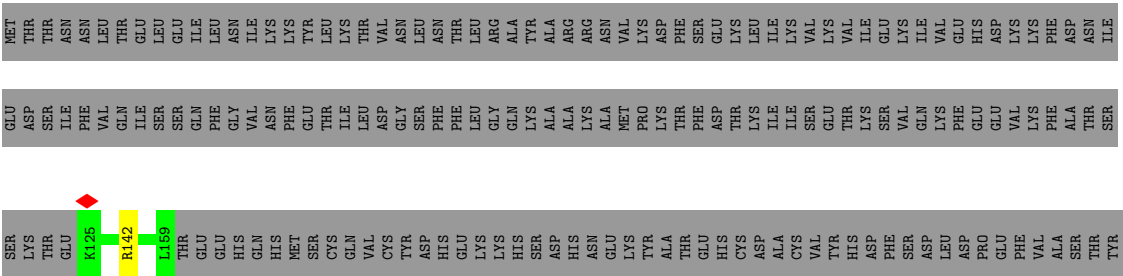


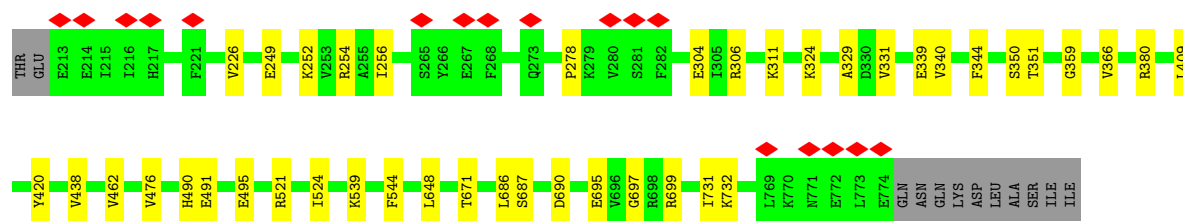


• Molecule 1: G1-ATPase subunit beta



• Molecule 1: G1-ATPase subunit beta





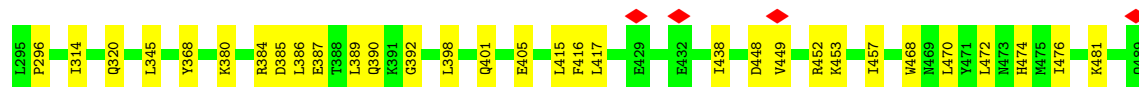
- Molecule 2: G1-ATPase subunit alpha

Chain D: 90% 10%



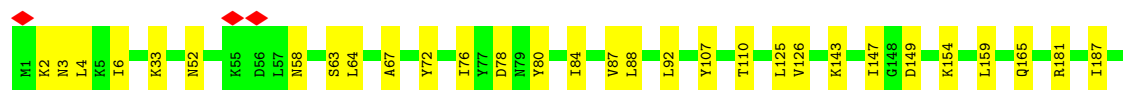
- Molecule 2: G1-ATPase subunit alpha

Chain E: 87% 13%



- Molecule 2: G1-ATPase subunit alpha

Chain F: 84% 16%



- Molecule 2: G1-ATPase subunit alpha

- Chain L: 87% 13%

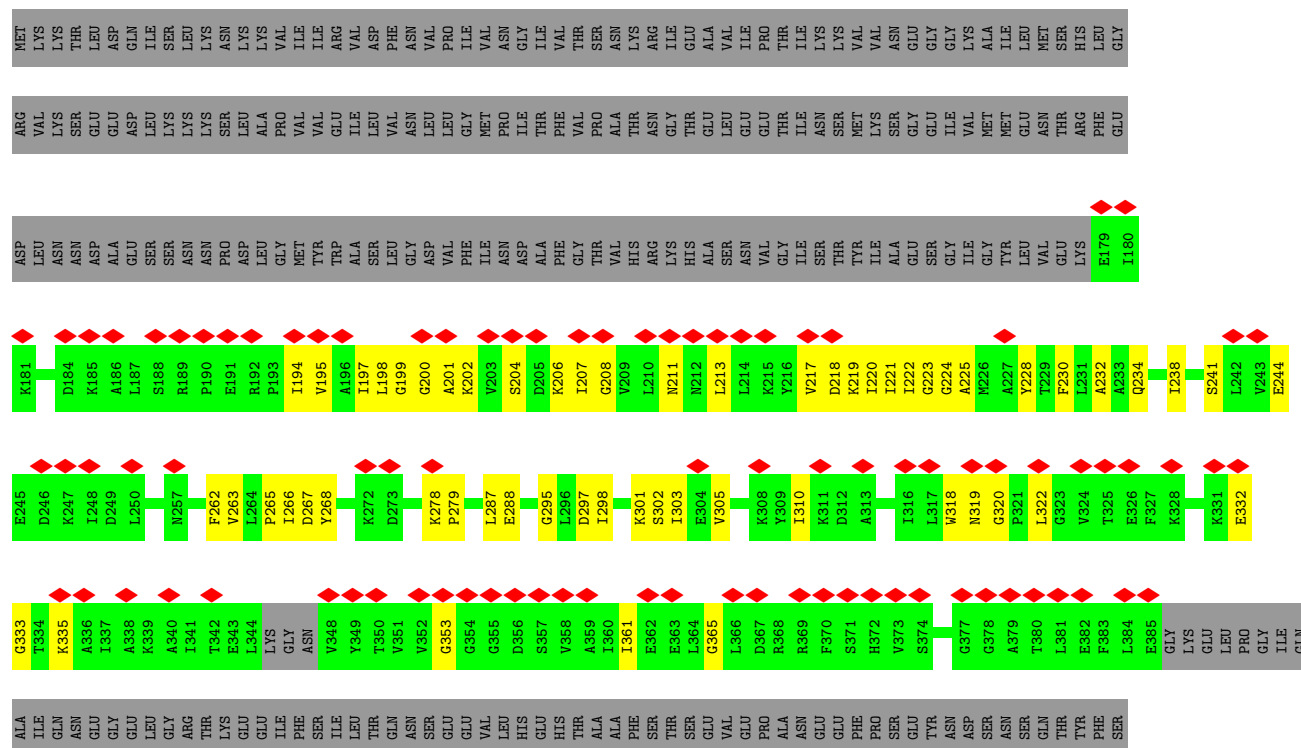
[illegible]

- Chain M:  85% 15%

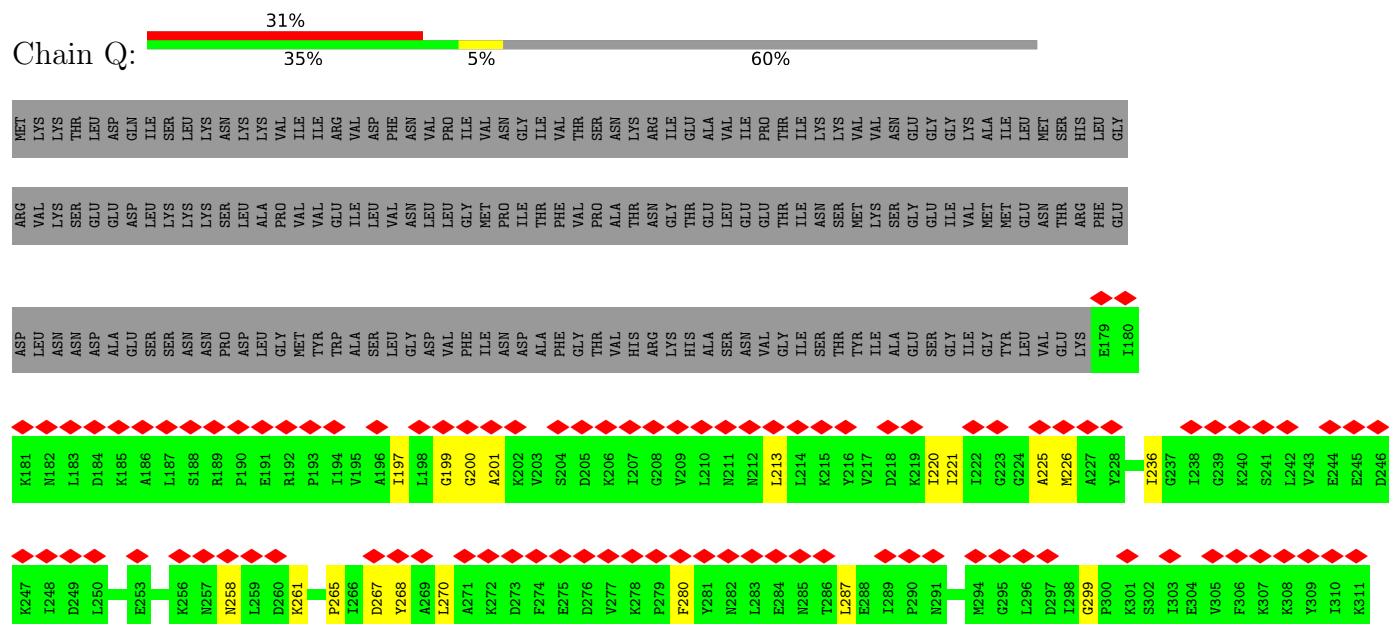
Category	Item	Value	Color
Category 1	L415	100	Green
	F416	100	Green
	L417	100	Green
	T431	100	Green
	L438	100	Green
	D448	100	Green
	R452	100	Green
	K453	100	Green
	M454	100	Green
	D464	100	Green
Category 2	S465	100	Green
	W468	100	Green
	L472	100	Green
	M473	100	Green
	H474	100	Green
	L477	100	Green
	K481	100	Green
	Y482	100	Green
	H483	100	Green
	L488	100	Green
Category 3	Q489	100	Green
	Y490	100	Green
	L491	100	Green
	R495	100	Green
	F501	100	Green
	I510	100	Green
	A513	100	Green
	T514	100	Green
	E515	100	Green
	R516	100	Green
Category 4	K517	100	Green
	R521	100	Green
	K528	100	Green
	M162	100	Yellow
	Q165	100	Yellow
	T168	100	Yellow
	D169	100	Yellow
	V170	100	Yellow
	I171	100	Yellow
	N172	100	Yellow
Category 5	I175	100	Yellow
	R181	100	Yellow
	I187	100	Yellow
	K199	100	Yellow
	I202	100	Yellow
	P218	100	Yellow
	W222	100	Yellow
	F227	100	Yellow
	D234	100	Yellow
	W239	100	Yellow
Category 6	D240	100	Yellow
	D241	100	Yellow
	T292	100	Yellow
	T293	100	Yellow
	I297	100	Yellow
	G307	100	Yellow
	T311	100	Yellow
	R373	100	Yellow
	L374	100	Yellow
	S375	100	Yellow
Category 7	S376	100	Yellow
	F377	100	Yellow
	S378	100	Yellow
	S379	100	Yellow
	K380	100	Yellow
	I381	100	Yellow
	S382	100	Yellow
	H383	100	Yellow
	L386	100	Yellow
	E387	100	Yellow
Category 8	I399	100	Yellow
	D400	100	Yellow
	D401	100	Yellow
	M1	100	Red
	I6	100	Red
	I14	100	Red
	K40	100	Red
	D43	100	Red
	L47	100	Red
	I50	100	Red
N58	100	Red	
Category 9	S63	100	Red
	Y72	100	Red
	I76	100	Red
	Y77	100	Red
	D78	100	Red
	N79	100	Red
	Y80	100	Red
	L81	100	Red
	I84	100	Red
	W87	100	Red
Category 10	L92	100	Red
	R98	100	Red
	D104	100	Red
	K105	100	Red
	I115	100	Red
	L125	100	Red
	V126	100	Red
	T127	100	Red
	G128	100	Red
	V131	100	Red
G134	100	Red	
Category 11	V138	100	Red
	G139	100	Red
	R140	100	Red
	E144	100	Red
	D149	100	Red
	K154	100	Red
	L159	100	Red

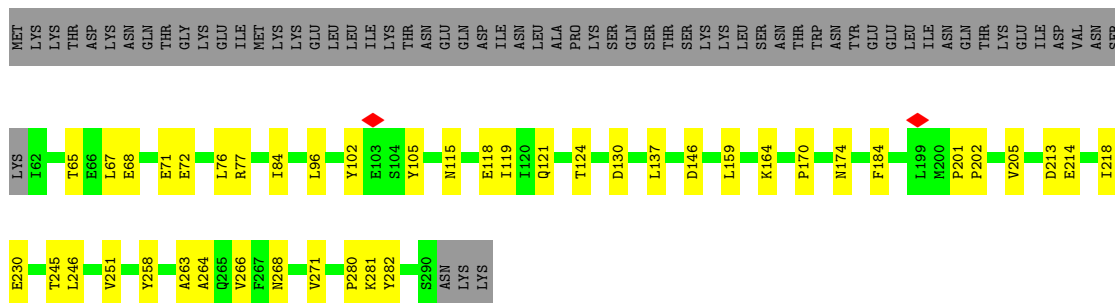
- Chain G:

Category	Item	Value
Amino acids	F1	0.00
	K2	0.00
	K8	0.00
	K9	0.00
	K10	0.00
	Q11	0.00
	I22	0.00
	V27	0.00
	L38	0.00
	K42	0.00
	G46	0.00
	E47	0.00
	L51	0.00
	L52	0.00
	N53	0.00
R54	0.00	
L55	0.00	
L56	0.00	
ASN	0.00	
LYS	0.00	
TRP	0.00	
PHE	0.00	
PRO	0.00	
HIS	0.00	
ASN	0.00	
SER	0.00	
ASN	0.00	
ILE	0.00	
TYR	0.00	
HIS	0.00	
GLU	0.00	
LEU	0.00	
HIS	0.00	
GLU	0.00	
ASN	0.00	
ASP	0.00	
R76	0.00	
I81	0.00	
L82	0.00	
I83	0.00	
D84	0.00	
P85	0.00	
V103	0.00	
I107	0.00	
D110	0.00	
K111	0.00	

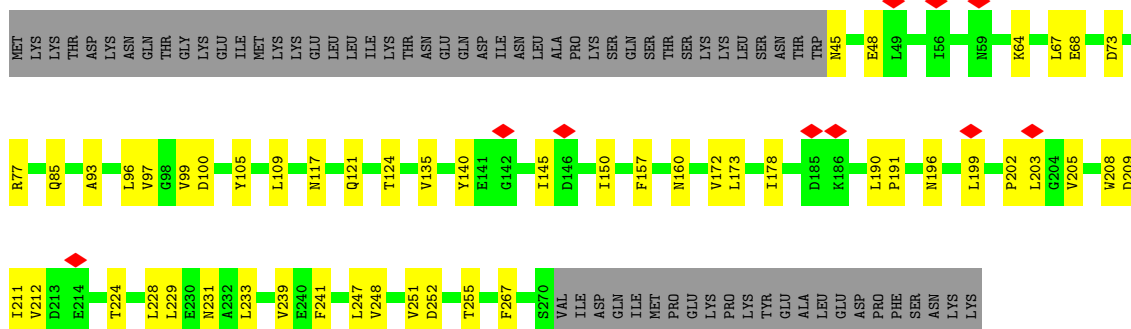


Chain P:

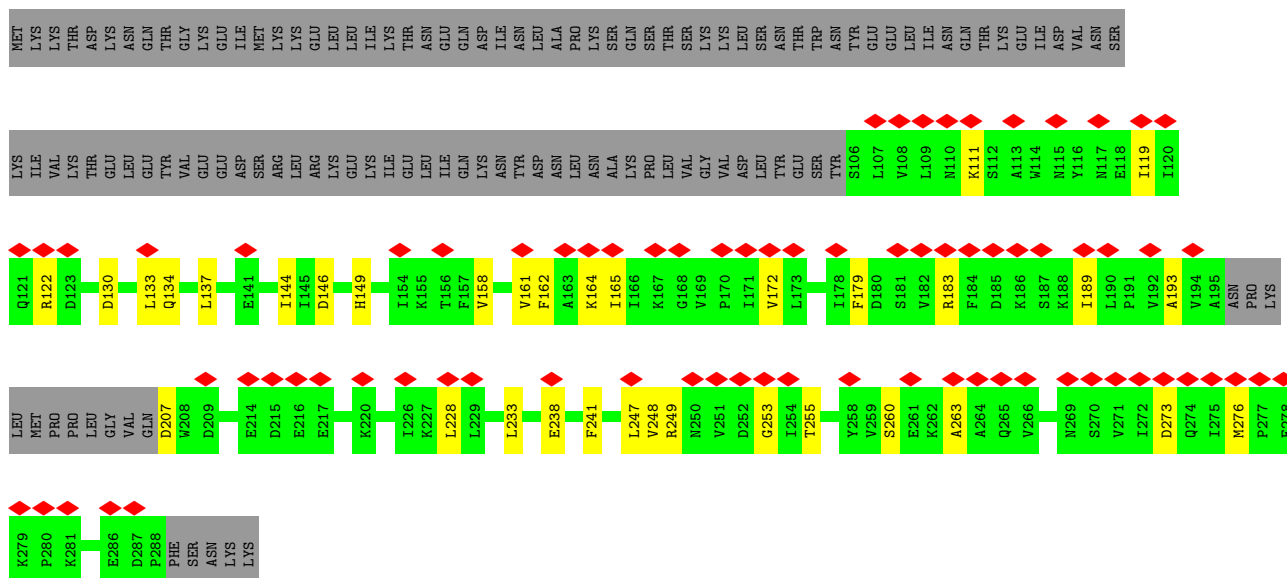




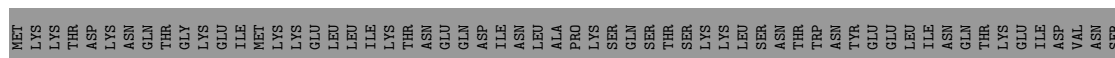
- Molecule 5: G1-ATPase subunit D

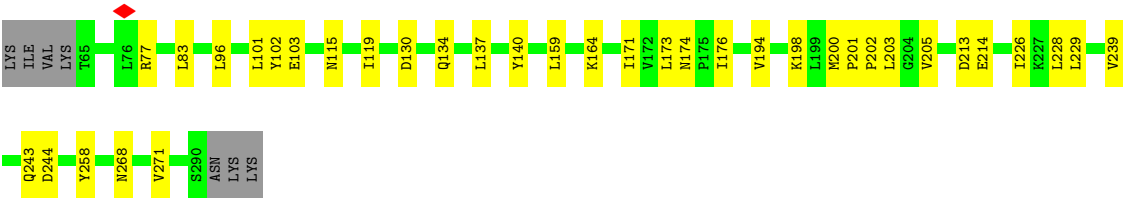


- Molecule 5: G1-ATPase subunit D



- Molecule 5: G1-ATPase subunit D

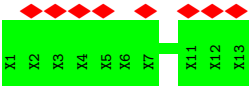




• Molecule 6: G1-ATPase subunit E



• Molecule 7: UNKNOWN HELIX



• Molecule 8: UNKNOWN HELIX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.943	Depositor
Minimum map value	-1.819	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	459.36002, 459.36002, 459.36002	wwPDB
Map dimensions	528, 528, 528	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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: PO4, MG, ATP, ADP

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	0.10	0/3969	0.25	0/5356
1	B	0.10	0/4551	0.25	0/6145
1	C	0.10	0/4481	0.26	0/6047
1	H	0.14	0/3966	0.29	0/5354
1	I	0.14	0/4547	0.29	0/6142
1	J	0.10	0/4770	0.24	0/6432
2	D	0.16	0/4218	0.27	0/5696
2	E	0.14	0/4182	0.28	0/5653
2	F	0.16	0/4208	0.29	0/5684
2	K	0.18	0/4218	0.30	1/5696 (0.0%)
2	L	0.16	0/4196	0.30	0/5669
2	M	0.16	0/4188	0.30	0/5661
3	G	0.13	0/2178	0.22	0/2914
3	N	0.12	0/2143	0.25	0/2868
4	O	0.14	0/1397	0.33	0/1902
4	P	0.20	0/1328	0.38	1/1806 (0.1%)
4	Q	0.13	0/1245	0.32	0/1706
5	R	0.15	0/1806	0.46	0/2449
5	S	0.07	0/987	0.23	0/1349
5	T	0.12	0/1888	0.33	0/2563
5	U	0.17	0/1862	0.47	0/2526
5	V	0.10	0/1281	0.26	0/1743
5	W	0.13	0/1852	0.34	0/2516
6	X	0.14	0/931	0.38	0/1257
All	All	0.14	0/70392	0.30	2/95134 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	321	PRO	N-CA-C	-5.54	101.05	112.47
2	K	309	ILE	O-C-N	5.19	123.74	120.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3899	0	3992	37	0
1	B	4470	0	4590	56	0
1	C	4403	0	4530	40	0
1	H	3896	0	3978	48	0
1	I	4466	0	4573	54	0
1	J	4690	0	4809	28	0
2	D	4147	0	4267	35	0
2	E	4111	0	4190	48	0
2	F	4137	0	4247	54	0
2	K	4147	0	4267	42	0
2	L	4125	0	4223	40	0
2	M	4118	0	4206	51	0
3	G	2153	0	2255	22	0
3	N	2119	0	2222	27	0
4	O	1377	0	1233	36	0
4	P	1314	0	1139	30	0
4	Q	1232	0	949	16	0
5	R	1778	0	1838	36	0
5	S	984	0	752	16	0
5	T	1854	0	1911	30	0
5	U	1832	0	1888	37	0
5	V	1263	0	1196	24	0
5	W	1818	0	1856	29	0
6	X	913	0	919	19	0
7	Y	65	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Z	45	0	11	0	0
9	A	31	0	12	1	0
9	D	31	0	12	0	0
9	E	31	0	12	0	0
9	F	31	0	12	0	0
9	H	31	0	12	3	0
9	K	31	0	12	0	0
9	L	31	0	12	0	0
9	M	31	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	K	1	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	B	27	0	12	0	0
11	I	27	0	12	4	0
12	B	5	0	0	0	0
12	I	5	0	0	0	0
All	All	69678	0	70176	773	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 6.

All (773) 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)
4:P:199:GLY:HA3	4:P:320:GLY:HA3	1.51	0.92
3:N:103:VAL:HG13	3:N:107:ILE:HD12	1.58	0.86
2:E:51:LEU:HD21	2:E:216:LEU:HD12	1.66	0.78
1:B:547:ASN:HB3	1:B:550:ARG:HG3	1.67	0.75
5:U:67:LEU:HD22	6:X:98:LEU:HD21	1.68	0.73
4:P:199:GLY:CA	4:P:320:GLY:HA3	2.17	0.73
5:T:258:TYR:HE1	5:U:96:LEU:HB2	1.54	0.72
1:C:304:GLU:HB3	1:C:311:LYS:HB2	1.68	0.72
5:R:172:VAL:HG23	5:R:178:ILE:HG12	1.72	0.72
4:Q:201:ALA:HA	4:Q:225:ALA:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:89:ALA:HB1	6:X:103:PHE:HB3	1.70	0.72
1:C:750:VAL:HG11	1:C:756:ILE:HD11	1.73	0.71
4:P:200:GLY:HA3	4:P:226:MET:HE2	1.73	0.70
3:G:83:ILE:HB	3:G:171:ILE:HG12	1.72	0.69
1:I:219:LEU:O	4:P:285:ASN:ND2	2.24	0.69
1:C:699:ARG:NH1	1:C:742:ILE:O	2.26	0.69
5:V:119:ILE:HA	5:V:122:ARG:HD3	1.75	0.69
2:L:168:THR:O	2:L:199:LYS:NZ	2.26	0.68
1:I:660:ILE:HD11	1:I:732:LYS:HD3	1.76	0.68
3:N:82:LEU:HB2	3:N:116:THR:HG22	1.75	0.67
5:R:73:ASP:OD2	5:W:77:ARG:NH1	2.27	0.67
1:C:259:LEU:O	1:C:263:GLN:NE2	2.27	0.67
2:M:14:ILE:HD12	2:M:50:ILE:HD11	1.77	0.67
4:P:273:ASP:HB2	4:P:277:VAL:HG21	1.77	0.67
5:U:117:ASN:O	5:U:121:GLN:HG2	1.95	0.67
1:B:304:GLU:HB2	1:B:311:LYS:HB2	1.77	0.66
1:J:340:VAL:HA	1:J:351:THR:HG22	1.77	0.66
2:F:474:HIS:O	2:F:505:ARG:NH2	2.28	0.66
1:H:301:GLU:OE2	1:H:313:ARG:NH2	2.29	0.66
5:U:99:VAL:HG12	5:U:100:ASP:H	1.60	0.65
1:B:545:MET:HE1	1:B:582:LEU:HD11	1.79	0.65
2:M:489:GLN:HG2	5:W:83:LEU:HD21	1.78	0.65
4:P:200:GLY:CA	4:P:226:MET:HE2	2.27	0.65
4:O:303:ILE:HD11	4:O:333:GLY:HA2	1.79	0.64
5:R:256:SER:HB3	5:W:203:LEU:HD22	1.79	0.64
3:N:80:TYR:HB2	3:N:114:VAL:HG22	1.79	0.64
1:J:491:GLU:O	1:J:495:GLU:HG2	1.97	0.64
4:Q:314:LYS:O	4:Q:349:TYR:N	2.30	0.64
1:H:322:LEU:HD21	2:L:58:ASN:HB3	1.78	0.64
2:M:149:ASP:O	2:M:154:LYS:NZ	2.31	0.64
5:U:172:VAL:HG23	5:U:178:ILE:HG12	1.79	0.64
1:A:451:LEU:HG	1:A:600:MET:HB3	1.79	0.64
2:M:474:HIS:ND1	5:W:130:ASP:OD1	2.30	0.64
4:O:319:ASN:ND2	4:O:353:GLY:O	2.30	0.64
1:B:491:GLU:O	1:B:495:GLU:HG2	1.98	0.63
4:Q:197:ILE:HG12	4:Q:221:ILE:HD12	1.79	0.63
1:I:461:ILE:HD11	1:I:636:PRO:HB2	1.79	0.63
1:H:609:ASP:OD1	2:K:262:ARG:NH2	2.32	0.63
1:H:329:ALA:HB2	1:H:366:VAL:HG12	1.79	0.62
2:F:505:ARG:NH1	2:F:507:ASP:OD2	2.32	0.62
2:L:501:PHE:HA	2:L:504:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:416:GLU:OE2	2:M:181:ARG:NH1	2.33	0.62
3:G:103:VAL:HG13	3:G:107:ILE:HD12	1.79	0.62
2:L:106:LYS:HD2	2:L:227:PHE:HB2	1.82	0.62
1:I:220:LEU:HD23	4:P:285:ASN:HB2	1.80	0.62
5:T:174:ASN:ND2	5:T:230:GLU:OE1	2.33	0.62
2:E:125:LEU:HD22	2:E:293:THR:HG21	1.81	0.62
1:I:284:PRO:HB2	1:I:287:PRO:HG3	1.82	0.61
1:I:664:THR:HG23	1:I:700:LEU:HD13	1.83	0.61
5:W:101:LEU:HG	5:W:103:GLU:HG3	1.82	0.61
2:M:162:MET:HE3	2:M:172:ASN:HB3	1.81	0.61
2:M:140:ARG:NH1	2:M:234:ASP:OD2	2.29	0.61
1:J:344:PHE:HE2	1:J:350:SER:HB3	1.66	0.61
4:Q:201:ALA:O	4:Q:225:ALA:HB3	2.00	0.61
1:A:466:ILE:HG23	1:A:470:ILE:HD12	1.83	0.61
5:W:202:PRO:HB2	5:W:205:VAL:CG1	2.31	0.60
1:C:244:ARG:NH1	1:C:263:GLN:OE1	2.33	0.60
2:K:448:ASP:OD1	5:U:231:ASN:ND2	2.29	0.60
1:H:547:ASN:HD21	1:H:601:TYR:HB2	1.67	0.60
5:U:178:ILE:HG21	5:U:202:PRO:HG2	1.83	0.60
1:H:549:PHE:HB2	1:H:600:MET:HE3	1.84	0.60
5:V:162:PHE:HE2	5:V:276:MET:HG2	1.67	0.60
2:L:371:LEU:HB3	2:L:389:LEU:HD21	1.82	0.60
4:Q:318:TRP:NE1	4:Q:320:GLY:O	2.34	0.60
1:A:609:ASP:OD1	2:D:262:ARG:NH2	2.35	0.60
2:M:453:LYS:NZ	5:W:140:TYR:O	2.31	0.60
2:E:509:ARG:NH2	5:S:236:GLY:O	2.36	0.59
1:A:329:ALA:HB2	1:A:366:VAL:HG12	1.82	0.59
2:E:294:ILE:HG22	2:E:296:PRO:HD3	1.84	0.59
5:U:45:ASN:HB2	5:U:48:GLU:HG2	1.83	0.59
5:W:243:GLN:HG3	5:W:244:ASP:OD1	2.02	0.59
1:B:254:ARG:HH12	1:B:755:GLU:HG2	1.66	0.59
1:J:331:VAL:HG11	1:J:359:GLY:HA3	1.85	0.59
2:L:91:SER:OG	2:L:98:ARG:NH2	2.36	0.59
2:E:527:TYR:O	2:E:528:LYS:C	2.46	0.59
1:A:513:ASN:HB3	2:D:278:GLU:HG2	1.85	0.59
1:B:437:ASP:HB3	1:B:724:LEU:HD13	1.85	0.59
6:X:4:ASN:HB3	6:X:7:ALA:HB2	1.83	0.59
6:X:33:TYR:HE1	6:X:35:GLN:HG2	1.68	0.59
2:L:474:HIS:ND1	5:V:130:ASP:OD1	2.33	0.59
1:I:322:LEU:HD21	2:M:58:ASN:HB3	1.85	0.58
4:P:218:ASP:HA	4:P:261:LYS:HZ2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:683:PHE:HE1	1:H:691:LYS:HG2	1.68	0.58
1:I:445:GLY:H	1:I:595:THR:HB	1.69	0.58
5:T:268:ASN:HA	5:T:271:VAL:HG12	1.86	0.58
1:C:251:ASN:HB3	1:C:254:ARG:HG2	1.86	0.58
1:A:572:GLN:NE2	1:A:578:GLU:OE1	2.34	0.58
2:F:159:LEU:HD11	2:F:187:ILE:HG12	1.86	0.58
5:U:241:PHE:HB2	5:U:247:LEU:HD22	1.85	0.58
1:B:329:ALA:HB2	1:B:366:VAL:HG12	1.86	0.57
2:E:481:LYS:NZ	2:E:501:PHE:O	2.36	0.57
3:G:186:ARG:HD3	3:G:189:PRO:HD2	1.86	0.57
1:H:572:GLN:NE2	1:H:578:GLU:OE1	2.37	0.57
1:J:339:GLU:OE2	1:J:521:ARG:NH2	2.34	0.57
2:K:401:GLN:NE2	2:K:405:GLU:O	2.38	0.57
4:O:222:ILE:HD13	4:O:230:PHE:HE2	1.69	0.57
2:F:516:ARG:HD3	5:U:85:GLN:OE1	2.04	0.57
4:P:201:ALA:O	4:P:225:ALA:HB3	2.04	0.57
2:F:520:GLU:HG3	2:F:527:TYR:OH	2.05	0.57
2:F:149:ASP:O	2:F:154:LYS:NZ	2.38	0.57
1:H:545:MET:HB2	1:H:598:GLN:HG2	1.86	0.57
1:H:387:ASP:HB3	1:H:393:LEU:HD11	1.87	0.57
6:X:37:ALA:HB1	6:X:46:VAL:HG13	1.87	0.57
3:N:52:LEU:HD13	3:N:247:PHE:HD2	1.70	0.57
3:N:85:PRO:HD3	3:N:172:ALA:HB3	1.87	0.57
2:E:91:SER:OG	2:E:98:ARG:NH2	2.38	0.56
4:O:202:LYS:HA	4:O:244:GLU:OE2	2.05	0.56
2:F:126:VAL:O	2:F:165:GLN:NE2	2.39	0.56
2:M:125:LEU:HD22	2:M:293:THR:HG21	1.87	0.56
5:R:108:VAL:HG11	5:W:200:MET:HE1	1.88	0.56
1:A:387:ASP:OD1	1:A:391:LYS:N	2.39	0.56
6:X:46:VAL:HB	6:X:67:ALA:HB3	1.88	0.56
2:F:229:GLN:OE1	2:F:230:GLN:NE2	2.39	0.56
2:M:72:TYR:OH	2:M:87:VAL:O	2.23	0.55
2:M:515:GLU:OE2	5:R:77:ARG:NH2	2.33	0.55
2:M:138:VAL:HG22	2:M:144:GLU:HG3	1.88	0.55
3:N:81:ILE:HB	3:N:169:LEU:HD23	1.87	0.55
1:I:485:ARG:NH1	1:I:488:GLU:OE1	2.40	0.55
2:L:142:GLN:NE2	2:L:144:GLU:OE1	2.40	0.55
1:B:426:ASN:OD1	1:J:142:ARG:NH2	2.39	0.55
3:G:38:LEU:HD21	3:G:42:LYS:HE2	1.88	0.55
2:K:426:PHE:HB2	2:K:484:LEU:HD21	1.88	0.55
4:O:199:GLY:O	4:O:320:GLY:HA3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:270:LEU:N	4:Q:280:PHE:O	2.39	0.55
1:I:534:ARG:HD3	1:I:594:ILE:HG13	1.89	0.55
1:A:451:LEU:HD23	1:A:602:ILE:HD11	1.87	0.55
1:B:252:LYS:O	1:B:256:ILE:HG13	2.07	0.55
2:F:294:ILE:HG22	2:F:296:PRO:HD3	1.87	0.55
1:I:750:VAL:HG21	1:I:756:ILE:HD11	1.89	0.55
5:S:260:SER:H	5:S:263:ALA:HB3	1.71	0.55
1:B:416:GLU:OE2	2:F:181:ARG:NH1	2.40	0.55
1:J:304:GLU:HB3	1:J:311:LYS:HB2	1.88	0.55
2:D:149:ASP:O	2:D:154:LYS:NZ	2.39	0.55
5:T:251:VAL:HB	5:U:93:ALA:HB1	1.89	0.55
5:V:134:GLN:HG2	5:V:228:LEU:HD13	1.88	0.55
1:C:699:ARG:NH2	1:C:740:ASN:O	2.40	0.55
1:H:547:ASN:ND2	1:H:601:TYR:HB2	2.22	0.54
1:H:447:LYS:NZ	1:H:583:GLN:O	2.29	0.54
1:C:397:ILE:HD11	1:J:380:ARG:HD3	1.90	0.54
1:B:231:LEU:O	4:O:234:GLN:NE2	2.40	0.54
1:C:572:GLN:NE2	1:C:578:GLU:OE1	2.39	0.54
2:F:373:ARG:HG3	2:F:374:LEU:HG	1.90	0.54
3:G:27:VAL:HG13	3:G:268:LEU:HD22	1.90	0.54
5:R:97:VAL:HG11	5:W:102:TYR:CE2	2.42	0.54
1:I:304:GLU:HB2	1:I:311:LYS:HB3	1.90	0.54
2:L:125:LEU:HD22	2:L:293:THR:HG21	1.90	0.54
5:T:96:LEU:HD11	5:T:119:ILE:HD11	1.90	0.54
1:I:387:ASP:HB3	1:I:393:LEU:HD11	1.90	0.54
1:B:284:PRO:HB2	1:B:287:PRO:HG3	1.89	0.54
2:E:159:LEU:HD11	2:E:187:ILE:HG12	1.89	0.54
2:E:526:ASP:C	2:E:528:LYS:H	2.15	0.54
1:B:206:VAL:HG12	1:B:278:PRO:HD3	1.89	0.53
1:B:634:VAL:HG13	1:B:705:THR:HG22	1.89	0.53
1:C:463:GLN:HB3	1:C:710:VAL:HG21	1.89	0.53
2:F:125:LEU:HD22	2:F:293:THR:HG21	1.90	0.53
6:X:68:THR:HG23	6:X:69:THR:HG23	1.89	0.53
1:A:306:ARG:HG3	2:D:40:LYS:HG2	1.91	0.53
1:B:387:ASP:OD1	1:B:391:LYS:N	2.39	0.53
1:I:680:ILE:HD12	3:N:22:ILE:HD13	1.88	0.53
5:S:136:HIS:HE1	5:S:144:ILE:HG23	1.73	0.53
2:L:73:LYS:HE2	2:L:107:TYR:CZ	2.44	0.53
5:S:172:VAL:O	5:S:207:ASP:N	2.41	0.53
5:U:248:VAL:O	5:U:255:THR:HA	2.08	0.53
1:A:384:ARG:NH2	1:A:399:THR:O	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:368:TYR:CG	2:E:392:GLY:HA3	2.43	0.53
2:L:145:LEU:HB2	2:L:317:THR:HG21	1.91	0.53
5:W:268:ASN:HA	5:W:271:VAL:HG12	1.90	0.53
1:A:618:HIS:HA	2:E:180:LYS:HD3	1.90	0.53
1:H:466:ILE:HG23	1:H:470:ILE:HD12	1.89	0.53
2:K:521:ARG:HE	5:U:251:VAL:HG21	1.73	0.53
2:L:126:VAL:O	2:L:165:GLN:NE2	2.42	0.53
4:O:208:GLY:HA2	4:O:211:ASN:HD22	1.74	0.53
5:R:64:LYS:O	5:R:68:GLU:HG3	2.09	0.53
1:A:420:TYR:CE1	2:E:92:LEU:HD13	2.44	0.53
2:K:182:ASP:OD1	2:K:183:GLU:N	2.42	0.53
1:B:465:LEU:HD13	1:B:597:ILE:HD13	1.91	0.53
2:F:4:LEU:HD11	2:F:67:ALA:HB2	1.90	0.53
1:H:542:LEU:HD23	1:H:595:THR:HB	1.91	0.53
1:I:460:VAL:HG12	1:I:708:PHE:HD2	1.73	0.53
1:H:451:LEU:HG	1:H:600:MET:HB3	1.91	0.53
5:S:226:ILE:HA	5:S:229:LEU:HD12	1.91	0.53
2:M:84:ILE:HG22	2:M:92:LEU:HD12	1.91	0.52
2:K:450:LEU:HD23	2:K:475:MET:HE2	1.90	0.52
2:F:487:GLU:OE2	2:F:521:ARG:NH1	2.42	0.52
4:O:198:LEU:HD22	4:O:206:LYS:HZ1	1.73	0.52
2:K:363:LYS:NZ	2:K:367:GLU:OE2	2.34	0.52
1:A:440:LEU:HD13	1:A:623:ILE:HG12	1.92	0.52
2:L:238:VAL:HG22	2:L:295:LEU:HB2	1.91	0.52
2:L:421:LYS:HB3	2:L:423:PHE:HE1	1.75	0.52
2:M:104:ASP:OD1	2:M:105:LYS:N	2.40	0.52
2:M:464:ASP:OD1	2:M:465:SER:N	2.42	0.52
5:U:229:LEU:O	5:U:233:LEU:HD13	2.10	0.52
2:D:482:TYR:HE2	2:D:511:LEU:HD23	1.73	0.52
1:H:450:LEU:HD23	1:H:623:ILE:HB	1.91	0.52
4:O:220:ILE:HD12	4:O:262:PHE:HE1	1.74	0.52
4:O:297:ASP:OD1	4:O:298:ILE:N	2.42	0.52
4:P:259:LEU:HD23	5:R:50:ILE:HD12	1.92	0.52
4:Q:201:ALA:C	4:Q:225:ALA:HB3	2.35	0.52
3:G:85:PRO:HD3	3:G:172:ALA:HB3	1.92	0.52
3:N:147:PHE:O	3:N:151:ILE:HG12	2.10	0.52
2:D:367:GLU:O	2:D:371:LEU:HD13	2.10	0.51
4:Q:258:ASN:HB3	4:Q:261:LYS:HB2	1.93	0.51
1:H:441:PRO:HG2	1:H:647:MET:HB2	1.92	0.51
1:I:482:ILE:N	1:I:546:ASP:O	2.44	0.51
1:I:514:GLU:O	1:I:519:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:GLN:NE2	2:F:405:GLU:O	2.42	0.51
1:C:620:ASP:OD1	2:D:180:LYS:NZ	2.43	0.51
4:Q:199:GLY:O	4:Q:320:GLY:HA3	2.11	0.51
1:B:294:LYS:NZ	1:B:319:GLU:OE2	2.43	0.51
5:V:161:VAL:HG22	5:V:164:LYS:HE2	1.92	0.51
4:O:195:VAL:HG23	4:O:219:LYS:HG2	1.92	0.51
2:M:472:LEU:HG	2:M:477:LEU:HG	1.93	0.51
4:P:306:PHE:O	4:P:310:ILE:HG12	2.11	0.51
5:V:161:VAL:HA	5:V:164:LYS:HE2	1.93	0.51
2:E:448:ASP:O	2:E:452:ARG:HG3	2.11	0.51
9:H:800:ATP:O1A	2:K:344:ARG:NH2	2.43	0.51
4:O:223:GLY:HA3	4:O:322:LEU:HB2	1.93	0.51
1:A:322:LEU:HD21	2:E:58:ASN:HB3	1.92	0.51
1:B:381:LEU:HD13	1:B:401:VAL:HG11	1.93	0.51
2:E:206:ALA:N	2:E:209:ASP:OD2	2.43	0.51
4:Q:213:LEU:O	4:Q:220:ILE:HD11	2.11	0.51
1:H:481:GLY:HA2	1:H:546:ASP:O	2.11	0.51
1:I:709:VAL:O	1:I:712:GLU:HG3	2.11	0.51
1:B:423:SER:O	1:B:588:SER:OG	2.29	0.50
1:C:301:GLU:HG2	1:C:365:LYS:HD3	1.93	0.50
4:P:204:SER:HA	4:P:207:ILE:HG13	1.93	0.50
1:I:388:PRO:HG3	1:I:522:SER:HA	1.93	0.50
2:L:421:LYS:HB3	2:L:423:PHE:CE1	2.47	0.50
4:P:209:VAL:HG12	4:P:213:LEU:HG	1.93	0.50
2:L:461:HIS:CD2	5:V:144:ILE:HD11	2.47	0.50
6:X:28:LEU:HD13	6:X:86:PHE:HD1	1.77	0.50
2:E:134:GLY:HA3	2:E:416:PHE:HE2	1.77	0.50
2:E:501:PHE:HA	2:E:504:ILE:HD13	1.93	0.50
2:K:125:LEU:HD22	2:K:293:THR:HG21	1.92	0.50
1:A:634:VAL:HG13	1:A:705:THR:HG22	1.92	0.50
1:B:343:ILE:HG23	1:B:349:VAL:HG12	1.93	0.50
2:M:488:LEU:HD12	2:M:491:LEU:HD11	1.92	0.50
1:C:409:LEU:HD23	1:C:524:ILE:HG21	1.94	0.50
1:C:670:LYS:HD3	1:C:693:VAL:HG11	1.93	0.50
2:E:453:LYS:O	2:E:457:ILE:HG12	2.12	0.50
3:G:170:LEU:HD13	3:G:184:GLN:HB3	1.94	0.50
5:T:65:THR:HB	5:T:68:GLU:HG3	1.93	0.50
2:F:84:ILE:HG12	2:F:202:ILE:HB	1.94	0.50
4:O:197:ILE:HD11	4:O:310:ILE:HD11	1.94	0.50
2:D:81:LEU:HD22	2:D:199:LYS:HA	1.94	0.49
2:E:415:LEU:HD11	2:E:438:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:418:LEU:HD21	2:F:472:LEU:HD11	1.94	0.49
1:H:750:VAL:HG21	1:H:756:ILE:HD11	1.94	0.49
1:J:476:VAL:HG13	1:J:539:LYS:HD2	1.94	0.49
2:K:482:TYR:CD2	2:K:508:GLY:HA3	2.48	0.49
1:B:649:SER:O	1:B:653:THR:OG1	2.27	0.49
5:T:170:PRO:HG2	5:T:205:VAL:HA	1.94	0.49
1:C:329:ALA:HB2	1:C:366:VAL:HG12	1.94	0.49
1:C:381:LEU:HD13	1:C:401:VAL:HG11	1.94	0.49
4:O:221:ILE:HG13	4:O:263:VAL:CG2	2.43	0.49
5:R:176:ILE:O	5:R:197:PRO:HG2	2.13	0.49
1:H:420:TYR:CE1	2:L:92:LEU:HD13	2.47	0.49
1:H:440:LEU:HD13	1:H:623:ILE:HG12	1.94	0.49
1:H:689:ASP:N	1:H:689:ASP:OD1	2.45	0.49
2:K:467:VAL:HG23	5:U:140:TYR:HD2	1.77	0.49
4:O:265:PRO:O	4:O:268:TYR:OH	2.29	0.49
1:J:329:ALA:HB2	1:J:366:VAL:HG12	1.94	0.49
2:D:134:GLY:HA3	2:D:416:PHE:CE2	2.47	0.49
1:J:409:LEU:HD23	1:J:524:ILE:HG21	1.94	0.49
2:M:222:MET:HE1	2:M:292:ILE:HG21	1.93	0.49
3:G:110:ASP:OD1	3:G:111:LYS:N	2.46	0.49
1:I:306:ARG:NH2	1:I:561:LEU:O	2.45	0.49
4:Q:200:GLY:O	4:Q:226:MET:HG2	2.13	0.49
1:A:447:LYS:HE2	1:A:586:ILE:HB	1.95	0.49
1:B:301:GLU:OE1	1:B:365:LYS:NZ	2.46	0.49
1:H:483:GLY:HA3	1:H:550:ARG:HG3	1.94	0.49
5:T:264:ALA:O	5:T:268:ASN:ND2	2.29	0.49
2:E:384:ARG:O	2:E:387:GLU:HG2	2.13	0.48
2:K:31:SER:HB3	2:K:57:LEU:HD13	1.95	0.48
4:Q:236:ILE:HD13	4:Q:287:LEU:HD21	1.95	0.48
1:B:378:SER:OG	1:B:402:HIS:O	2.27	0.48
1:I:457:GLY:H	11:I:801:ADP:C5'	2.26	0.48
2:M:483:HIS:NE2	2:M:521:ARG:O	2.45	0.48
5:T:84:ILE:HD11	5:U:77:ARG:NH2	2.28	0.48
2:D:159:LEU:HD11	2:D:187:ILE:HG12	1.95	0.48
2:K:439:GLY:O	2:K:443:VAL:HG23	2.13	0.48
2:D:125:LEU:HD22	2:D:293:THR:HG21	1.94	0.48
2:D:318:ASP:HA	2:D:344:ARG:HD2	1.94	0.48
1:B:545:MET:HB2	1:B:598:GLN:HG2	1.95	0.48
1:I:453:GLY:HA2	1:I:456:VAL:CG2	2.42	0.48
2:K:165:GLN:O	2:K:199:LYS:NZ	2.37	0.48
2:L:78:ASP:OD2	2:L:99:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ILE:HG23	2:E:115:ILE:HG22	1.95	0.48
2:F:209:ASP:O	2:F:214:ARG:NH1	2.47	0.48
1:H:683:PHE:CE1	2:K:377:PHE:HB2	2.48	0.48
1:I:453:GLY:HA3	11:I:801:ADP:O3B	2.14	0.48
1:I:209:THR:HG21	1:I:278:PRO:HB3	1.95	0.48
1:C:321:VAL:O	2:D:60:THR:OG1	2.23	0.48
1:I:387:ASP:OD2	1:I:391:LYS:HB3	2.13	0.48
1:J:344:PHE:CE2	1:J:350:SER:HB3	2.47	0.48
2:L:471:TYR:CE1	5:V:133:LEU:HD21	2.49	0.48
4:P:199:GLY:HA2	4:P:223:GLY:O	2.14	0.48
5:R:96:LEU:HB2	5:W:258:TYR:HE1	1.79	0.48
5:W:174:ASN:HD21	5:W:176:ILE:HB	1.77	0.48
1:A:420:TYR:HH	2:E:204:SER:HG	1.60	0.48
2:M:307:GLY:O	2:M:311:THR:OG1	2.25	0.48
5:V:233:LEU:HD21	5:V:247:LEU:HB3	1.95	0.48
3:G:166:TYR:CD1	3:G:189:PRO:HD3	2.49	0.48
2:M:84:ILE:HG12	2:M:202:ILE:HB	1.95	0.48
5:R:134:GLN:HB3	5:R:228:LEU:HD13	1.95	0.48
9:A:800:ATP:O3'	2:D:344:ARG:HG2	2.14	0.47
2:D:72:TYR:CE2	2:D:108:VAL:HG21	2.50	0.47
2:D:364:ILE:HD13	2:D:391:LYS:HD2	1.96	0.47
5:R:166:ILE:HD11	5:R:267:PHE:CD2	2.48	0.47
6:X:39:LYS:HB3	6:X:43:GLU:HA	1.96	0.47
5:S:150:ILE:O	5:S:154:ILE:HG12	2.13	0.47
1:C:534:ARG:HD3	1:C:594:ILE:HG13	1.96	0.47
2:D:447:LYS:O	2:D:452:ARG:NH2	2.47	0.47
1:I:376:LYS:NZ	1:I:401:VAL:O	2.39	0.47
5:T:118:GLU:O	5:T:121:GLN:HG3	2.14	0.47
2:E:398:LEU:HD11	2:E:415:LEU:HB3	1.96	0.47
2:F:147:ILE:HD11	2:F:310:PRO:HB3	1.96	0.47
2:F:206:ALA:N	2:F:209:ASP:OD2	2.42	0.47
1:H:431:THR:HG21	1:H:442:ILE:HD12	1.97	0.47
2:M:481:LYS:HD2	2:M:501:PHE:HB3	1.96	0.47
3:N:114:VAL:O	3:N:132:ILE:HA	2.14	0.47
5:R:177:ILE:HD11	5:R:233:LEU:HD12	1.97	0.47
1:A:482:ILE:HG12	1:A:522:SER:HB2	1.97	0.47
1:A:683:PHE:CE1	2:D:377:PHE:HB2	2.50	0.47
1:I:455:GLY:HA2	11:I:801:ADP:H4'	1.97	0.47
1:C:438:VAL:HG21	1:C:731:ILE:HD12	1.97	0.47
2:E:4:LEU:HD11	2:E:67:ALA:HB2	1.97	0.47
3:G:287:LYS:HB3	3:G:287:LYS:HE2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:294:ILE:HG22	2:K:296:PRO:HD3	1.96	0.47
4:O:213:LEU:O	4:O:217:VAL:N	2.34	0.47
5:R:164:LYS:O	5:R:169:VAL:HG12	2.15	0.47
5:V:183:ARG:HA	5:V:189:ILE:HA	1.97	0.47
5:W:173:LEU:HD23	5:W:226:ILE:HG12	1.97	0.47
5:W:202:PRO:HB2	5:W:205:VAL:HG13	1.95	0.47
1:C:451:LEU:HD12	1:C:624:ILE:HG12	1.97	0.47
2:L:398:LEU:HD11	2:L:415:LEU:HB3	1.97	0.47
4:P:267:ASP:HB2	4:P:301:LYS:HB2	1.95	0.47
2:E:417:LEU:HD13	2:E:468:TRP:CE2	2.50	0.47
2:K:143:LYS:HD3	2:K:277:LEU:O	2.15	0.47
5:V:172:VAL:O	5:V:207:ASP:N	2.48	0.47
2:D:4:LEU:HD11	2:D:67:ALA:HB2	1.96	0.47
2:K:318:ASP:C	2:K:344:ARG:HD3	2.40	0.47
3:N:167:VAL:HB	3:N:188:VAL:HB	1.97	0.47
3:N:169:LEU:O	3:N:184:GLN:HA	2.15	0.47
5:R:152:LYS:HB3	5:R:152:LYS:HE2	1.63	0.47
5:R:153:ILE:O	5:R:156:THR:HG22	2.15	0.47
3:G:81:ILE:HG12	3:G:115:ILE:HB	1.96	0.46
1:I:420:TYR:CE1	2:M:92:LEU:HD13	2.50	0.46
2:L:481:LYS:HD3	2:L:501:PHE:HD2	1.79	0.46
2:M:417:LEU:HD13	2:M:468:TRP:CE2	2.50	0.46
5:R:75:ARG:O	5:R:79:GLU:OE1	2.34	0.46
1:B:339:GLU:OE1	1:B:521:ARG:NH2	2.30	0.46
1:J:252:LYS:O	1:J:256:ILE:HG13	2.16	0.46
5:T:202:PRO:HB2	5:T:205:VAL:HB	1.98	0.46
5:W:134:GLN:HB3	5:W:228:LEU:HD13	1.97	0.46
1:C:310:TYR:OH	1:C:357:GLU:OE1	2.28	0.46
2:D:482:TYR:CG	2:D:508:GLY:HA3	2.51	0.46
2:F:33:LYS:O	2:F:52:ASN:ND2	2.47	0.46
2:F:222:MET:HE1	2:F:292:ILE:HG21	1.97	0.46
1:H:683:PHE:CE1	1:H:691:LYS:HG2	2.50	0.46
1:I:516:PRO:HB2	1:I:558:ILE:HG13	1.98	0.46
2:M:43:ASP:OD1	2:M:43:ASP:N	2.48	0.46
4:O:232:ALA:HB2	4:O:238:ILE:HG21	1.96	0.46
2:F:447:LYS:HB2	2:F:523:ILE:HD11	1.96	0.46
1:H:340:VAL:HA	1:H:351:THR:HG22	1.98	0.46
2:K:454:MET:HE1	2:K:476:ILE:HG13	1.98	0.46
1:A:745:SER:O	2:D:384:ARG:NH2	2.49	0.46
1:C:340:VAL:HA	1:C:351:THR:HG22	1.97	0.46
2:E:314:ILE:HG12	2:E:320:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:368:TYR:CG	2:L:392:GLY:HA3	2.50	0.46
2:M:510:ILE:HD12	2:M:510:ILE:H	1.81	0.46
5:T:72:GLU:O	5:T:76:LEU:HD23	2.15	0.46
5:U:239:VAL:O	5:U:247:LEU:HD23	2.15	0.46
2:E:241:ASP:N	2:E:241:ASP:OD1	2.48	0.46
6:X:35:GLN:HG3	6:X:49:PRO:HG2	1.97	0.46
1:B:666:GLN:O	1:B:669:GLU:HG3	2.16	0.46
2:D:140:ARG:NH1	2:D:234:ASP:OD2	2.44	0.46
2:E:142:GLN:OE1	2:E:345:LEU:HD12	2.14	0.46
5:U:145:ILE:HG21	5:U:150:ILE:HD11	1.97	0.46
1:C:387:ASP:OD1	1:C:391:LYS:N	2.48	0.46
2:E:125:LEU:HD21	2:E:236:LEU:HD13	1.97	0.46
1:I:228:GLN:OE1	4:P:235:GLY:HA3	2.16	0.46
3:N:175:SER:HB2	3:N:183:VAL:HG12	1.97	0.46
1:B:234:ILE:HD11	1:B:252:LYS:HG3	1.98	0.46
1:H:387:ASP:OD2	1:H:391:LYS:HB3	2.16	0.46
2:M:134:GLY:HA3	2:M:416:PHE:CE2	2.50	0.46
2:F:494:ASN:O	2:F:498:ILE:HD12	2.16	0.46
3:G:292:LYS:HE2	3:G:292:LYS:HB3	1.68	0.46
5:R:179:PHE:HZ	5:R:247:LEU:HD11	1.80	0.46
5:S:115:ASN:O	5:S:118:GLU:HG3	2.16	0.46
5:U:109:LEU:HD21	5:U:190:LEU:HD13	1.98	0.46
1:H:546:ASP:HA	1:H:547:ASN:HA	1.71	0.45
1:I:461:ILE:O	1:I:465:LEU:HG	2.17	0.45
2:L:14:ILE:HG13	2:L:50:ILE:HD11	1.98	0.45
5:W:164:LYS:HG2	5:W:171:ILE:HD11	1.98	0.45
6:X:34:ILE:HD12	6:X:50:LEU:HG	1.98	0.45
1:A:771:ASN:O	1:A:774:GLU:HG3	2.16	0.45
1:B:483:GLY:O	1:B:550:ARG:NH1	2.50	0.45
1:B:542:LEU:HG	1:B:544:PHE:CE1	2.51	0.45
2:F:472:LEU:HG	2:F:477:LEU:HG	1.98	0.45
1:I:340:VAL:HA	1:I:351:THR:HG22	1.98	0.45
5:R:101:LEU:HD22	5:W:194:VAL:HG11	1.98	0.45
5:R:194:VAL:HG23	5:W:201:PRO:HG2	1.98	0.45
5:V:260:SER:H	5:V:263:ALA:HB3	1.81	0.45
2:D:448:ASP:O	2:D:452:ARG:HG3	2.16	0.45
2:F:395:PHE:O	2:F:399:ILE:HG12	2.15	0.45
4:O:222:ILE:HD13	4:O:230:PHE:CE2	2.51	0.45
5:T:102:TYR:CZ	5:U:97:VAL:HG21	2.51	0.45
2:D:434:LEU:O	2:D:438:ILE:HG12	2.16	0.45
2:E:470:LEU:HD12	2:E:474:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:411:MET:HE3	1:I:411:MET:HB3	1.87	0.45
2:K:147:ILE:HD11	2:K:310:PRO:HB3	1.97	0.45
2:L:249:TYR:CE2	2:L:272:VAL:HG21	2.52	0.45
4:O:204:SER:HA	4:O:207:ILE:HD11	1.98	0.45
4:O:332:GLU:HA	4:O:335:LYS:HE3	1.97	0.45
5:T:77:ARG:NH1	5:U:73:ASP:OD2	2.38	0.45
5:U:209:ASP:O	5:U:212:VAL:HG22	2.17	0.45
1:I:212:GLU:O	1:I:216:ILE:HG12	2.17	0.45
2:K:484:LEU:HG	2:K:491:LEU:HD13	1.97	0.45
3:N:80:TYR:CE2	3:N:107:ILE:HG12	2.51	0.45
5:R:97:VAL:HG21	5:W:102:TYR:CZ	2.52	0.45
5:R:172:VAL:HG12	5:R:206:GLN:O	2.16	0.45
5:T:263:ALA:O	5:T:266:VAL:HG12	2.17	0.45
3:G:144:ILE:HG12	3:G:260:LYS:HG2	1.99	0.45
1:J:438:VAL:HG11	1:J:731:ILE:HD12	1.98	0.45
2:M:76:ILE:HG21	2:M:227:PHE:CE2	2.52	0.45
5:T:146:ASP:OD2	5:T:282:TYR:OH	2.34	0.45
1:B:414:ASP:OD1	1:B:415:SER:N	2.49	0.45
1:B:494:LYS:HA	1:B:494:LYS:HD3	1.65	0.45
1:I:329:ALA:HB2	1:I:366:VAL:HG12	1.99	0.45
2:L:6:ILE:HD12	2:L:63:SER:HB2	1.98	0.45
4:Q:350:THR:HB	4:Q:370:PHE:HA	1.99	0.45
6:X:25:HIS:ND1	6:X:103:PHE:HE1	2.14	0.45
1:A:362:ILE:HB	2:D:21:GLN:HA	1.99	0.45
2:F:491:LEU:HD23	2:F:491:LEU:HA	1.83	0.45
3:G:140:LEU:HG	3:G:147:PHE:HB2	1.97	0.45
1:J:686:LEU:HB3	1:J:690:ASP:HB2	1.99	0.45
2:K:453:LYS:O	2:K:457:ILE:HG12	2.17	0.45
4:O:200:GLY:O	4:O:224:GLY:HA3	2.16	0.45
4:P:321:PRO:C	4:P:323:GLY:N	2.74	0.45
5:T:281:LYS:HE3	5:T:281:LYS:HB2	1.76	0.45
1:A:304:GLU:HB2	1:A:311:LYS:HB3	1.99	0.45
1:A:542:LEU:HD23	1:A:595:THR:HB	1.99	0.45
1:B:249:GLU:HG3	1:B:251:ASN:H	1.81	0.45
1:I:546:ASP:HA	1:I:547:ASN:HA	1.65	0.45
4:P:270:LEU:O	4:P:280:PHE:N	2.43	0.45
2:D:294:ILE:HG22	2:D:296:PRO:HD3	1.99	0.45
2:D:438:ILE:HG22	2:D:442:LYS:HE2	1.99	0.45
2:M:488:LEU:HB2	2:M:491:LEU:HG	1.99	0.45
5:R:166:ILE:HD11	5:R:267:PHE:HD2	1.81	0.45
1:C:653:THR:HB	1:C:658:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:310:SER:HA	3:N:313:LYS:HG2	1.99	0.44
1:A:324:LYS:HD3	1:A:409:LEU:HD13	2.00	0.44
1:C:695:GLU:O	1:C:699:ARG:HG3	2.17	0.44
2:E:385:ASP:O	2:E:389:LEU:HD23	2.17	0.44
2:K:34:VAL:HG21	2:K:57:LEU:HD22	1.99	0.44
5:S:172:VAL:HA	5:S:178:ILE:HA	1.98	0.44
1:B:420:TYR:CE1	2:F:92:LEU:HD13	2.52	0.44
1:B:546:ASP:HA	1:B:547:ASN:HA	1.69	0.44
2:E:134:GLY:HA3	2:E:416:PHE:CE2	2.52	0.44
2:F:78:ASP:OD1	2:F:78:ASP:N	2.50	0.44
2:F:519:TYR:CD1	6:X:80:ARG:HD2	2.52	0.44
1:I:411:MET:HE1	1:I:585:ARG:HG2	1.99	0.44
2:L:215:TYR:O	2:L:245:HIS:NE2	2.48	0.44
5:T:102:TYR:CE2	5:U:97:VAL:HG21	2.52	0.44
5:U:173:LEU:HD23	5:U:208:TRP:HB3	2.00	0.44
1:B:635:TYR:HA	1:B:637:ALA:N	2.33	0.44
3:G:8:GLU:O	3:G:11:GLN:HG2	2.17	0.44
1:H:634:VAL:HG13	1:H:705:THR:HG22	1.99	0.44
2:M:448:ASP:O	2:M:452:ARG:HG3	2.16	0.44
3:N:38:LEU:HD13	3:N:265:ILE:HD12	2.00	0.44
4:O:302:SER:HA	4:O:305:VAL:HG22	1.98	0.44
5:V:273:ASP:OD1	5:V:273:ASP:N	2.50	0.44
2:E:104:ASP:OD1	2:E:105:LYS:N	2.50	0.44
1:H:635:TYR:HB3	9:H:800:ATP:C6	2.53	0.44
4:P:198:LEU:HD11	4:P:213:LEU:HD12	1.98	0.44
5:U:105:TYR:O	5:U:109:LEU:HD23	2.18	0.44
5:V:162:PHE:HA	5:V:165:ILE:HG12	1.98	0.44
1:A:481:GLY:HA2	1:A:546:ASP:O	2.17	0.44
1:B:302:ILE:HD12	1:B:364:THR:HB	1.98	0.44
1:C:344:PHE:CE2	1:C:350:SER:HB3	2.53	0.44
1:H:428:ILE:HD13	1:H:441:PRO:HB2	2.00	0.44
1:I:454:ALA:H	11:I:801:ADP:PB	2.40	0.44
2:K:135:VAL:HG13	2:K:362:LYS:HB2	1.99	0.44
4:O:218:ASP:OD1	4:O:218:ASP:N	2.48	0.44
4:P:206:LYS:HE2	4:P:226:MET:HE1	1.99	0.44
5:W:164:LYS:HA	5:W:164:LYS:HD3	1.76	0.44
2:K:148:GLY:O	2:K:299:GLN:HA	2.18	0.44
2:M:240:ASP:HA	2:M:241:ASP:HA	1.70	0.44
5:R:167:LYS:O	5:R:167:LYS:HG2	2.18	0.44
5:U:64:LYS:O	5:U:68:GLU:HG3	2.17	0.44
2:F:435:LYS:HE2	2:F:435:LYS:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:671:THR:OG1	1:J:697:GLY:HA3	2.17	0.44
2:M:240:ASP:OD1	2:M:297:ILE:HD12	2.18	0.44
2:F:307:GLY:O	2:F:311:THR:OG1	2.27	0.44
3:N:6:VAL:HG21	3:N:293:TRP:CD2	2.53	0.44
5:S:153:ILE:HD11	5:S:218:ILE:HG23	1.99	0.44
5:U:99:VAL:HG12	5:U:100:ASP:N	2.30	0.44
5:U:224:THR:O	5:U:228:LEU:HD23	2.17	0.44
5:W:229:LEU:HD13	5:W:239:VAL:HG11	2.00	0.44
1:C:629:LEU:HD23	1:C:629:LEU:HA	1.90	0.43
2:F:427:TYR:CZ	2:F:434:LEU:HD23	2.53	0.43
2:K:149:ASP:O	2:K:154:LYS:NZ	2.51	0.43
3:N:116:THR:HB	3:N:121:VAL:HG23	2.00	0.43
4:P:204:SER:HA	4:P:207:ILE:CD1	2.48	0.43
2:D:76:ILE:HG21	2:D:227:PHE:CE2	2.54	0.43
1:H:387:ASP:CG	1:H:391:LYS:HB3	2.43	0.43
1:I:635:TYR:HA	1:I:637:ALA:N	2.33	0.43
2:L:76:ILE:HG21	2:L:227:PHE:CE2	2.53	0.43
5:T:115:ASN:O	5:T:119:ILE:HG13	2.18	0.43
1:A:465:LEU:HD13	1:A:597:ILE:HD13	1.99	0.43
5:R:202:PRO:O	5:R:205:VAL:HG13	2.17	0.43
1:B:219:LEU:HD22	4:O:288:GLU:HG2	1.99	0.43
2:F:417:LEU:HD13	2:F:468:TRP:CE2	2.53	0.43
2:K:76:ILE:HG21	2:K:227:PHE:CE2	2.54	0.43
2:L:114:PRO:O	2:L:117:THR:OG1	2.36	0.43
5:U:160:ASN:ND2	5:U:211:ILE:O	2.52	0.43
5:U:202:PRO:HB2	5:U:205:VAL:CG1	2.48	0.43
5:U:203:LEU:HD23	5:U:203:LEU:HA	1.89	0.43
5:U:251:VAL:HG13	5:U:252:ASP:OD1	2.19	0.43
1:C:241:LEU:HD22	1:C:246:LEU:HB3	2.00	0.43
2:D:328:PHE:O	2:D:333:ARG:NH1	2.38	0.43
2:F:6:ILE:HD12	2:F:63:SER:HB2	2.00	0.43
2:F:52:ASN:ND2	2:F:88:LEU:HD12	2.32	0.43
2:F:422:GLY:O	2:F:425:ASN:ND2	2.52	0.43
5:V:158:VAL:HG21	5:V:241:PHE:O	2.18	0.43
5:V:249:ARG:HG3	5:V:253:GLY:O	2.18	0.43
1:B:750:VAL:HG21	1:B:756:ILE:HD11	2.01	0.43
2:F:72:TYR:OH	2:F:87:VAL:O	2.35	0.43
2:F:474:HIS:ND1	5:T:130:ASP:OD1	2.51	0.43
1:I:339:GLU:OE2	1:I:521:ARG:NH2	2.52	0.43
3:G:249:LYS:O	3:G:253:LYS:HG2	2.18	0.43
1:H:339:GLU:OE2	1:H:521:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:392:ILE:HD11	1:H:401:VAL:HG23	2.00	0.43
5:V:161:VAL:HA	5:V:164:LYS:HG2	1.99	0.43
1:A:450:LEU:HD23	1:A:623:ILE:HB	1.99	0.43
2:F:208:ASP:OD1	2:F:208:ASP:N	2.50	0.43
1:H:690:ASP:HA	1:H:693:VAL:HG12	2.00	0.43
2:L:134:GLY:HA3	2:L:416:PHE:CE2	2.54	0.43
2:M:454:MET:HE2	5:W:137:LEU:HD11	1.99	0.43
5:R:150:ILE:HD13	5:R:221:ILE:HD13	2.01	0.43
5:W:115:ASN:O	5:W:119:ILE:HG13	2.17	0.43
5:W:213:ASP:OD1	5:W:214:GLU:N	2.52	0.43
2:F:2:LYS:HB3	2:F:64:LEU:HB3	2.00	0.43
1:J:732:LYS:HA	1:J:732:LYS:HD2	1.75	0.43
2:K:500:LYS:HA	2:K:500:LYS:HD2	1.80	0.43
2:L:417:LEU:HD13	2:L:468:TRP:CE2	2.53	0.43
2:M:126:VAL:O	2:M:165:GLN:NE2	2.49	0.43
3:N:45:LYS:HD2	3:N:255:GLU:HG2	2.00	0.43
5:U:135:VAL:HG22	5:U:224:THR:HG22	2.01	0.43
3:G:2:LYS:HD3	3:G:2:LYS:HA	1.85	0.43
1:I:211:THR:HB	1:I:214:GLU:HG3	2.01	0.43
4:Q:350:THR:O	4:Q:371:SER:N	2.51	0.43
5:T:105:TYR:HB2	5:T:184:PHE:CD2	2.54	0.43
5:V:276:MET:HE3	5:V:276:MET:HB2	1.92	0.43
1:B:746:TYR:HB3	1:B:756:ILE:HG23	2.01	0.42
2:F:3:ASN:OD1	2:F:3:ASN:N	2.51	0.42
2:F:125:LEU:HD21	2:F:236:LEU:HD13	2.00	0.42
1:H:305:ILE:HG12	2:K:41:ALA:HB3	2.00	0.42
1:I:228:GLN:NE2	4:P:234:GLN:O	2.52	0.42
2:L:72:TYR:OH	2:L:88:LEU:HA	2.18	0.42
2:L:475:MET:HE1	5:V:137:LEU:HD12	2.00	0.42
1:A:546:ASP:HA	1:A:547:ASN:HA	1.69	0.42
2:D:509:ARG:HE	2:D:509:ARG:HB2	1.69	0.42
2:E:453:LYS:HA	2:E:453:LYS:HD2	1.95	0.42
1:H:454:ALA:HA	9:H:800:ATP:O3G	2.19	0.42
1:H:524:ILE:HD13	1:H:582:LEU:HD13	2.01	0.42
1:J:695:GLU:OE1	1:J:699:ARG:NH1	2.45	0.42
2:M:78:ASP:OD1	2:M:79:ASN:N	2.52	0.42
5:R:244:ASP:HB2	5:R:263:ALA:HB2	2.00	0.42
5:T:164:LYS:HA	5:T:164:LYS:HD3	1.77	0.42
5:V:247:LEU:HG	5:V:255:THR:HG23	2.00	0.42
1:A:342:ASP:HB3	2:E:10:LYS:HG2	2.01	0.42
1:C:322:LEU:HD23	2:D:60:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:141:PHE:O	3:G:260:LYS:NZ	2.52	0.42
1:H:482:ILE:HG23	1:H:522:SER:HB3	2.01	0.42
2:L:512:LEU:HA	2:L:515:GLU:HG2	2.01	0.42
2:M:175:ILE:HD13	2:M:218:PRO:HA	2.01	0.42
4:Q:265:PRO:HB2	4:Q:268:TYR:HE1	1.84	0.42
5:S:152:LYS:HG3	5:S:281:LYS:C	2.45	0.42
5:W:159:LEU:HD23	5:W:159:LEU:HA	1.83	0.42
1:A:683:PHE:CE1	1:A:691:LYS:HG2	2.54	0.42
1:H:479:PHE:HD1	1:H:509:PHE:HE1	1.67	0.42
2:K:208:ASP:OD1	2:K:208:ASP:N	2.46	0.42
2:L:324:SER:HB3	2:L:327:LEU:HB2	2.00	0.42
5:R:115:ASN:O	5:R:119:ILE:HG13	2.20	0.42
1:H:387:ASP:OD1	1:H:391:LYS:N	2.49	0.42
2:K:249:TYR:CE2	2:K:272:VAL:HG21	2.53	0.42
1:C:226:VAL:HG22	1:C:260:LEU:HD21	2.01	0.42
1:C:699:ARG:NE	1:C:740:ASN:HA	2.35	0.42
1:I:462:VAL:HG13	1:I:544:PHE:CE1	2.54	0.42
1:J:687:SER:HA	3:N:101:GLN:NE2	2.34	0.42
2:L:4:LEU:HD23	2:L:18:GLY:HA3	2.02	0.42
2:M:168:THR:HG22	2:M:170:VAL:HG23	2.01	0.42
2:M:415:LEU:HD11	2:M:438:ILE:HG12	2.02	0.42
3:N:83:ILE:HG12	3:N:117:VAL:CG1	2.50	0.42
5:U:157:PHE:HZ	5:U:173:LEU:HD21	1.85	0.42
5:U:191:PRO:HG3	5:U:267:PHE:CZ	2.55	0.42
6:X:51:GLN:HG3	6:X:62:ASP:OD1	2.19	0.42
1:A:387:ASP:HB2	1:A:388:PRO:HD2	2.01	0.42
3:G:10:LYS:HD3	3:G:290:ILE:HD11	2.01	0.42
1:I:426:ASN:OD1	1:I:426:ASN:N	2.51	0.42
2:L:385:ASP:HA	2:L:388:THR:HG22	2.02	0.42
5:R:248:VAL:O	5:R:255:THR:HA	2.19	0.42
6:X:41:ASN:HB2	6:X:45:ARG:HD3	2.02	0.42
2:E:449:VAL:O	2:E:453:LYS:HG2	2.20	0.42
1:H:569:VAL:HG12	1:H:569:VAL:O	2.20	0.42
2:K:310:PRO:O	2:K:314:ILE:HG13	2.19	0.42
3:N:117:VAL:HG23	3:N:136:TYR:HB2	2.01	0.42
4:O:225:ALA:HA	4:O:228:TYR:HD2	1.84	0.42
4:P:253:GLU:HA	4:P:256:LYS:HZ3	1.85	0.42
5:V:111:LYS:HB3	5:V:111:LYS:HE2	1.86	0.42
5:V:179:PHE:HA	5:V:193:ALA:HA	2.02	0.42
5:V:238:GLU:HB3	5:V:248:VAL:HG22	2.02	0.42
1:J:226:VAL:HG21	6:X:86:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:98:ARG:HG2	2:L:100:ASN:H	1.84	0.42
2:M:131:VAL:HG22	2:M:399:ILE:HG12	2.02	0.42
2:M:175:ILE:HD12	2:M:239:MET:HG2	2.02	0.42
5:S:226:ILE:HG13	5:S:227:LYS:N	2.34	0.42
2:D:126:VAL:O	2:D:165:GLN:NE2	2.53	0.42
2:E:457:ILE:HD11	5:S:140:TYR:CG	2.55	0.42
2:F:143:LYS:HE3	2:F:143:LYS:HB2	1.84	0.42
1:I:387:ASP:HB2	1:I:388:PRO:HD2	2.01	0.42
2:K:72:TYR:CD2	2:K:108:VAL:HG21	2.55	0.42
2:M:79:ASN:CG	2:M:98:ARG:HB3	2.45	0.42
4:P:209:VAL:O	4:P:213:LEU:HG	2.20	0.42
4:P:268:TYR:HB2	4:P:270:LEU:HD11	2.02	0.42
5:S:153:ILE:HG21	5:S:221:ILE:HG21	2.01	0.42
1:A:289:LYS:H	1:A:412:GLN:NE2	2.18	0.41
2:E:76:ILE:HG21	2:E:227:PHE:CE2	2.54	0.41
2:F:454:MET:HE3	5:T:137:LEU:HD11	2.01	0.41
2:M:40:LYS:HB3	2:M:47:ILE:HD12	2.00	0.41
5:S:134:GLN:HB3	5:S:228:LEU:HD13	2.02	0.41
5:T:159:LEU:HD12	5:T:280:PRO:HG3	2.01	0.41
1:A:683:PHE:HE1	1:A:691:LYS:HG2	1.86	0.41
1:B:355:GLY:HA2	1:B:518:LEU:HD22	2.02	0.41
1:B:569:VAL:O	1:B:569:VAL:HG12	2.20	0.41
2:E:401:GLN:NE2	2:E:405:GLU:O	2.53	0.41
2:F:107:TYR:O	2:F:110:THR:OG1	2.31	0.41
3:G:116:THR:HB	3:G:121:VAL:HG23	2.02	0.41
2:L:482:TYR:OH	2:L:515:GLU:OE2	2.38	0.41
2:M:6:ILE:HD12	2:M:63:SER:HB2	2.02	0.41
6:X:33:TYR:CE1	6:X:35:GLN:HG2	2.52	0.41
1:A:494:LYS:HD3	1:A:494:LYS:HA	1.77	0.41
1:B:542:LEU:HD13	1:B:595:THR:HB	2.02	0.41
1:C:387:ASP:OD2	1:C:391:LYS:HB3	2.19	0.41
2:F:88:LEU:HD23	2:F:88:LEU:HA	1.80	0.41
1:I:377:ILE:HD12	1:I:406:TYR:HB2	2.02	0.41
4:O:241:SER:OG	4:O:295:GLY:N	2.41	0.41
4:P:195:VAL:HG23	4:P:219:LYS:HG3	2.01	0.41
5:S:225:PHE:CE2	5:S:229:LEU:HD11	2.55	0.41
5:T:213:ASP:OD1	5:T:214:GLU:N	2.53	0.41
5:V:146:ASP:HB3	5:V:149:HIS:HB3	2.01	0.41
1:B:497:GLU:HB2	1:B:502:LEU:HD22	2.01	0.41
1:B:534:ARG:HD3	1:B:594:ILE:HG13	2.03	0.41
1:B:651:LYS:HB2	1:B:651:LYS:HE3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:ILE:HG23	1:C:594:ILE:HG22	2.01	0.41
1:I:212:GLU:O	1:I:215:ILE:HG13	2.21	0.41
2:K:312:ASN:O	2:K:316:ILE:HG13	2.21	0.41
2:K:485:LEU:HD23	2:K:485:LEU:HA	1.85	0.41
3:N:9:LYS:HB3	3:N:9:LYS:HE3	1.92	0.41
5:R:128:ILE:HD12	5:R:154:ILE:HG21	2.02	0.41
5:R:155:LYS:HA	5:R:158:VAL:HG22	2.02	0.41
5:U:124:THR:HG22	5:U:124:THR:O	2.20	0.41
5:W:201:PRO:HA	5:W:202:PRO:HD3	1.92	0.41
2:D:437:ILE:HD12	2:D:437:ILE:HA	1.91	0.41
2:F:506:ASN:HB2	5:T:124:THR:HG22	2.03	0.41
1:I:435:VAL:HG22	1:I:704:LEU:HB3	2.02	0.41
4:O:278:LYS:HA	4:O:279:PRO:HD3	1.94	0.41
1:A:431:THR:HG22	1:A:469:PHE:CZ	2.55	0.41
2:E:472:LEU:HD12	2:E:476:ILE:HB	2.02	0.41
2:E:506:ASN:O	5:S:124:THR:HG22	2.21	0.41
2:F:80:TYR:HB3	2:F:201:ILE:HD13	2.03	0.41
1:H:338:LEU:HB3	1:H:351:THR:HB	2.02	0.41
1:I:345:ASP:OD1	1:I:348:LEU:HB2	2.20	0.41
1:J:462:VAL:HG22	1:J:544:PHE:CZ	2.55	0.41
3:N:54:ARG:HD3	3:N:54:ARG:HA	1.79	0.41
4:O:201:ALA:HA	4:O:225:ALA:H	1.86	0.41
4:O:318:TRP:HD1	4:O:319:ASN:N	2.18	0.41
5:T:67:LEU:O	5:T:71:GLU:HG2	2.19	0.41
5:T:245:THR:HG22	5:T:246:LEU:N	2.36	0.41
5:U:196:ASN:HB3	5:U:199:LEU:HB2	2.02	0.41
5:W:198:LYS:HD3	5:W:198:LYS:HA	1.93	0.41
1:B:470:ILE:HD12	1:B:501:PHE:HB2	2.02	0.41
1:B:517:GLY:N	1:B:558:ILE:HD11	2.35	0.41
1:B:680:ILE:HG21	3:G:22:ILE:HG21	2.03	0.41
1:C:264:THR:O	1:C:267:GLU:HG2	2.21	0.41
2:E:380:LYS:HB2	2:E:380:LYS:HE2	1.88	0.41
1:I:517:GLY:HA2	1:I:558:ILE:HD11	2.02	0.41
1:C:222:LYS:HD2	1:C:224:TYR:HE1	1.85	0.41
2:K:309:ILE:HB	2:K:310:PRO:HD3	2.02	0.41
2:M:81:LEU:HD12	2:M:199:LYS:HA	2.03	0.41
3:N:175:SER:HB2	3:N:183:VAL:CG1	2.51	0.41
4:O:266:ILE:HG22	4:O:287:LEU:HD21	2.03	0.41
4:P:267:ASP:CB	4:P:301:LYS:HB2	2.50	0.41
5:W:96:LEU:HD11	5:W:119:ILE:HD11	2.02	0.41
1:B:466:ILE:HG12	1:B:544:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LYS:HE3	1:C:336:ILE:HD11	2.03	0.41
1:C:632:GLU:OE1	1:C:701:LYS:NZ	2.35	0.41
2:E:192:LYS:HB2	2:E:197:LEU:HD22	2.03	0.41
2:E:398:LEU:HD11	2:E:415:LEU:HD13	2.03	0.41
2:E:528:LYS:HE2	2:E:528:LYS:HB3	1.84	0.41
1:H:295:GLU:O	1:H:297:THR:HG23	2.21	0.41
1:J:249:GLU:HG2	1:J:254:ARG:HG2	2.02	0.41
1:J:490:HIS:N	2:M:115:ILE:HD11	2.36	0.41
1:J:648:LEU:HD23	1:J:648:LEU:HA	1.94	0.41
2:K:80:TYR:HB3	2:K:201:ILE:HD13	2.03	0.41
2:K:528:LYS:HG3	5:T:218:ILE:HD11	2.02	0.41
4:O:220:ILE:HD12	4:O:262:PHE:CE1	2.53	0.41
4:O:267:ASP:HB2	4:O:301:LYS:HB2	2.03	0.41
1:B:286:ASN:N	1:B:287:PRO:HD3	2.36	0.41
2:D:458:LEU:HB2	2:D:468:TRP:NE1	2.36	0.41
2:E:386:LEU:O	2:E:390:GLN:HG2	2.21	0.41
1:H:431:THR:HG22	1:H:469:PHE:CZ	2.56	0.41
1:I:220:LEU:HD21	4:P:284:GLU:HB2	2.02	0.41
2:K:146:ILE:O	2:K:297:ILE:HA	2.21	0.41
2:L:454:MET:HA	2:L:457:ILE:HG22	2.03	0.41
2:M:513:ALA:O	2:M:517:LYS:HG3	2.21	0.41
3:N:96:LEU:HD23	3:N:96:LEU:HA	1.94	0.41
4:O:361:ILE:O	4:O:365:GLY:N	2.49	0.41
4:P:210:LEU:O	4:P:214:LEU:N	2.45	0.41
4:P:271:ALA:HB1	4:P:277:VAL:HB	2.03	0.41
5:R:84:ILE:HD13	5:R:84:ILE:HA	1.95	0.41
5:T:201:PRO:HA	5:T:202:PRO:HD3	1.98	0.41
1:B:246:LEU:HD11	1:B:262:LEU:HB2	2.03	0.40
1:C:379:LYS:HE2	1:C:379:LYS:HB3	1.85	0.40
1:C:418:THR:O	1:C:421:VAL:HG22	2.21	0.40
2:F:527:TYR:CE1	6:X:80:ARG:HD3	2.56	0.40
1:H:581:GLN:HA	2:L:208:ASP:OD1	2.21	0.40
3:N:295:ARG:O	3:N:299:GLU:HG3	2.21	0.40
5:R:107:LEU:HA	5:R:107:LEU:HD23	1.83	0.40
5:R:159:LEU:HD23	5:R:159:LEU:HA	1.92	0.40
5:R:164:LYS:HG3	5:R:211:ILE:HG21	2.03	0.40
1:B:483:GLY:O	1:B:512:MET:HE3	2.20	0.40
1:I:483:GLY:O	1:I:512:MET:HE3	2.21	0.40
2:M:159:LEU:HD21	2:M:187:ILE:HG12	2.03	0.40
4:O:219:LYS:HB2	4:O:219:LYS:HE3	1.92	0.40
4:Q:267:ASP:HB3	4:Q:299:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:HD12	1:B:444:LYS:HE2	2.04	0.40
2:E:39:LEU:HD11	2:E:252:LEU:HD22	2.03	0.40
1:J:306:ARG:HD3	2:M:40:LYS:HE3	2.03	0.40
1:J:324:LYS:HD2	1:J:409:LEU:HD13	2.02	0.40
1:J:420:TYR:CE1	2:K:92:LEU:HD13	2.57	0.40
6:X:64:TYR:CE2	6:X:100:ASN:HB2	2.56	0.40
1:A:691:LYS:O	1:A:695:GLU:HG2	2.22	0.40
1:B:387:ASP:OD2	1:B:391:LYS:HB3	2.22	0.40
2:D:135:VAL:HG13	2:D:362:LYS:HB2	2.04	0.40
2:F:147:ILE:HG23	2:F:322:TYR:HD1	1.86	0.40
3:G:155:VAL:HA	3:G:164:PHE:HZ	1.86	0.40
1:H:626:SER:HB3	1:H:629:LEU:HB2	2.02	0.40
2:M:128:GLY:O	2:M:401:GLN:NE2	2.47	0.40
3:N:10:LYS:HD3	3:N:290:ILE:HD11	2.03	0.40
4:O:263:VAL:HG23	4:O:263:VAL:O	2.21	0.40
5:R:128:ILE:HD13	5:R:128:ILE:HA	1.99	0.40
1:B:322:LEU:HD21	2:F:58:ASN:HB3	2.03	0.40
1:C:443:PRO:HB3	1:C:647:MET:SD	2.61	0.40
2:E:159:LEU:HD23	2:E:159:LEU:HA	1.91	0.40
2:F:76:ILE:HG21	2:F:227:PHE:CE2	2.56	0.40
2:F:231:ILE:HB	1:J:278:PRO:HA	2.04	0.40
1:I:499:LEU:HD12	1:I:501:PHE:HE1	1.85	0.40
2:K:33:LYS:HA	2:K:33:LYS:HD2	1.81	0.40
2:M:241:ASP:N	2:M:241:ASP:OD1	2.55	0.40
4:O:194:ILE:HD12	4:O:217:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	496/784 (63%)	483 (97%)	12 (2%)	1 (0%)	43 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	568/784 (72%)	547 (96%)	20 (4%)	1 (0%)	43	73
1	C	559/784 (71%)	546 (98%)	13 (2%)	0	100	100
1	H	497/784 (63%)	484 (97%)	12 (2%)	1 (0%)	43	73
1	I	569/784 (73%)	555 (98%)	14 (2%)	0	100	100
1	J	593/784 (76%)	579 (98%)	14 (2%)	0	100	100
2	D	526/528 (100%)	514 (98%)	12 (2%)	0	100	100
2	E	526/528 (100%)	507 (96%)	19 (4%)	0	100	100
2	F	526/528 (100%)	505 (96%)	21 (4%)	0	100	100
2	K	526/528 (100%)	509 (97%)	17 (3%)	0	100	100
2	L	526/528 (100%)	510 (97%)	16 (3%)	0	100	100
2	M	526/528 (100%)	504 (96%)	22 (4%)	0	100	100
3	G	254/336 (76%)	252 (99%)	2 (1%)	0	100	100
3	N	250/336 (74%)	249 (100%)	1 (0%)	0	100	100
4	O	200/511 (39%)	192 (96%)	8 (4%)	0	100	100
4	P	199/511 (39%)	192 (96%)	7 (4%)	0	100	100
4	Q	199/511 (39%)	194 (98%)	5 (2%)	0	100	100
5	R	216/293 (74%)	204 (94%)	12 (6%)	0	100	100
5	S	150/293 (51%)	147 (98%)	3 (2%)	0	100	100
5	T	227/293 (78%)	219 (96%)	8 (4%)	0	100	100
5	U	224/293 (76%)	209 (93%)	15 (7%)	0	100	100
5	V	168/293 (57%)	161 (96%)	7 (4%)	0	100	100
5	W	224/293 (76%)	217 (97%)	7 (3%)	0	100	100
6	X	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
All	All	8856/11947 (74%)	8582 (97%)	271 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	569	VAL
1	A	569	VAL
1	B	569	VAL

5.3.2 Protein sidechains ⓘ

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	428/693 (62%)	428 (100%)	0	100	100
1	B	490/693 (71%)	490 (100%)	0	100	100
1	C	483/693 (70%)	483 (100%)	0	100	100
1	H	426/693 (62%)	426 (100%)	0	100	100
1	I	487/693 (70%)	487 (100%)	0	100	100
1	J	513/693 (74%)	513 (100%)	0	100	100
2	D	443/443 (100%)	443 (100%)	0	100	100
2	E	433/443 (98%)	433 (100%)	0	100	100
2	F	440/443 (99%)	440 (100%)	0	100	100
2	K	443/443 (100%)	443 (100%)	0	100	100
2	L	437/443 (99%)	437 (100%)	0	100	100
2	M	432/443 (98%)	432 (100%)	0	100	100
3	G	242/317 (76%)	242 (100%)	0	100	100
3	N	240/317 (76%)	240 (100%)	0	100	100
4	O	107/442 (24%)	107 (100%)	0	100	100
4	P	93/442 (21%)	93 (100%)	0	100	100
4	Q	67/442 (15%)	67 (100%)	0	100	100
5	R	204/274 (74%)	204 (100%)	0	100	100
5	S	57/274 (21%)	57 (100%)	0	100	100
5	T	212/274 (77%)	212 (100%)	0	100	100
5	U	210/274 (77%)	210 (100%)	0	100	100
5	V	120/274 (44%)	120 (100%)	0	100	100
5	W	205/274 (75%)	205 (100%)	0	100	100
6	X	100/103 (97%)	100 (100%)	0	100	100
All	All	7312/10523 (70%)	7312 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	618	HIS
2	E	21	GLN
2	E	165	GLN
2	E	312	ASN
2	E	469	ASN
2	F	194	HIS
3	G	17	HIS
1	H	356	ASN
1	H	583	GLN
1	H	598	GLN
1	I	511	GLN
1	I	583	GLN
1	I	598	GLN
1	I	628	GLN
1	I	741	HIS
1	J	741	HIS
2	L	42	ASN
2	M	167	ASN
2	M	494	ASN
3	N	17	HIS
5	R	136	HIS
5	R	243	GLN
5	R	265	GLN
5	S	121	GLN
5	U	121	GLN
5	U	160	ASN
5	U	206	GLN
5	V	151	GLN
5	V	160	ASN
5	V	231	ASN
5	W	160	ASN
6	X	106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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
9	ATP	A	800	10	32,33,33	0.32	0	48,52,52	0.28	0
9	ATP	F	600	10	32,33,33	0.34	0	48,52,52	0.30	0
11	ADP	B	801	10	28,29,29	1.39	5 (17%)	43,45,45	1.84	10 (23%)
12	PO4	B	802	10	4,4,4	0.99	0	6,6,6	0.48	0
9	ATP	K	600	10	32,33,33	0.33	0	48,52,52	0.29	0
9	ATP	L	600	10	32,33,33	0.35	0	48,52,52	0.29	0
12	PO4	I	802	10	4,4,4	1.00	0	6,6,6	0.47	0
9	ATP	E	600	10	32,33,33	0.34	0	48,52,52	0.29	0
9	ATP	M	600	10	32,33,33	0.31	0	48,52,52	0.28	0
9	ATP	H	800	10	32,33,33	1.37	4 (12%)	48,52,52	1.75	9 (18%)
9	ATP	D	600	10	32,33,33	0.34	0	48,52,52	0.29	0
11	ADP	I	801	10	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)

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
9	ATP	A	800	10	-	3/22/38/38	0/3/3/3
9	ATP	F	600	10	-	1/22/38/38	0/3/3/3
11	ADP	B	801	10	-	2/16/32/32	0/3/3/3
9	ATP	K	600	10	-	2/22/38/38	0/3/3/3
9	ATP	L	600	10	-	2/22/38/38	0/3/3/3
9	ATP	E	600	10	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	M	600	10	-	2/22/38/38	0/3/3/3
9	ATP	H	800	10	-	3/22/38/38	0/3/3/3
9	ATP	D	600	10	-	1/22/38/38	0/3/3/3
11	ADP	I	801	10	-	0/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	800	ATP	C5-C4	4.65	1.47	1.39
11	I	801	ADP	C5-C4	4.61	1.47	1.39
11	B	801	ADP	C5-C4	4.51	1.47	1.39
11	I	801	ADP	C5-C6	2.73	1.48	1.41
11	B	801	ADP	C5-C6	2.65	1.48	1.41
9	H	800	ATP	C5-C6	2.63	1.48	1.41
9	H	800	ATP	C8-N7	2.35	1.36	1.31
11	B	801	ADP	C5-N7	-2.32	1.34	1.39
9	H	800	ATP	C5-N7	-2.31	1.34	1.39
11	I	801	ADP	C5-N7	-2.29	1.34	1.39
11	I	801	ADP	C8-N7	2.29	1.36	1.31
11	B	801	ADP	C8-N7	2.20	1.35	1.31
11	B	801	ADP	C4-N9	-2.01	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	801	ADP	C5-C4-N3	-5.84	118.67	126.72
9	H	800	ATP	C5-C4-N3	-5.83	118.69	126.72
11	B	801	ADP	C5-C4-N3	-5.78	118.76	126.72
9	H	800	ATP	N3-C4-N9	4.59	134.98	127.17
11	B	801	ADP	N3-C4-N9	4.59	134.97	127.17
11	I	801	ADP	N3-C4-N9	4.53	134.87	127.17
11	B	801	ADP	C2-N3-C4	3.68	120.82	111.83
11	I	801	ADP	C2-N3-C4	3.67	120.80	111.83
9	H	800	ATP	C2-N3-C4	3.65	120.74	111.83
11	I	801	ADP	C4-C5-N7	-3.54	106.53	110.58
11	B	801	ADP	C4-C5-N7	-3.50	106.58	110.58
9	H	800	ATP	C4-C5-N7	-3.42	106.67	110.58
11	B	801	ADP	N3-C2-N1	-3.21	123.72	128.58
11	I	801	ADP	N3-C2-N1	-3.16	123.80	128.58
9	H	800	ATP	N3-C2-N1	-3.07	123.94	128.58
11	B	801	ADP	C4-N9-C8	2.81	108.69	105.74
9	H	800	ATP	C4-N9-C8	2.63	108.50	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	801	ADP	C5-N7-C8	2.55	107.46	103.45
11	I	801	ADP	C5-N7-C8	2.54	107.44	103.45
9	H	800	ATP	C5-N7-C8	2.48	107.35	103.45
11	I	801	ADP	C4-N9-C8	2.46	108.33	105.74
11	B	801	ADP	C3'-C2'-C1'	2.45	106.10	101.46
9	H	800	ATP	C3'-C2'-C1'	2.43	106.06	101.46
11	I	801	ADP	C3'-C2'-C1'	2.33	105.87	101.46
11	B	801	ADP	C6-C5-N7	2.10	136.13	132.09
11	B	801	ADP	N9-C8-N7	-2.06	111.01	113.94
11	I	801	ADP	C6-C5-N7	2.05	136.05	132.09
9	H	800	ATP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

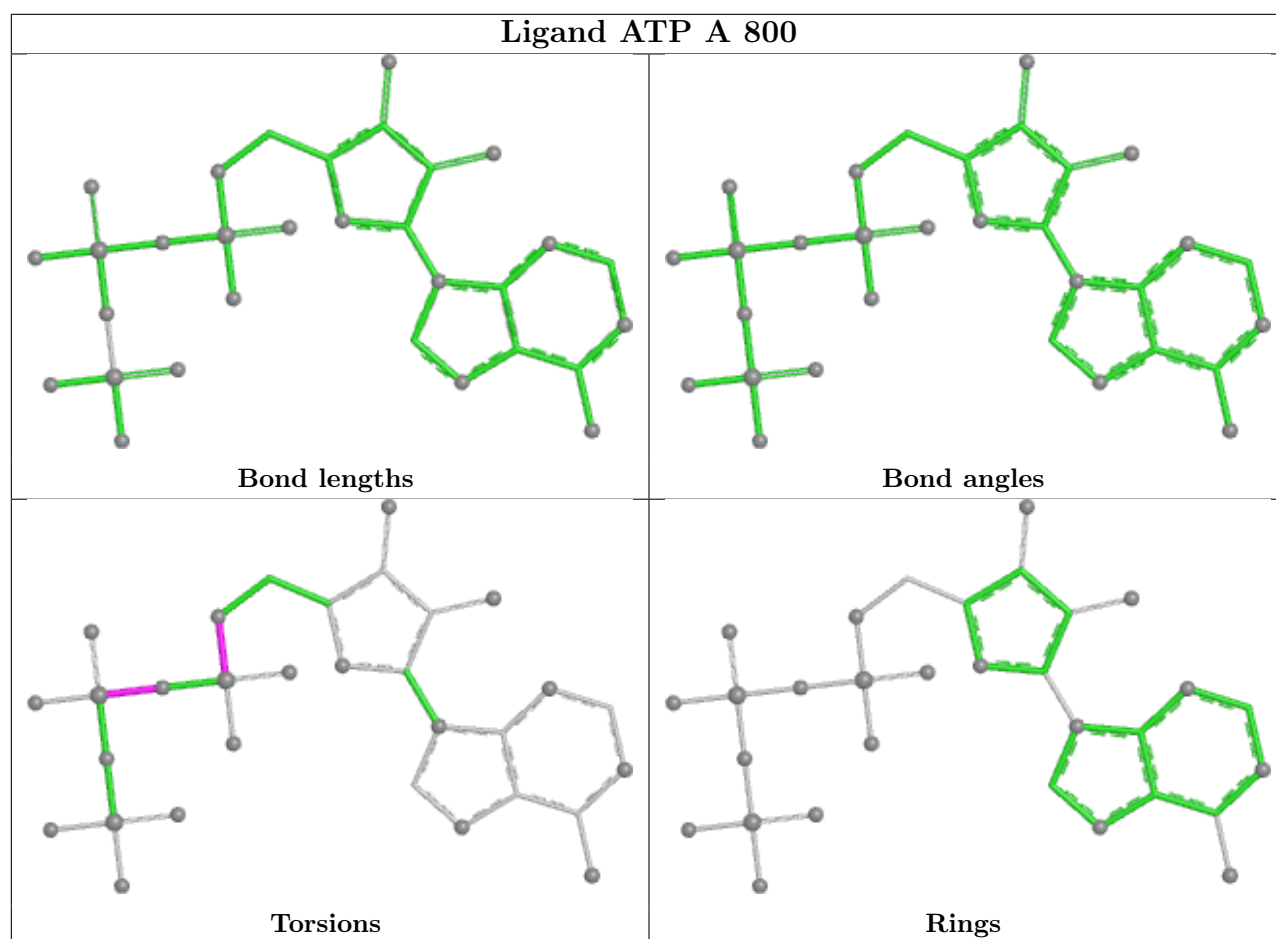
Mol	Chain	Res	Type	Atoms
9	E	600	ATP	C5'-O5'-PA-O2A
9	M	600	ATP	PB-O3B-PG-O2G
9	A	800	ATP	PA-O3A-PB-O2B
9	E	600	ATP	PA-O3A-PB-O2B
9	H	800	ATP	PB-O3A-PA-O2A
9	A	800	ATP	C5'-O5'-PA-O1A
9	E	600	ATP	C5'-O5'-PA-O1A
9	E	600	ATP	C5'-O5'-PA-O3A
9	H	800	ATP	C5'-O5'-PA-O1A
9	K	600	ATP	PA-O3A-PB-O2B
9	L	600	ATP	PA-O3A-PB-O1B
9	D	600	ATP	PB-O3B-PG-O1G
9	M	600	ATP	PB-O3B-PG-O1G
9	K	600	ATP	PA-O3A-PB-O1B
9	E	600	ATP	PB-O3B-PG-O2G
9	F	600	ATP	PB-O3B-PG-O3G
9	A	800	ATP	PA-O3A-PB-O1B
9	E	600	ATP	PA-O3A-PB-O1B
9	H	800	ATP	PB-O3A-PA-O1A
11	B	801	ADP	PB-O3A-PA-O1A
9	L	600	ATP	PA-O3A-PB-O2B
11	B	801	ADP	PB-O3A-PA-O2A

There are no ring outliers.

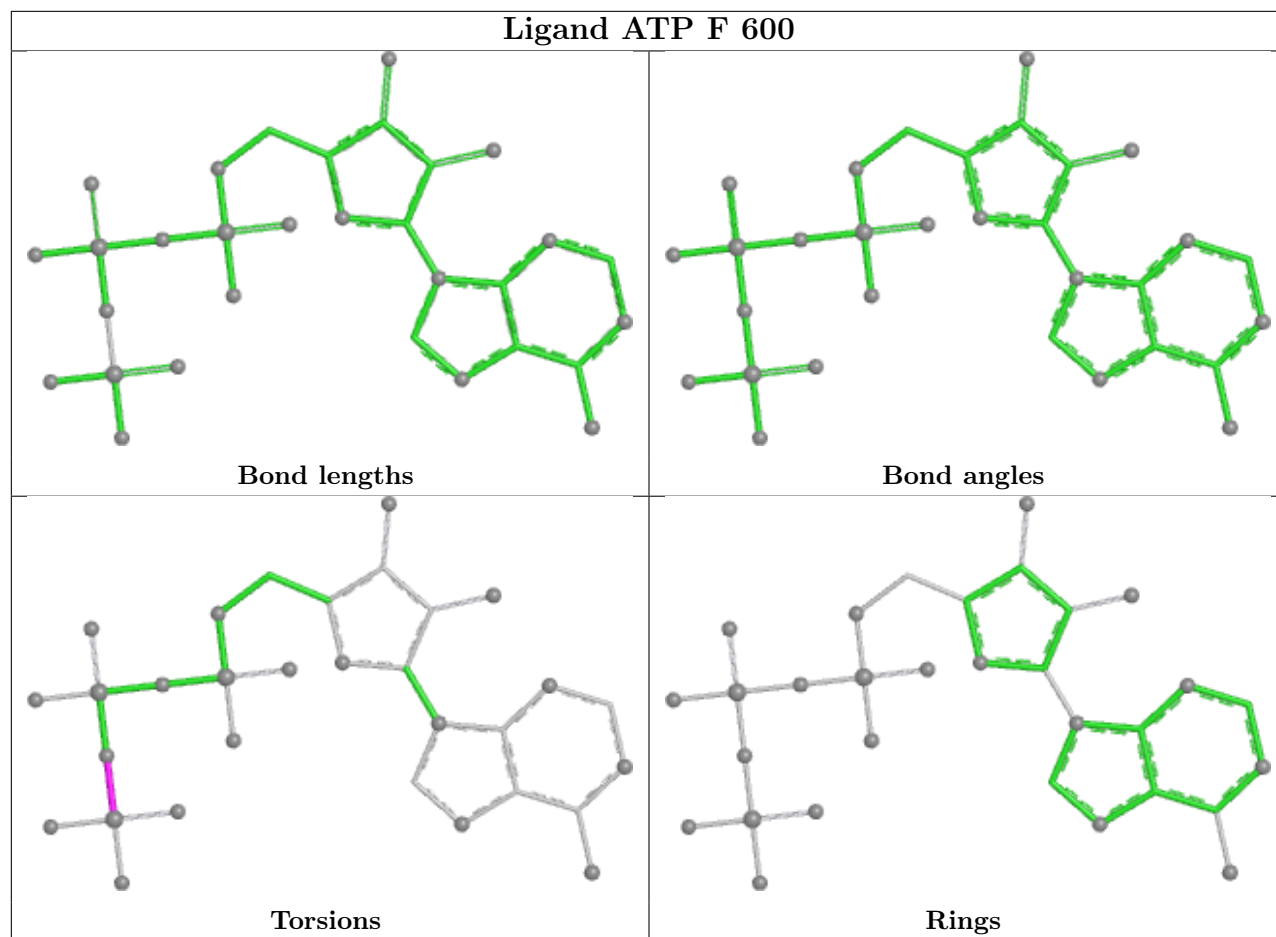
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	800	ATP	1	0
9	H	800	ATP	3	0
11	I	801	ADP	4	0

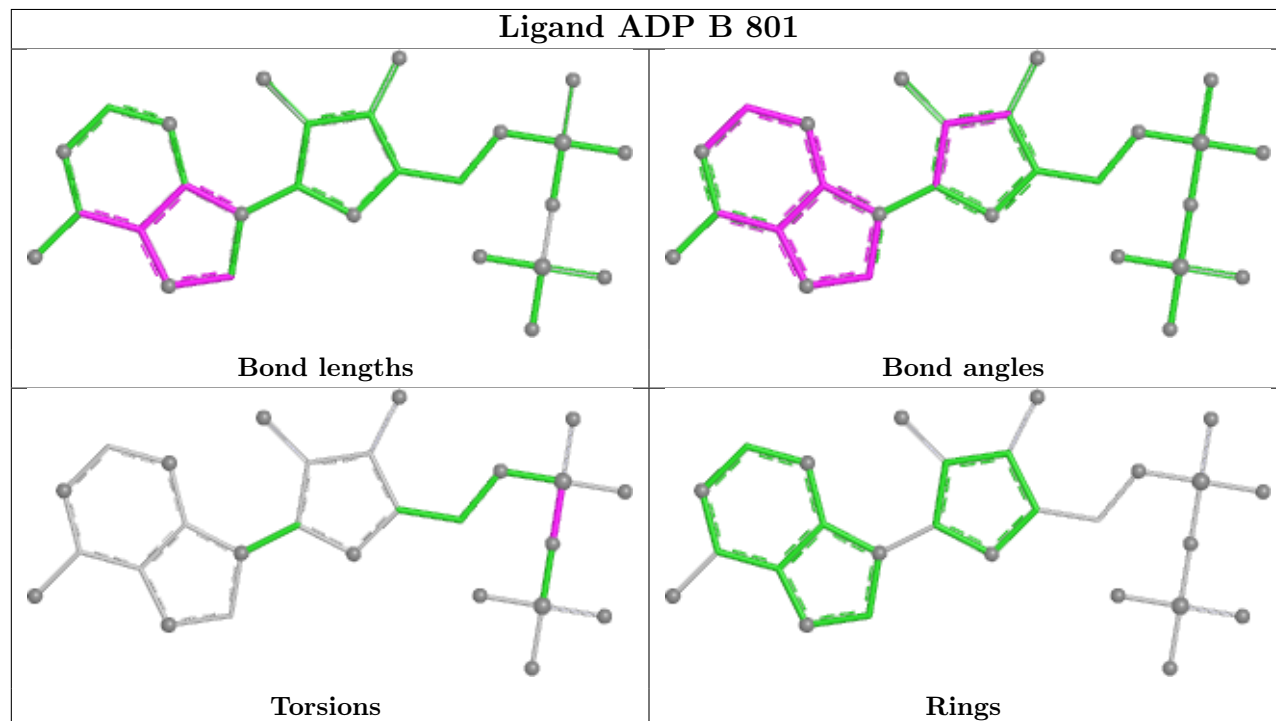
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

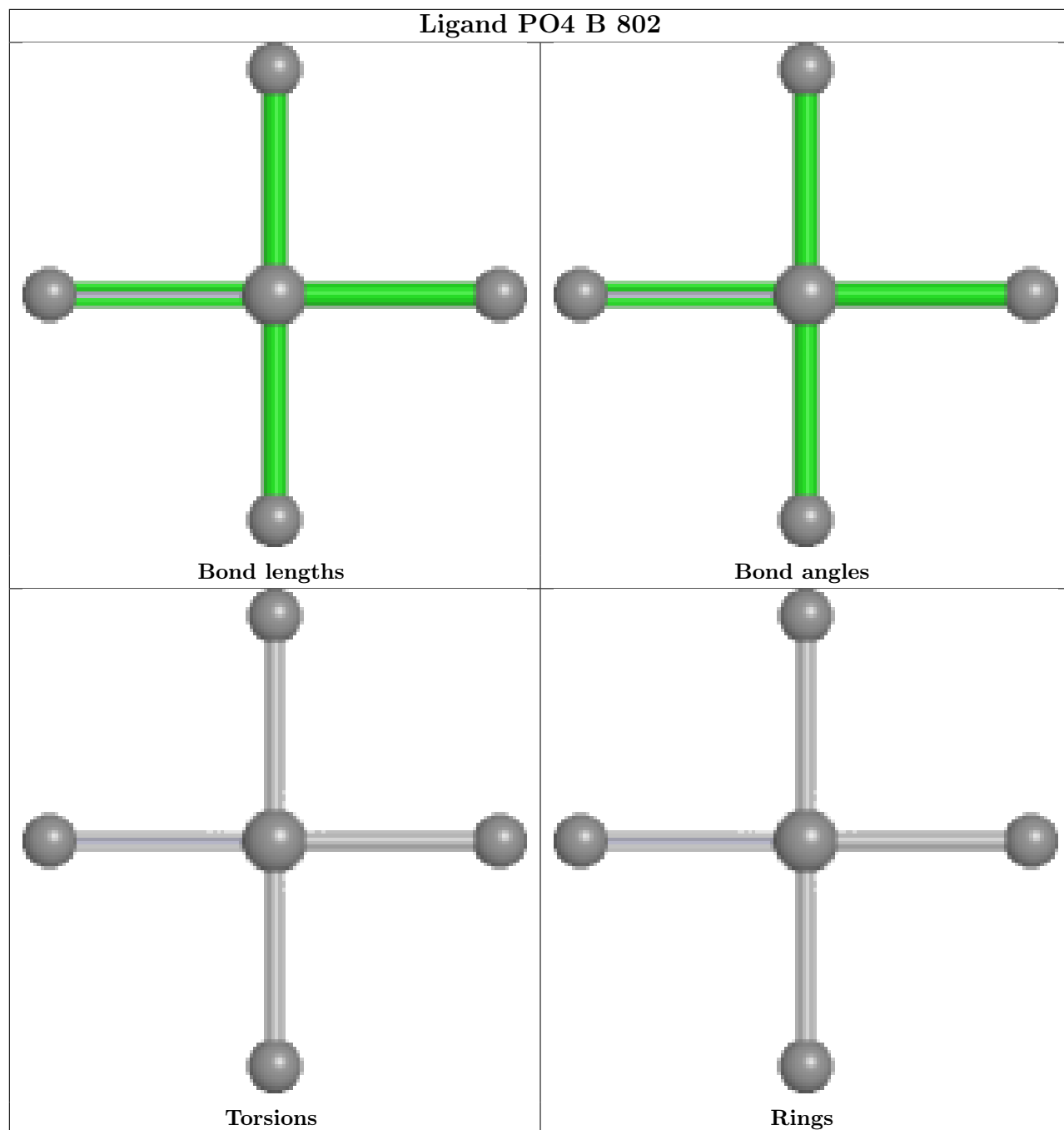


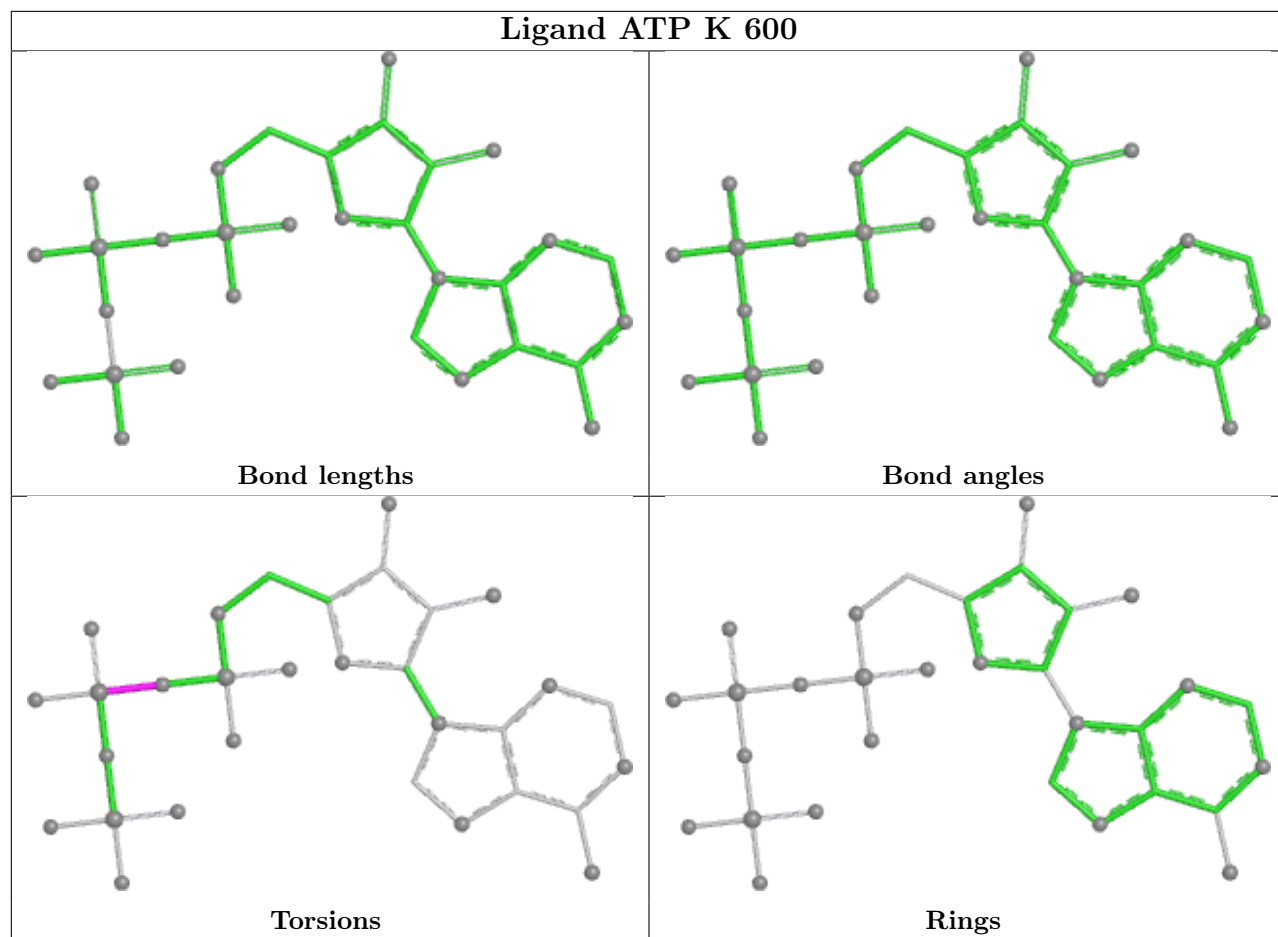
Ligand ATP F 600

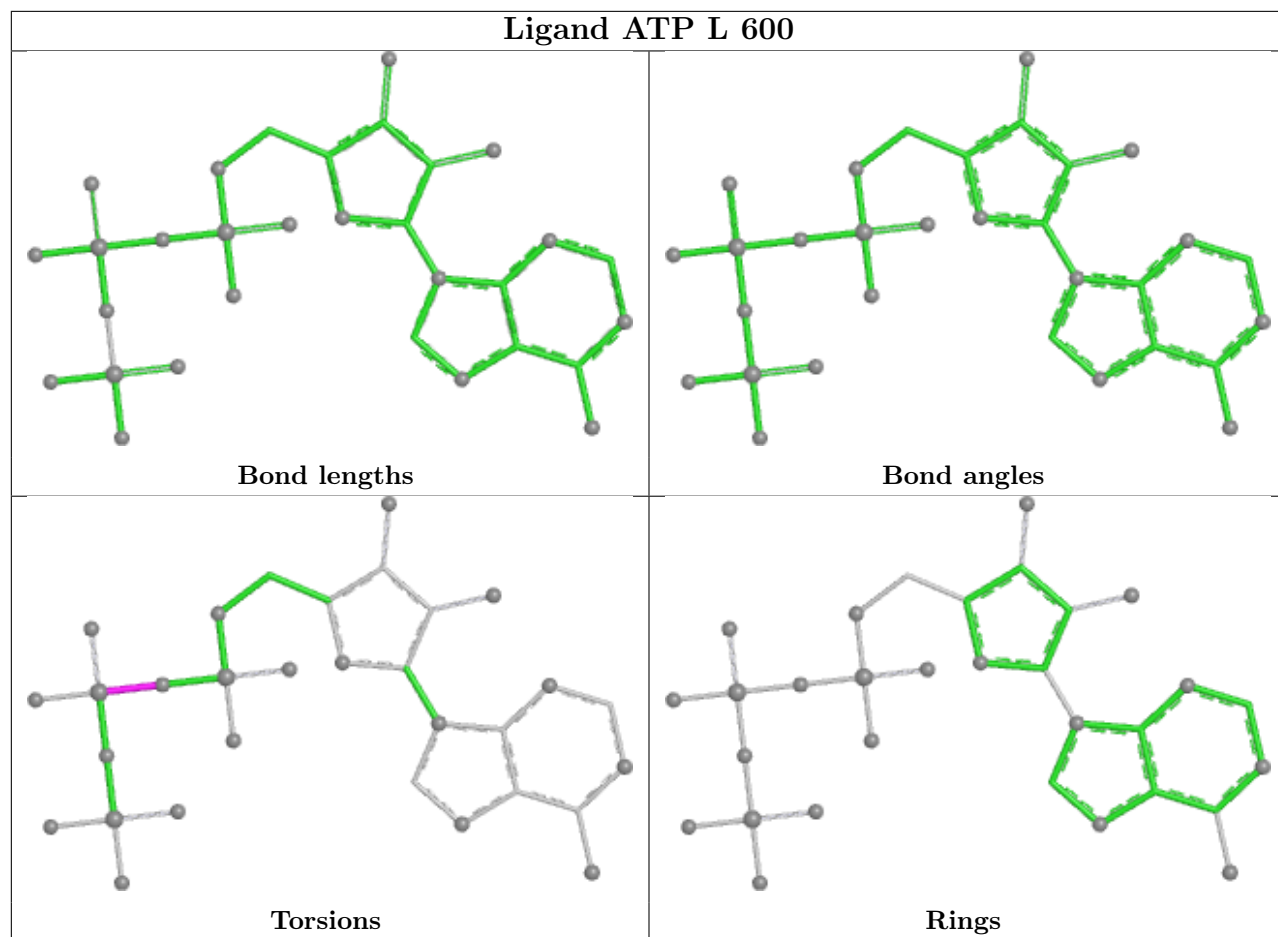


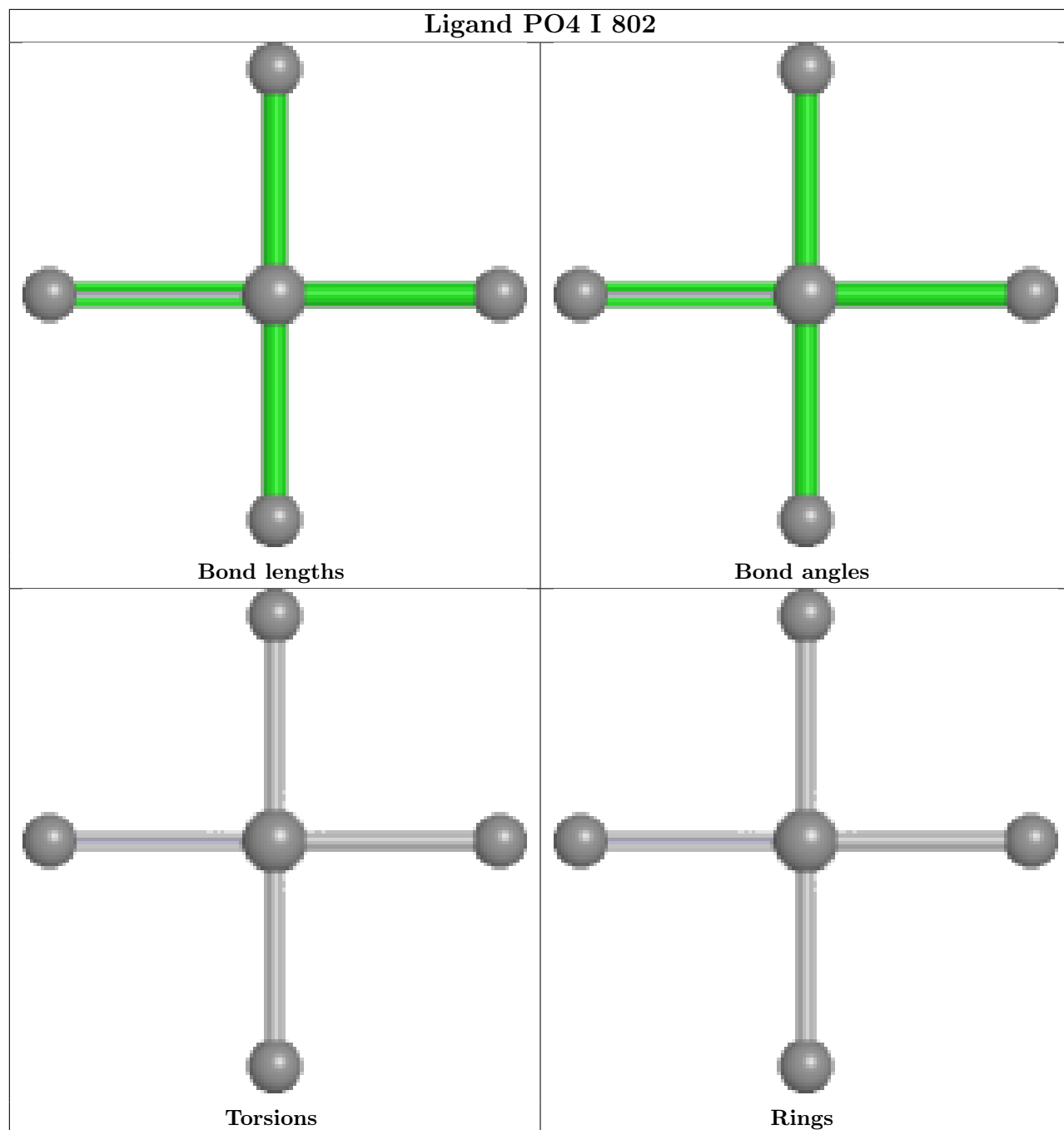
Ligand ADP B 801

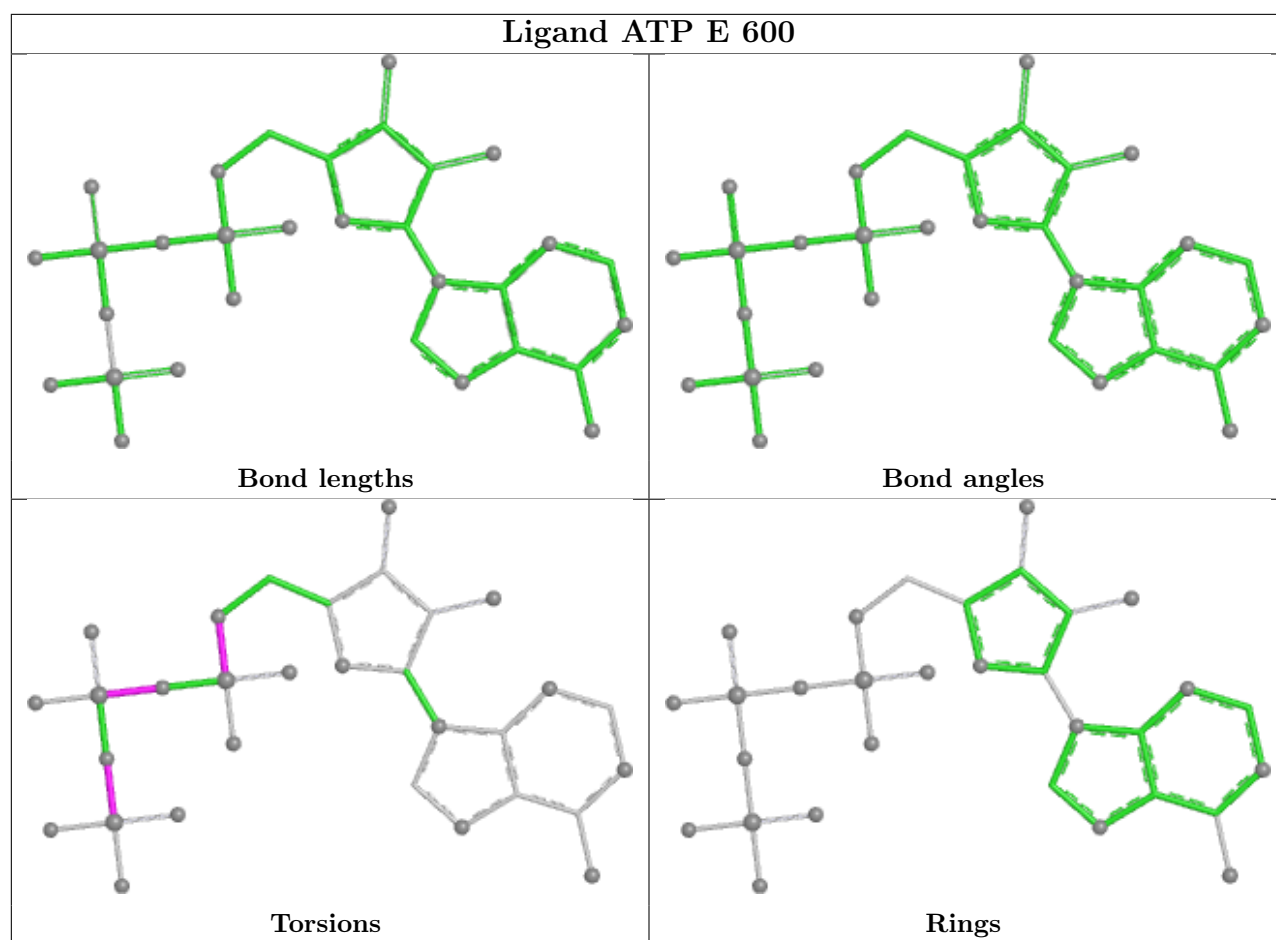


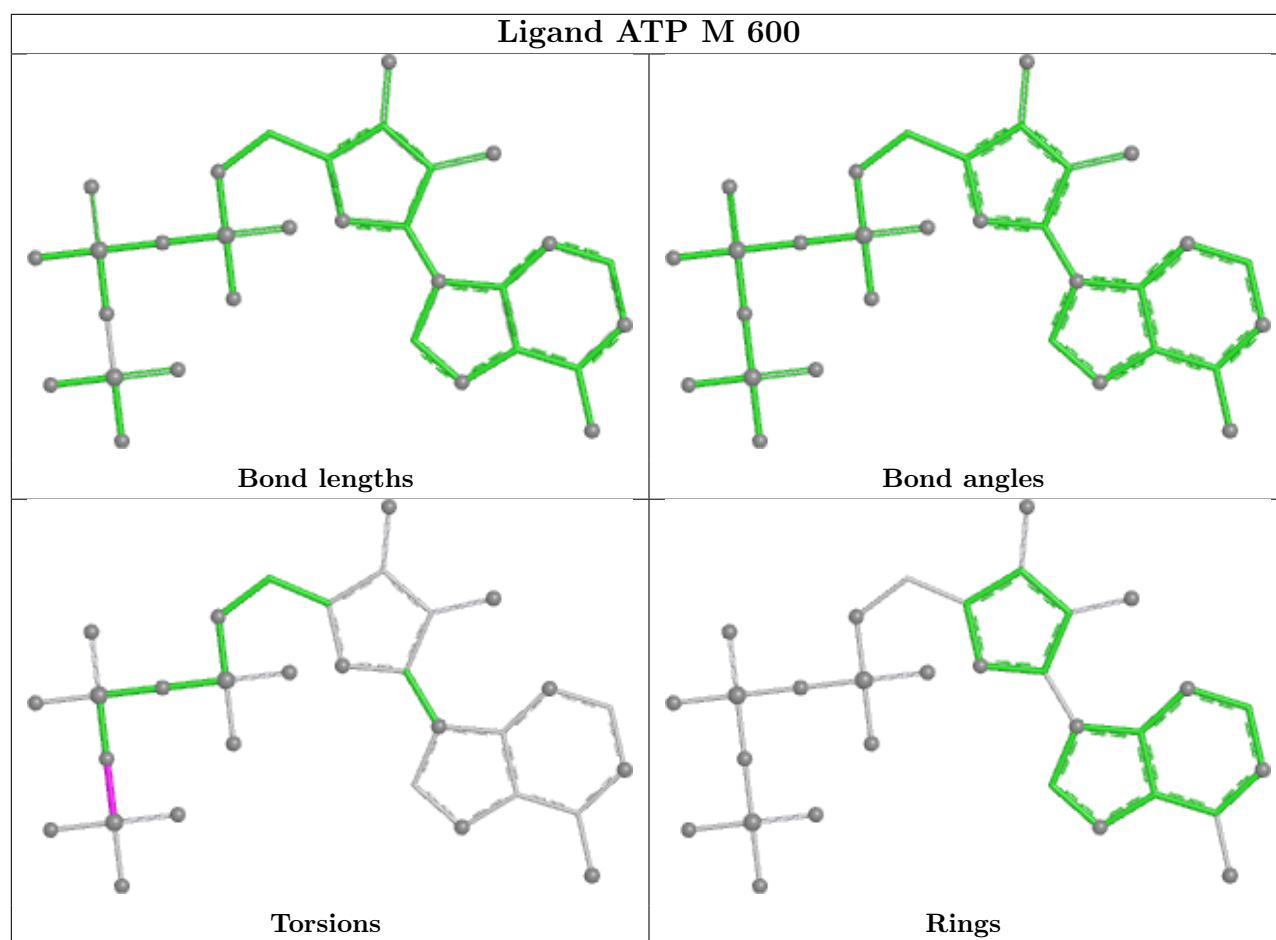


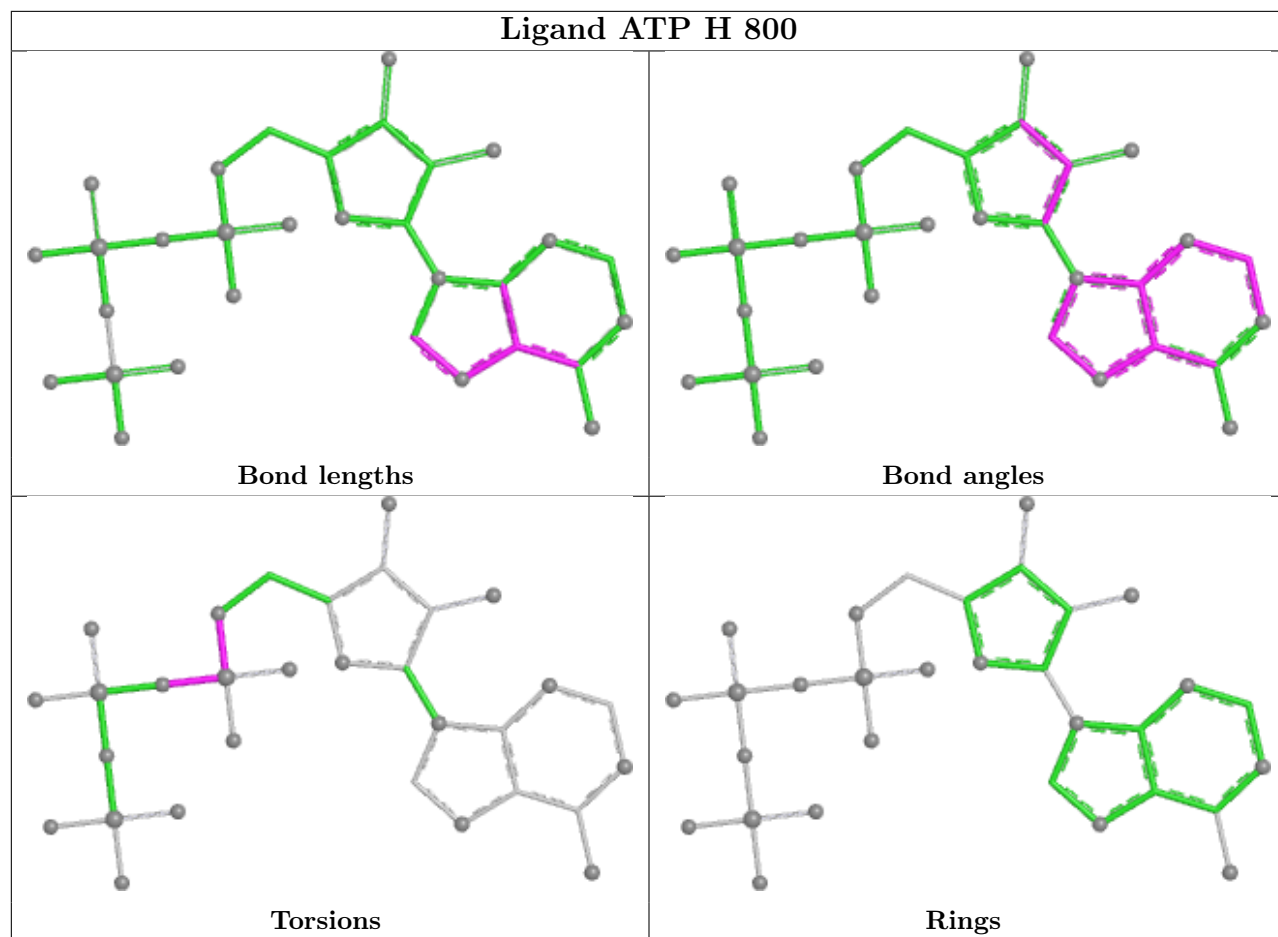


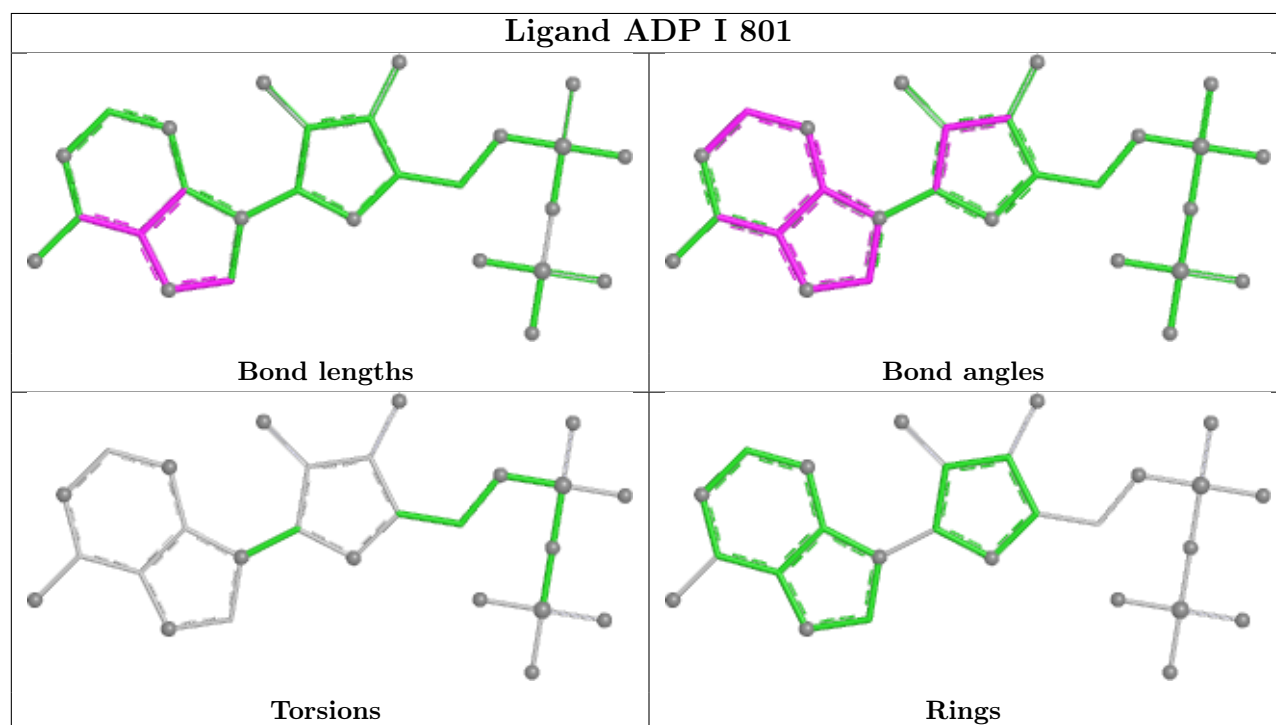
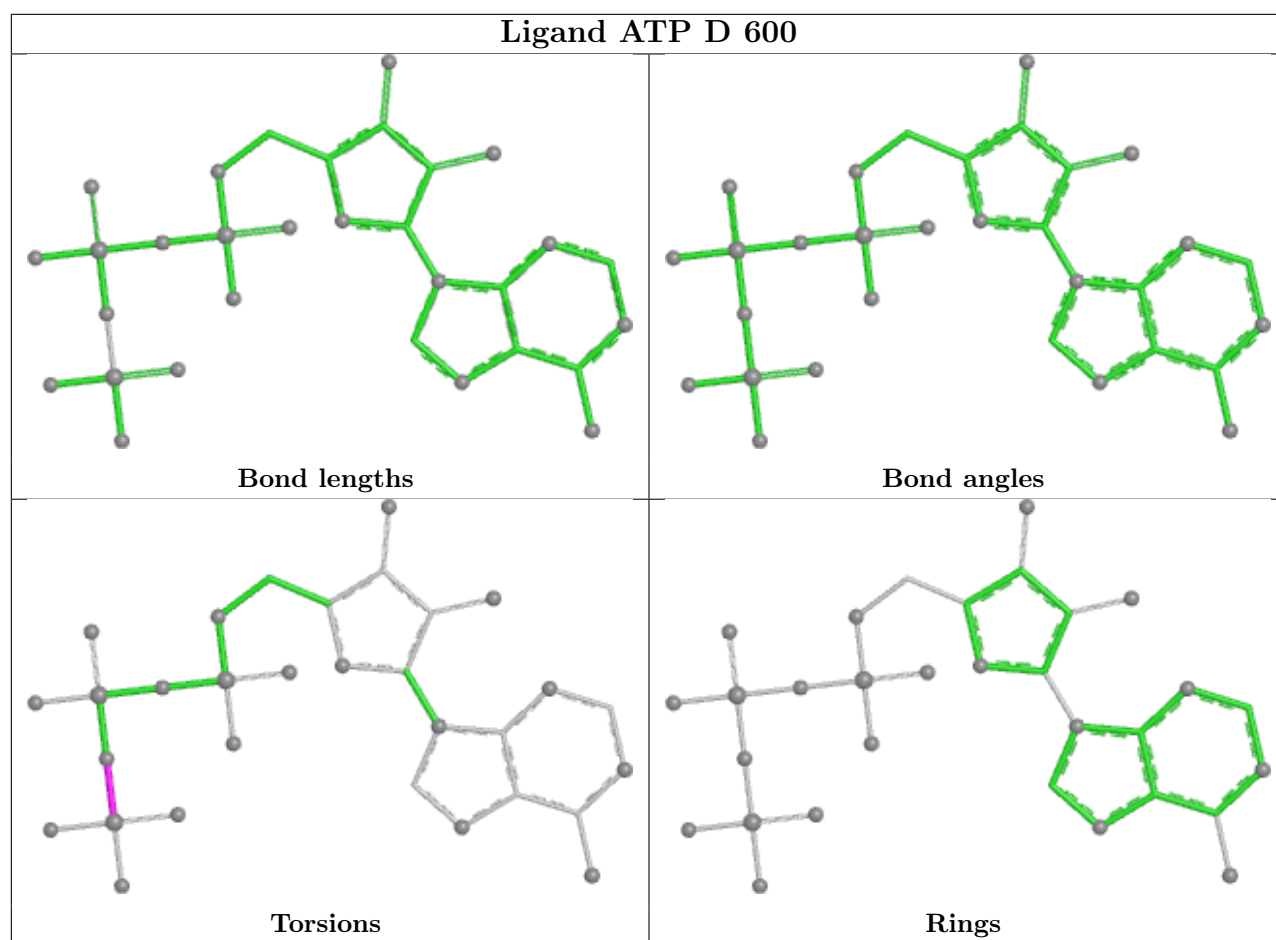












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

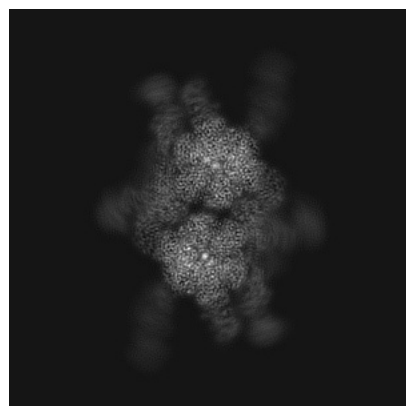
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60718. These allow visual inspection of the internal detail of the map and identification of artifacts.

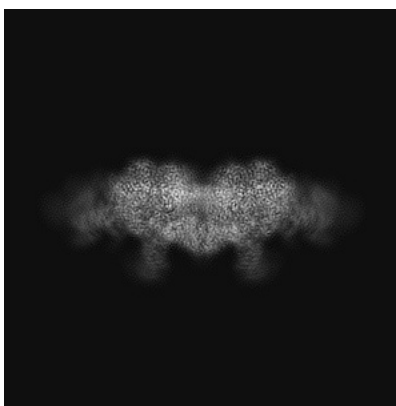
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

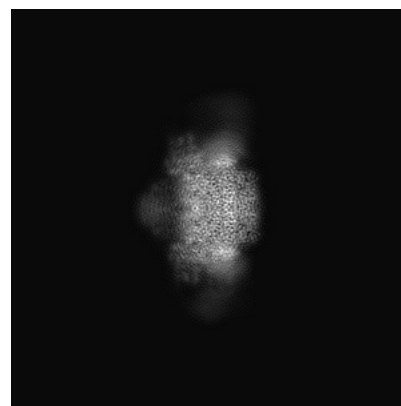
6.1.1 Primary map



X

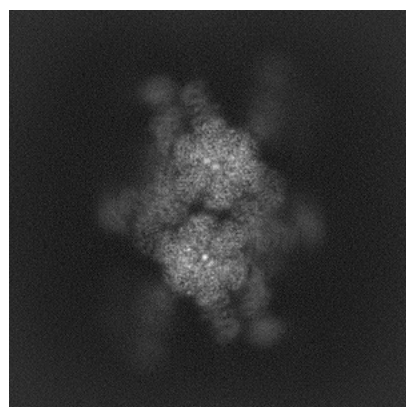


Y

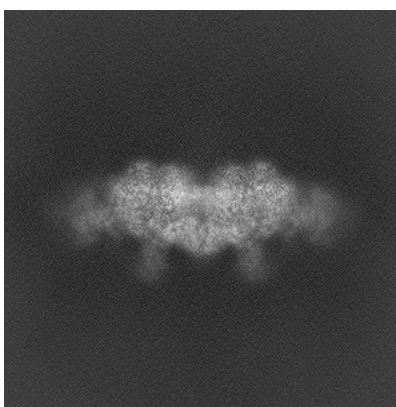


Z

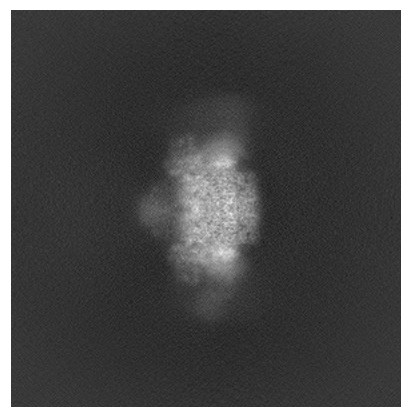
6.1.2 Raw map



X



Y

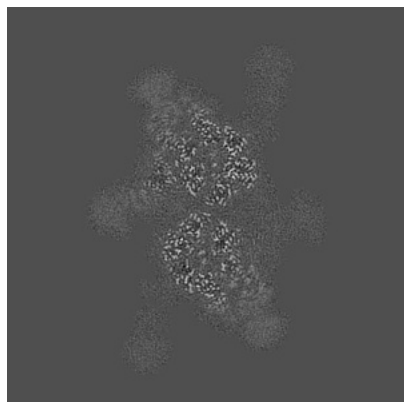


Z

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

6.2 Central slices [i](#)

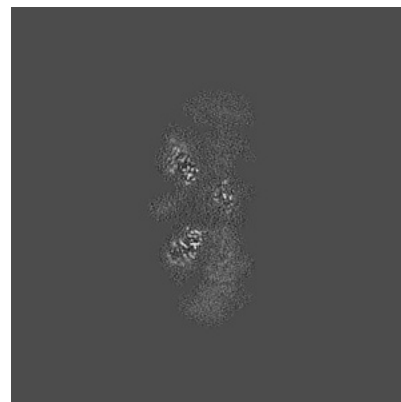
6.2.1 Primary map



X Index: 264

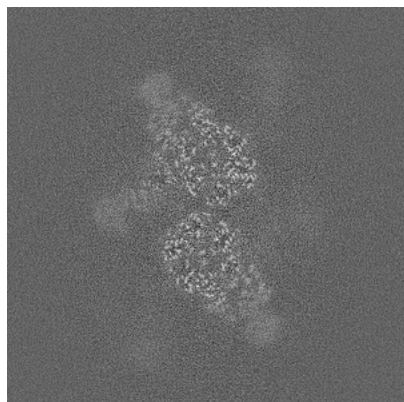


Y Index: 264

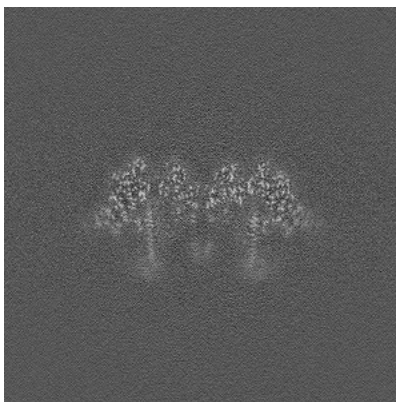


Z Index: 264

6.2.2 Raw map



X Index: 264



Y Index: 264

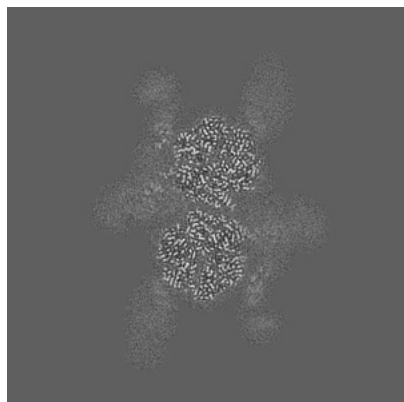


Z Index: 264

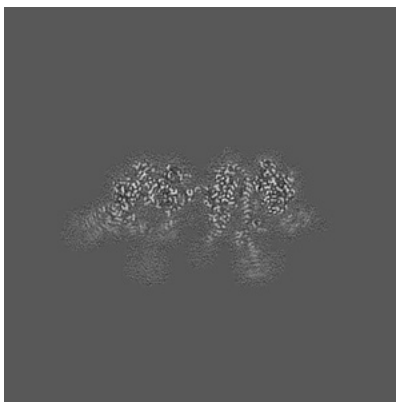
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

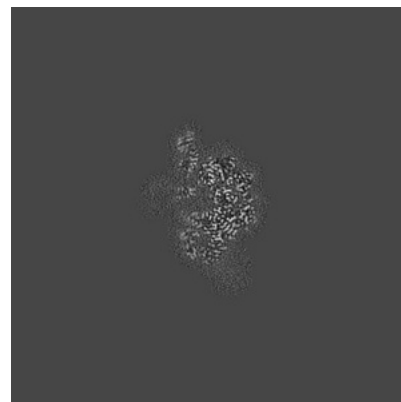
6.3.1 Primary map



X Index: 282

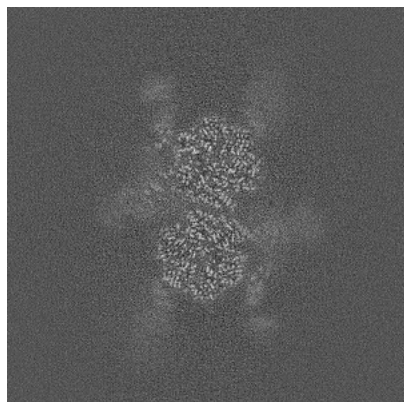


Y Index: 273

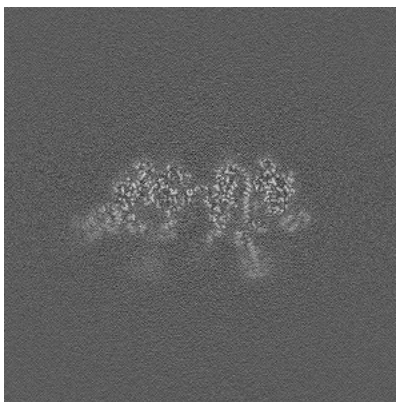


Z Index: 303

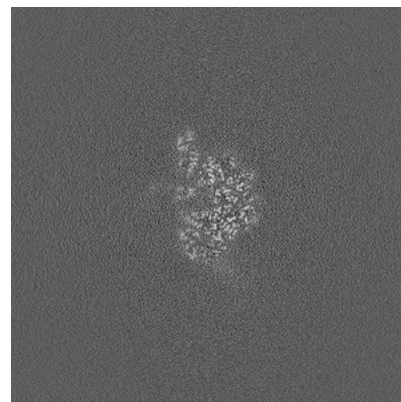
6.3.2 Raw map



X Index: 282



Y Index: 273

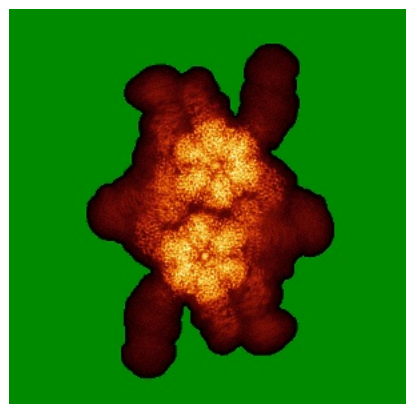


Z Index: 303

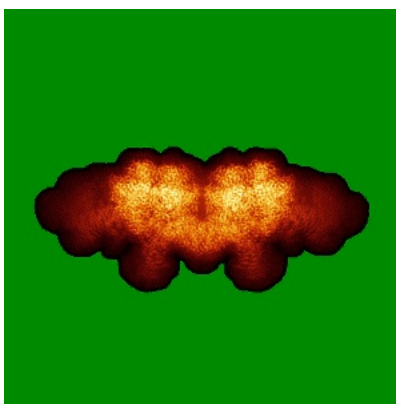
The images above show the largest variance slices of the map in three orthogonal directions.

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

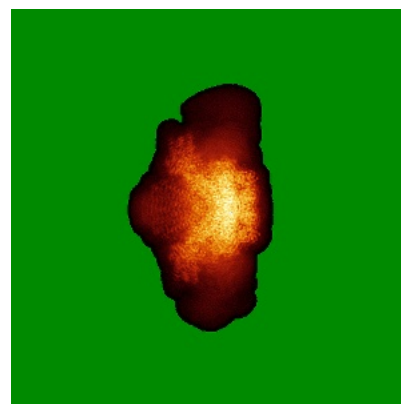
6.4.1 Primary map



X

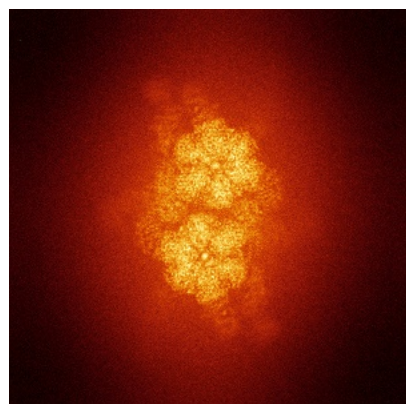


Y

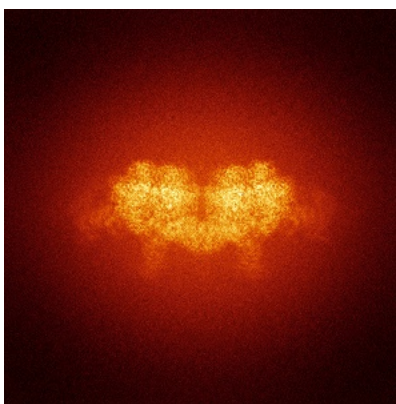


Z

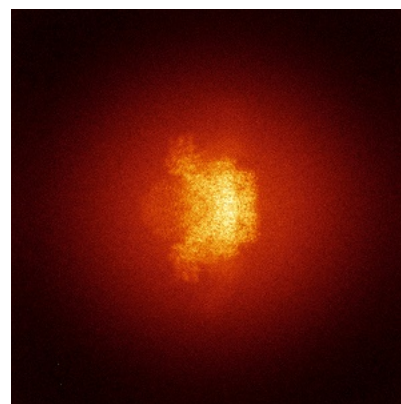
6.4.2 Raw map



X



Y

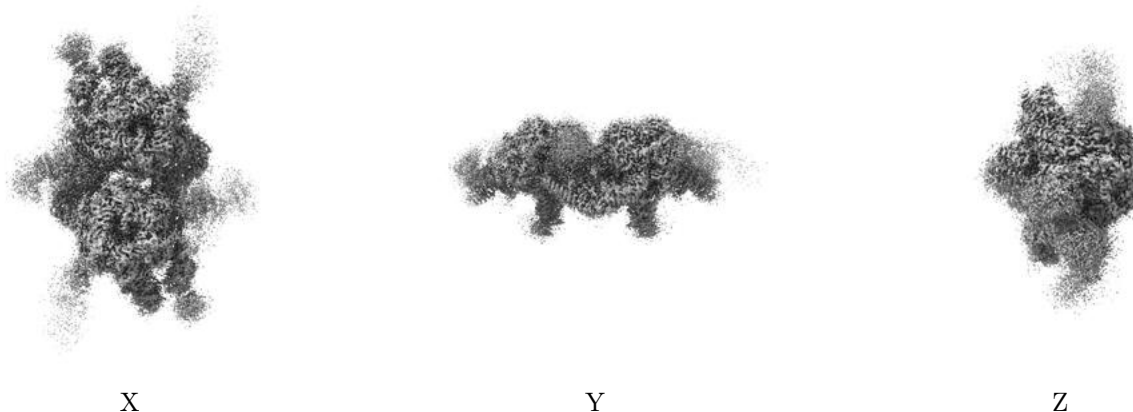


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

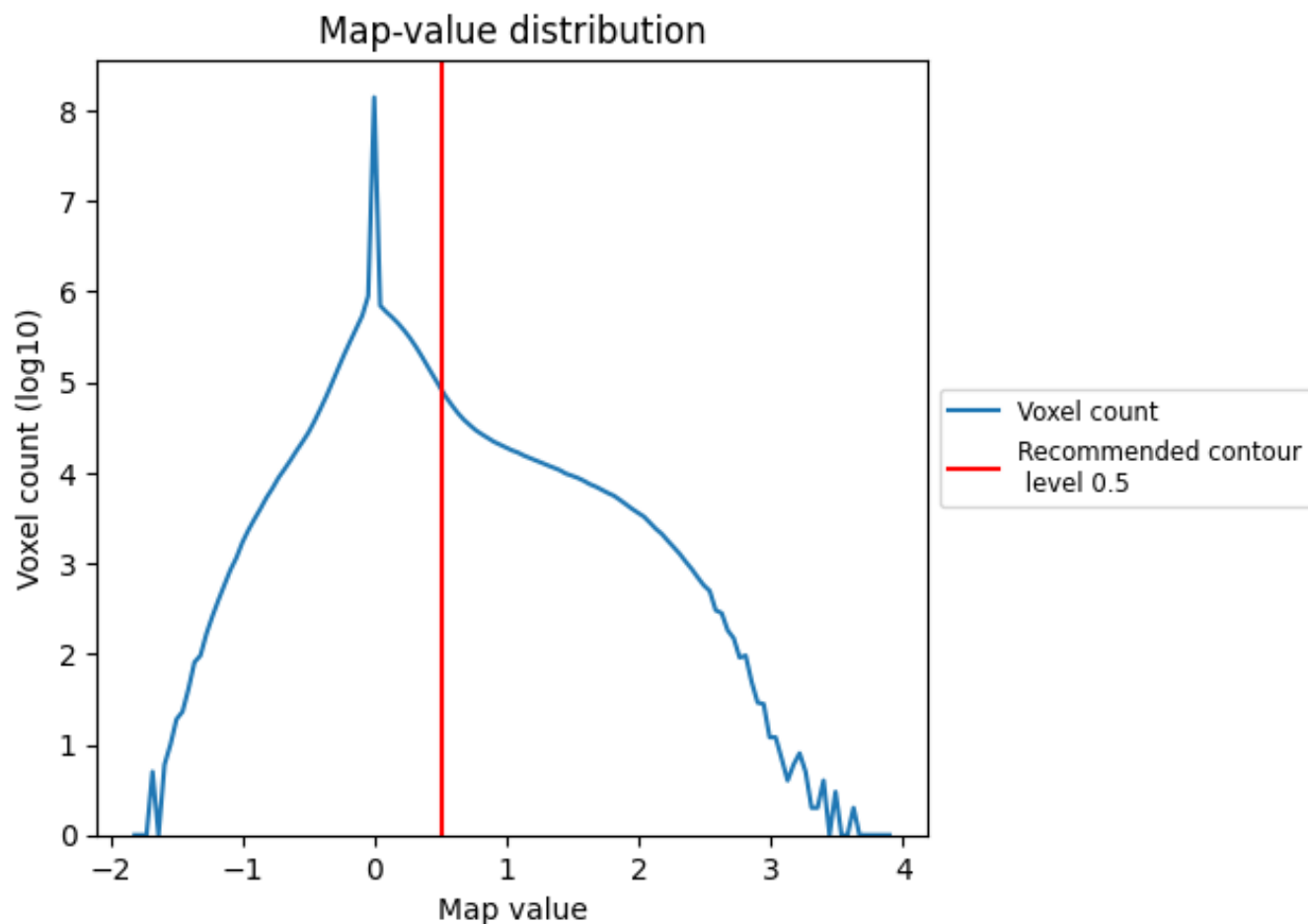
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

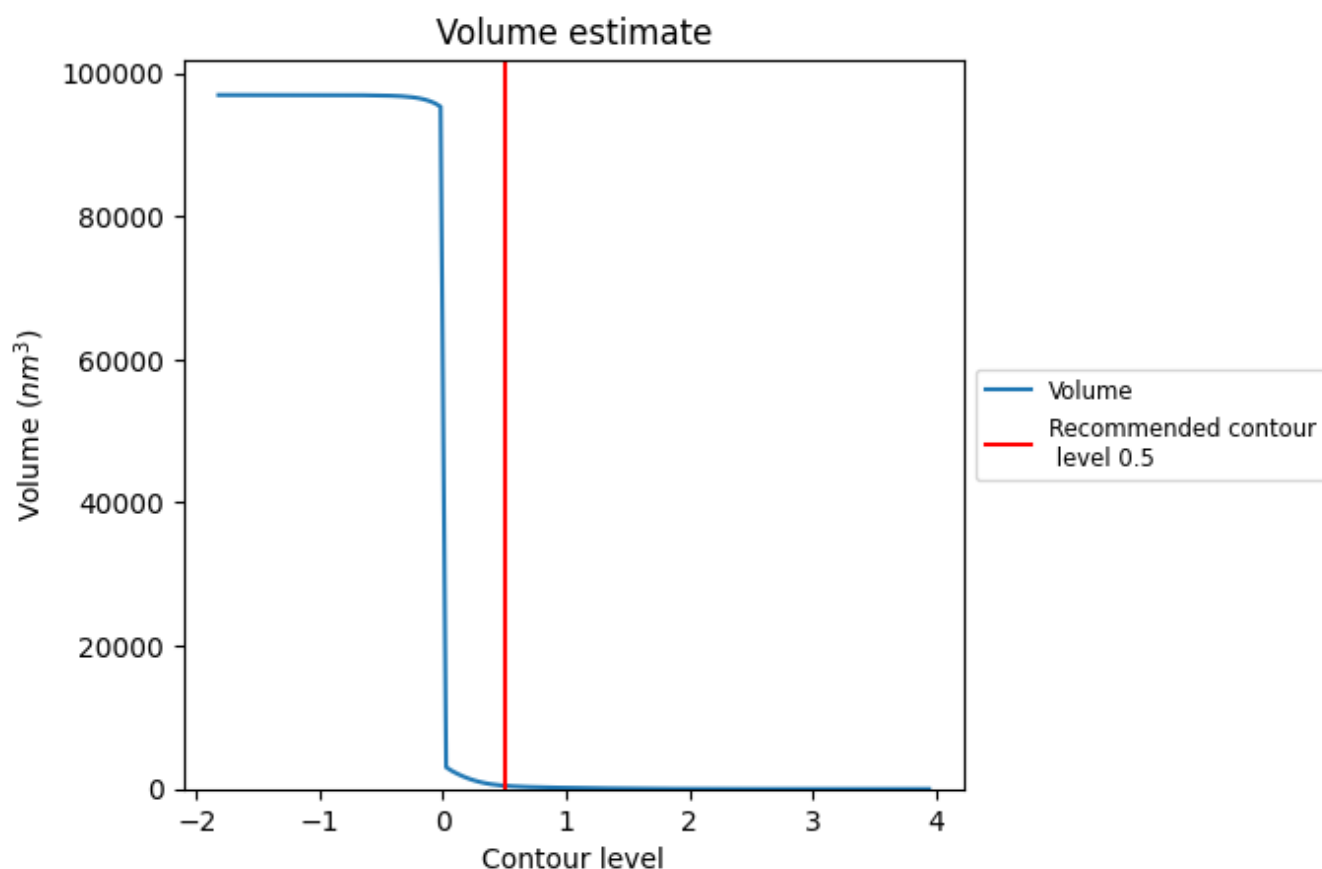
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

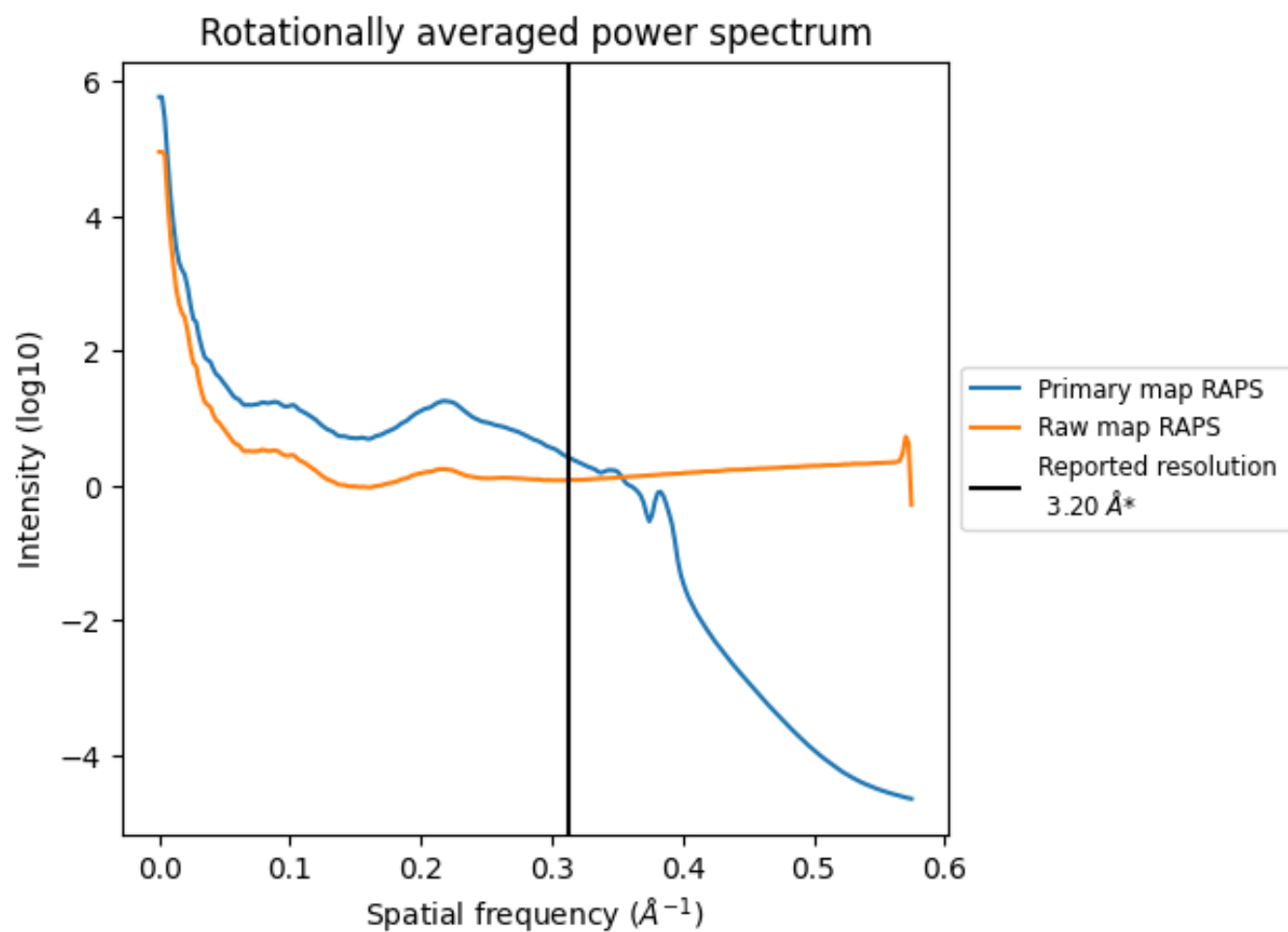
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm³; this corresponds to an approximate mass of 412 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 ⓘ

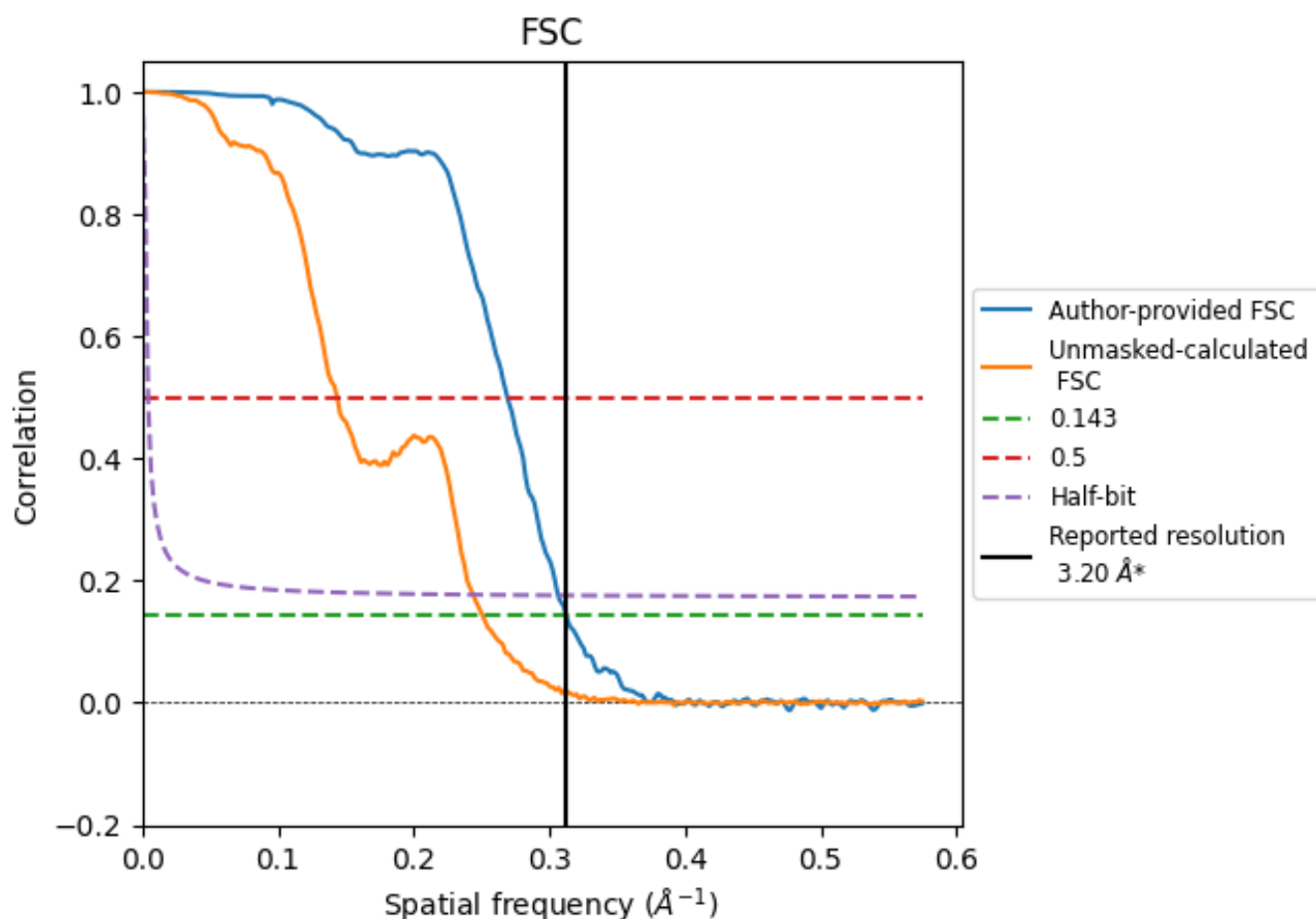


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

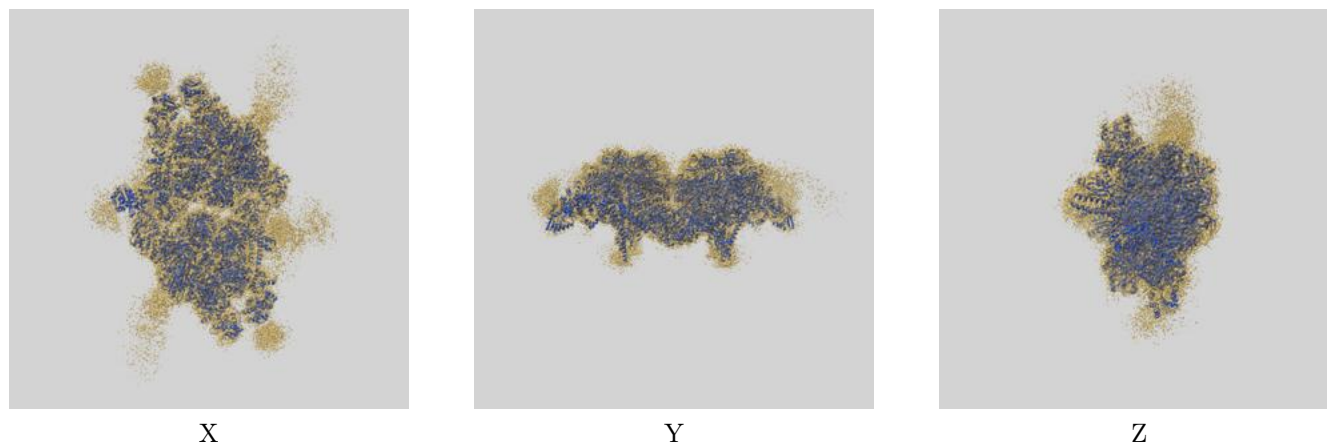
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.72	3.26
Unmasked-calculated*	3.99	6.96	4.10

*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 3.99 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

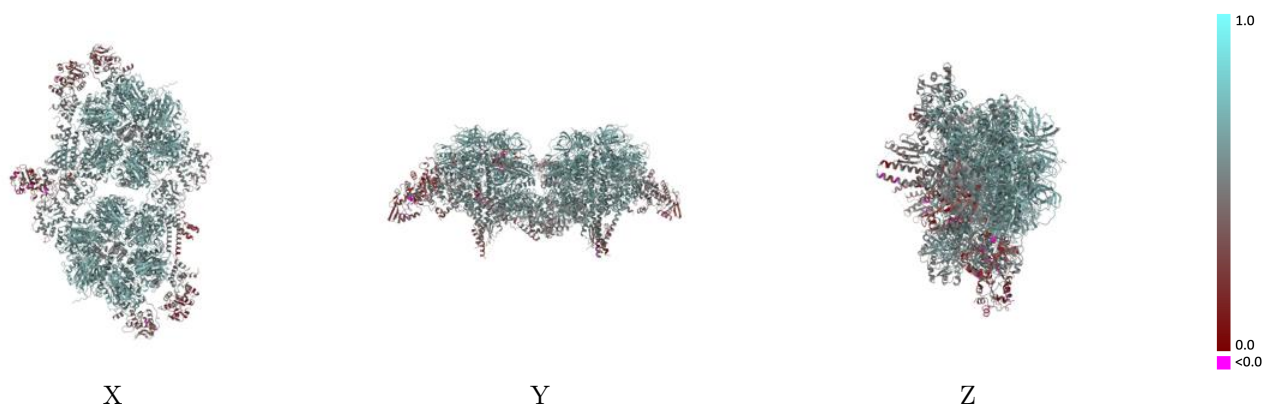
This section contains information regarding the fit between EMDB map EMD-60718 and PDB model 9IO5. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



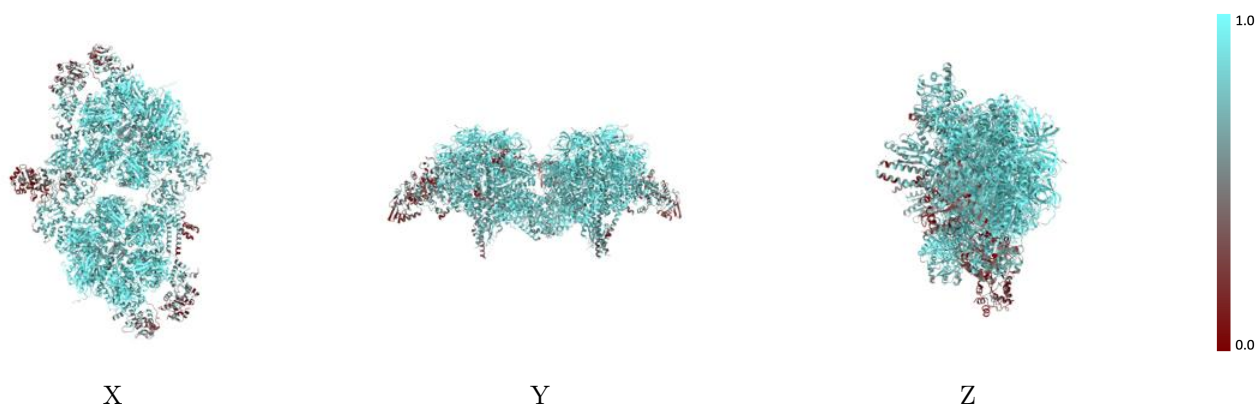
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



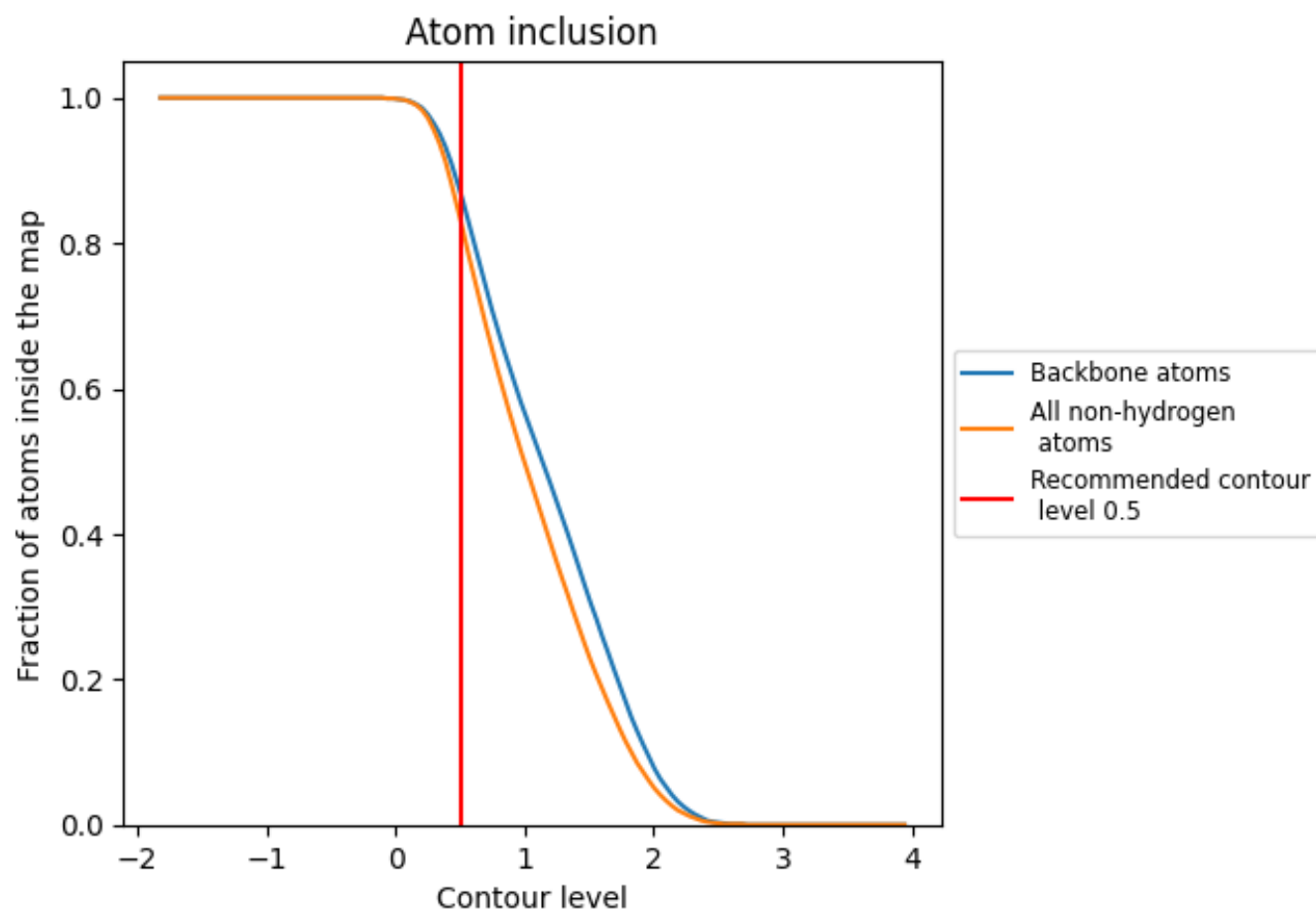
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.5540
A	 0.9210	 0.6030
B	 0.9030	 0.5890
C	 0.8550	 0.5710
D	 0.9270	 0.6050
E	 0.8920	 0.5830
F	 0.9170	 0.6020
G	 0.7330	 0.4880
H	 0.9190	 0.6020
I	 0.8670	 0.5670
J	 0.8750	 0.5820
K	 0.9190	 0.6000
L	 0.8920	 0.5820
M	 0.9120	 0.5950
N	 0.7210	 0.4830
O	 0.4900	 0.3700
P	 0.4270	 0.3350
Q	 0.3010	 0.3340
R	 0.7280	 0.4670
S	 0.4630	 0.3570
T	 0.8490	 0.5510
U	 0.7680	 0.5000
V	 0.4610	 0.3800
W	 0.8120	 0.5190
X	 0.8660	 0.5910
Y	 0.4460	 0.4520
Z	 0.4440	 0.3510

