



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:17 PM UTC

PDB ID : 9BYM / pdb_00009bym
EMDB ID : EMD-45038
Title : Cryo-EM structure of ATP synthase non-stator state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-23
Resolution : 3.11 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

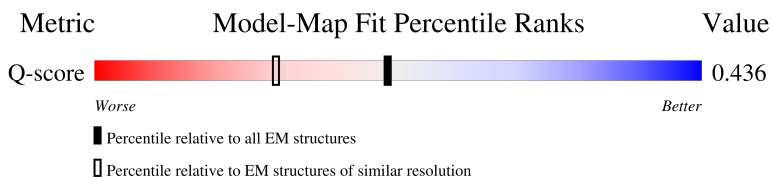
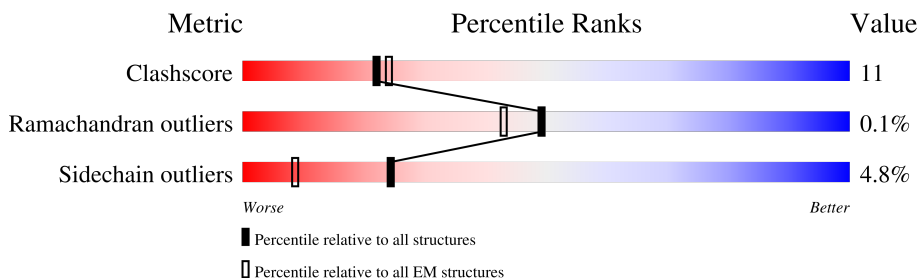
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	550	
1	B	550	
1	C	550	
2	D	570	

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Mol	Chain	Length	Quality of chain
2	E	570	
2	F	570	
3	J	108	
4	G	273	
5	H	168	
6	I	136	
7	K	141	
7	L	141	
7	M	141	
7	N	141	
7	O	141	
7	P	141	
7	Q	141	
7	R	141	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29873 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	489	Total	C	N	O	S	0	0
			3728	2350	658	708	12		
1	C	484	Total	C	N	O	S	0	0
			3689	2327	653	697	12		
1	B	489	Total	C	N	O	S	0	0
			3728	2350	658	708	12		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	470	Total	C	N	O	S	0	0
			3560	2256	604	688	12		
2	E	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		
2	F	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		

- Molecule 3 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	53	Total	C	N	O	0	0
			399	240	81	78		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2112	1332	366	407	7		

- Molecule 5 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			973	610	165	196	2		

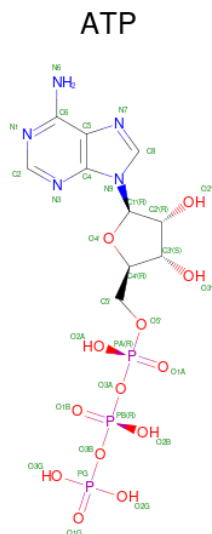
- Molecule 6 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	48	Total	C	N	O	S	0	0
			377	241	69	66	1		

- Molecule 7 is a protein called ATP synthase lipid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	L	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	N	72	Total	C	N	O	S	0	0
			510	339	80	89	2		
7	O	72	Total	C	N	O	S	0	0
			510	339	80	89	2		
7	P	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	Q	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	R	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
7	M	72	Total	C	N	O	S	0	0
			510	339	80	89	2		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total Mg 1 1	0
9	C	1	Total Mg 1 1	0
9	D	1	Total Mg 1 1	0
9	F	1	Total Mg 1 1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

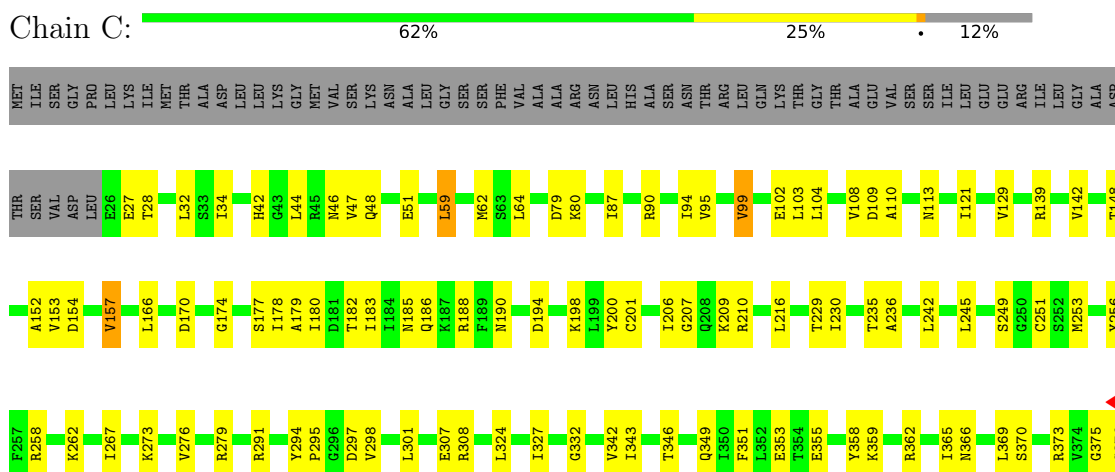
3 Residue-property plots

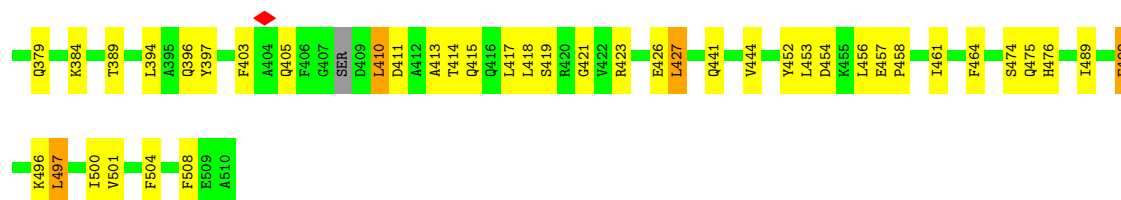
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP synthase subunit alpha



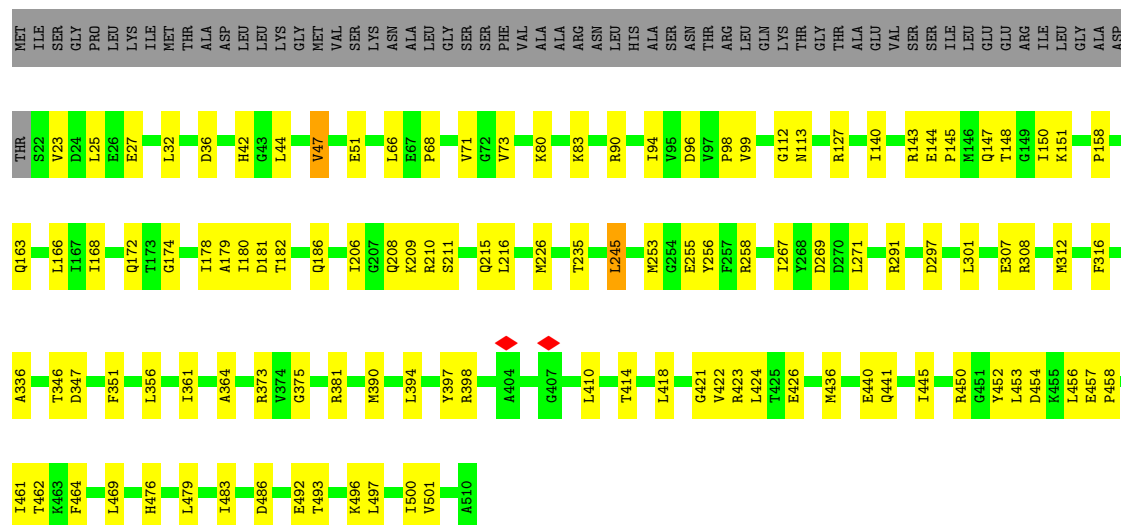
• Molecule 1: ATP synthase subunit alpha





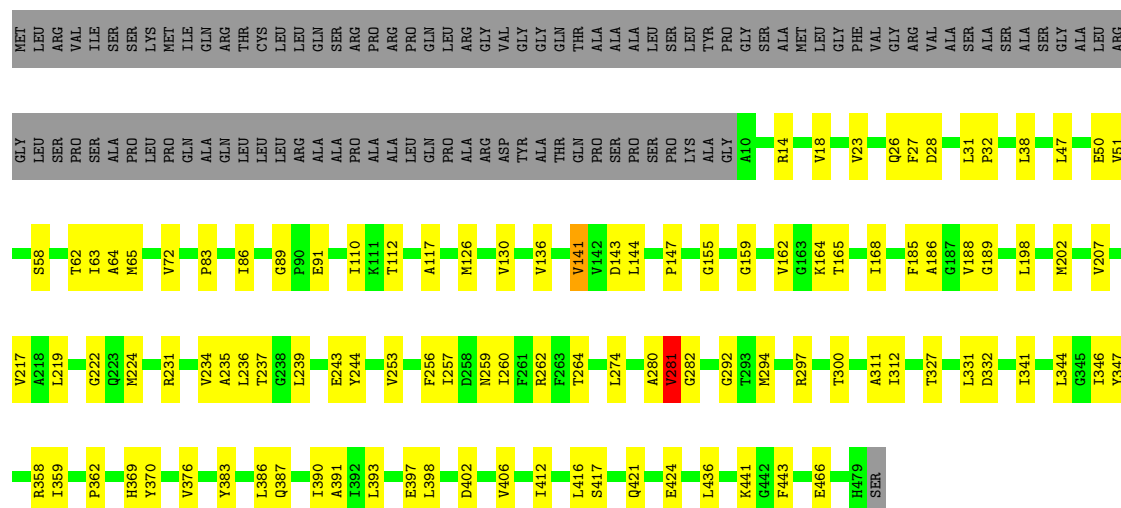
• Molecule 1: ATP synthase subunit alpha

Chain B:



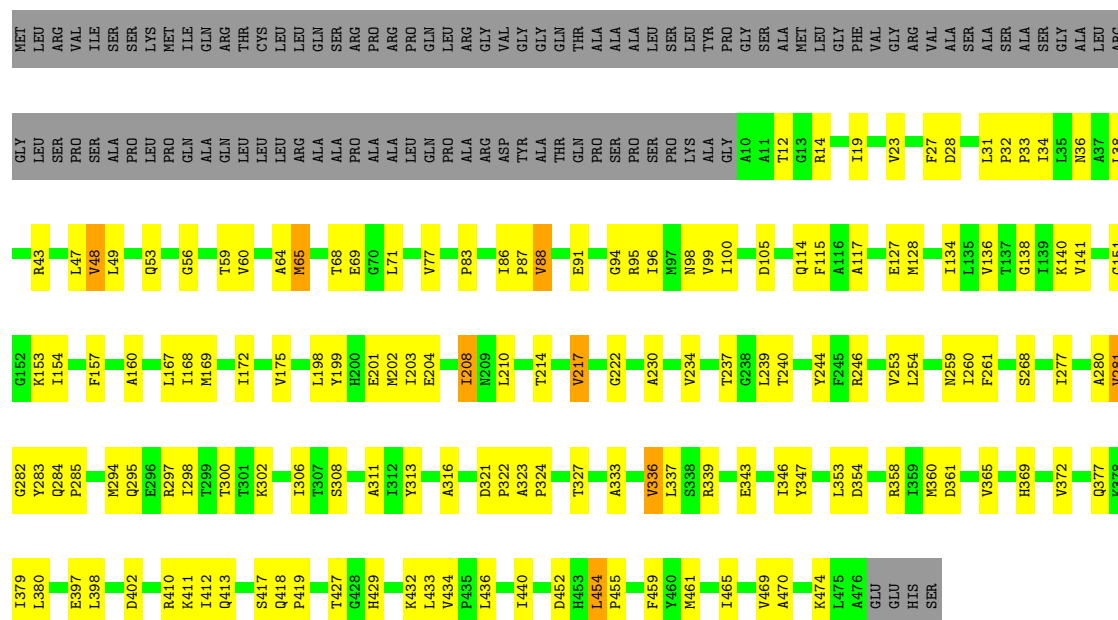
• Molecule 2: ATP synthase subunit beta

Chain D:



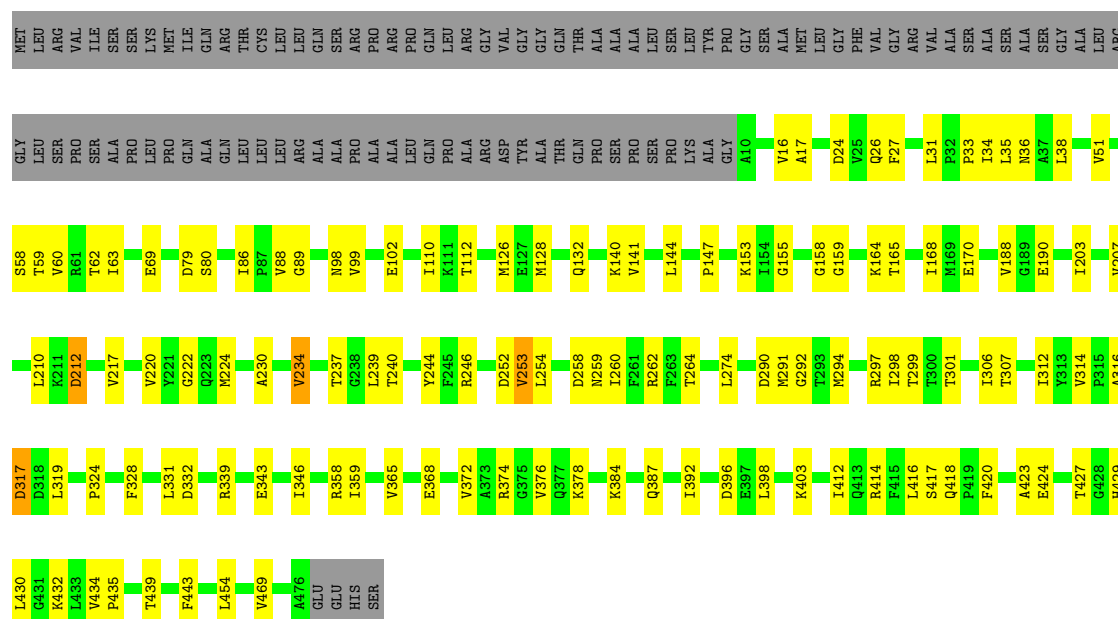
• Molecule 2: ATP synthase subunit beta

Chain E:



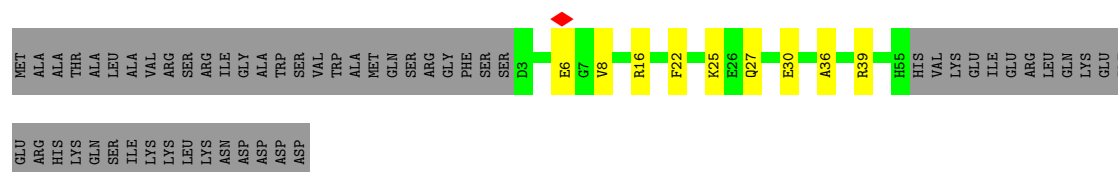
• Molecule 2: ATP synthase subunit beta

Chain F: 60% 21% 18%

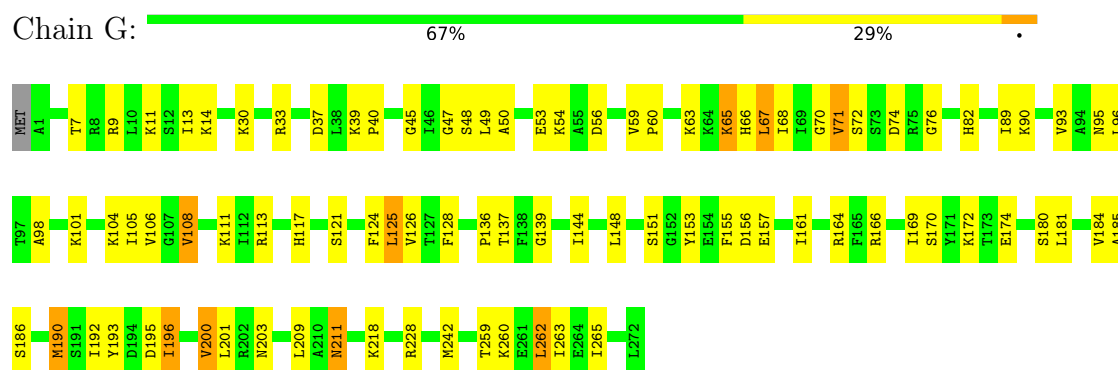


• Molecule 3: ATPase inhibitor, mitochondrial

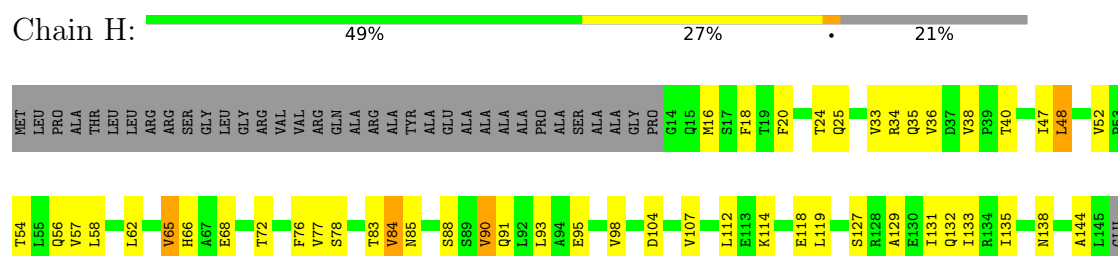
Chain J: 41% 8% 51%



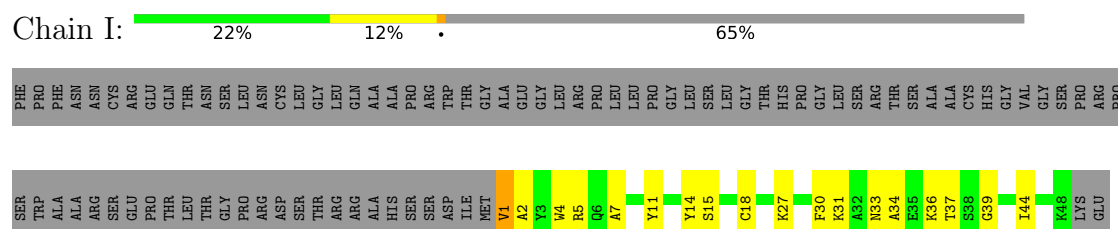
- Molecule 4: ATP synthase subunit gamma



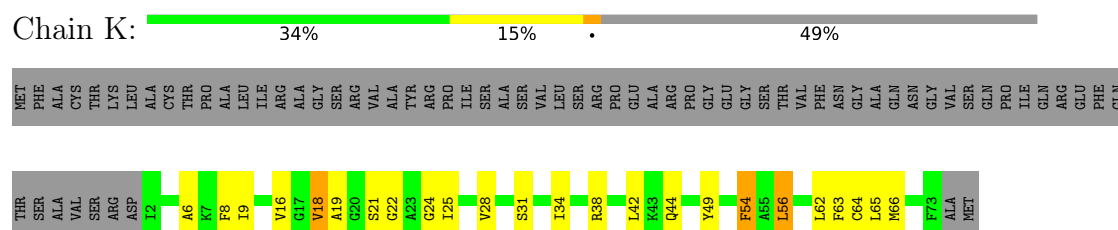
- Molecule 5: ATP synthase F1 subunit delta



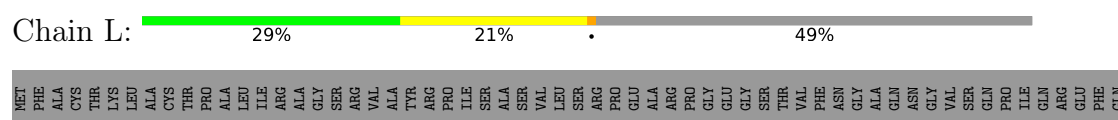
- Molecule 6: ATP synthase F1 subunit epsilon



- Molecule 7: ATP synthase lipid-binding protein

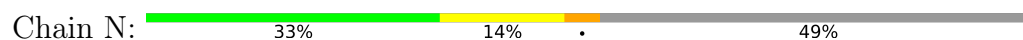


- Molecule 7: ATP synthase lipid-binding protein

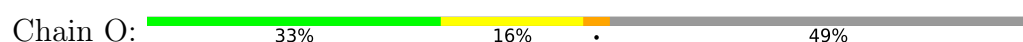




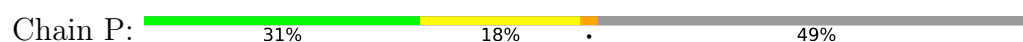
• Molecule 7: ATP synthase lipid-binding protein



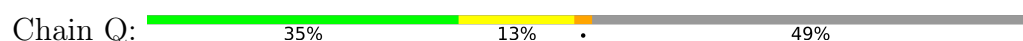
• Molecule 7: ATP synthase lipid-binding protein



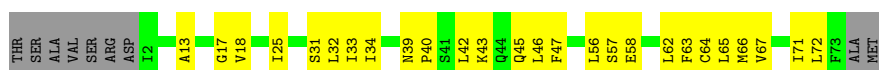
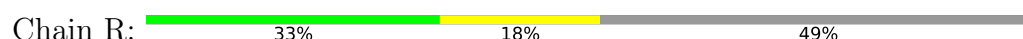
• Molecule 7: ATP synthase lipid-binding protein



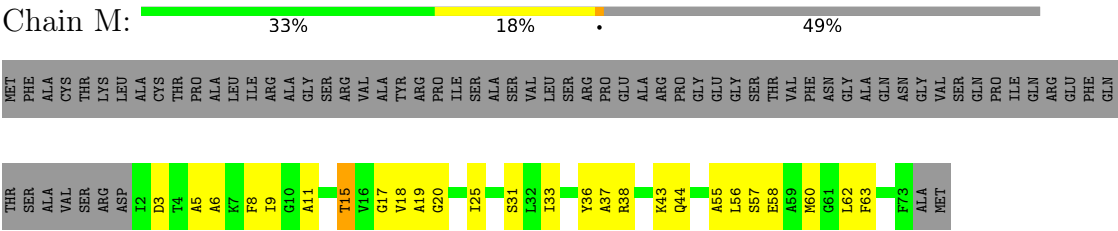
• Molecule 7: ATP synthase lipid-binding protein



• Molecule 7: ATP synthase lipid-binding protein



● Molecule 7: ATP synthase lipid-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.178	Depositor
Minimum map value	-0.301	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/3779	0.33	0/5099
1	B	0.17	0/3779	0.34	0/5099
1	C	0.18	0/3739	0.35	0/5043
2	D	0.16	0/3618	0.31	0/4907
2	E	0.17	0/3589	0.30	0/4868
2	F	0.19	0/3589	0.33	0/4868
3	J	0.10	0/404	0.28	0/539
4	G	0.14	0/2138	0.32	0/2874
5	H	0.14	0/986	0.32	0/1342
6	I	0.12	0/382	0.35	0/511
7	K	0.16	0/522	0.35	0/704
7	L	0.37	0/522	0.54	0/704
7	M	0.12	0/519	0.26	0/701
7	N	0.44	1/519 (0.2%)	0.53	1/701 (0.1%)
7	O	0.16	0/519	0.35	0/701
7	P	0.16	0/522	0.37	0/704
7	Q	0.40	0/522	0.61	0/704
7	R	0.31	0/519	0.47	0/700
All	All	0.19	1/30167 (0.0%)	0.35	1/40769 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	20	GLY	C-N	6.34	1.42	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	20	GLY	O-C-N	5.81	127.77	122.19

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	3728	0	3830	73	0
1	B	3728	0	3831	74	0
1	C	3689	0	3791	93	0
2	D	3560	0	3608	65	0
2	E	3532	0	3590	90	0
2	F	3532	0	3590	83	0
3	J	399	0	371	12	0
4	G	2112	0	2189	64	0
5	H	973	0	971	36	0
6	I	377	0	400	15	0
7	K	513	0	532	19	0
7	L	513	0	532	24	0
7	M	510	0	525	25	0
7	N	510	0	525	28	0
7	O	510	0	525	30	0
7	P	513	0	532	28	0
7	Q	513	0	532	24	0
7	R	510	0	523	24	0
8	A	31	0	12	1	0
8	B	31	0	12	1	0
8	C	31	0	12	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
10	D	27	0	12	2	0
10	F	27	0	12	3	0
All	All	29873	0	30457	692	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 11.

All (692) 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:C:327:ILE:HG13	1:C:342:VAL:HG11	1.53	0.88
2:F:427:THR:HG23	2:F:429:HIS:H	1.42	0.84
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.59	0.84
1:C:182:THR:HG22	1:C:186:GLN:HE22	1.42	0.83
4:G:63:LYS:HG3	4:G:157:GLU:HB2	1.64	0.80
1:C:201:CYS:HB2	1:C:229:THR:HG22	1.65	0.79
1:C:373:ARG:HD2	1:C:375:GLY:H	1.48	0.77
2:D:202:MET:HE1	2:D:219:LEU:HD21	1.66	0.77
2:D:393:LEU:HD22	2:D:397:GLU:HG2	1.65	0.76
2:E:427:THR:HG23	2:E:429:HIS:H	1.51	0.76
7:K:25:ILE:HD11	7:K:54:PHE:HD1	1.49	0.75
1:A:210:ARG:HG2	1:A:235:THR:HG21	1.69	0.74
2:F:259:ASN:HB3	2:F:262:ARG:HG2	1.71	0.73
2:E:379:ILE:HG21	2:E:412:ILE:HD12	1.70	0.73
1:A:423:ARG:NH2	1:A:456:LEU:O	2.22	0.72
2:F:140:LYS:HG3	2:F:434:VAL:HG21	1.72	0.72
4:G:166:ARG:HH21	4:G:170:SER:HB2	1.54	0.72
2:D:155:GLY:HA3	2:D:331:LEU:HD13	1.72	0.71
1:A:312:MET:HE2	1:A:316:PHE:HB3	1.72	0.71
7:L:33:ILE:HG21	7:N:32:LEU:HA	1.72	0.71
7:O:4:THR:HG21	7:P:3:ASP:HA	1.74	0.70
1:C:154:ASP:HB2	1:C:441:GLN:HE22	1.56	0.69
1:B:210:ARG:HG2	1:B:235:THR:HG21	1.73	0.69
1:A:148:THR:HA	1:A:182:THR:HG23	1.73	0.69
1:C:423:ARG:HA	1:C:461:ILE:HD13	1.75	0.69
1:A:479:LEU:HD13	1:A:496:LYS:HD3	1.74	0.69
2:F:239:LEU:HD21	2:F:297:ARG:HB2	1.74	0.69
2:E:140:LYS:HG2	2:E:434:VAL:HG21	1.75	0.68
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.76	0.68
2:F:316:ALA:HB2	1:B:291:ARG:NH1	2.09	0.68
1:B:423:ARG:HD3	1:B:454:ASP:HA	1.75	0.68
7:Q:15:THR:HG21	7:R:67:VAL:HG11	1.76	0.67
4:G:72:SER:HB3	4:G:82:HIS:HD2	1.59	0.67
2:F:239:LEU:HD13	2:F:298:ILE:HG12	1.76	0.67
7:P:25:ILE:HG13	7:P:54:PHE:HD1	1.60	0.67
10:F:501:ADP:O2A	1:B:373:ARG:NH1	2.29	0.66
4:G:76:GLY:O	4:G:228:ARG:NH2	2.29	0.66
7:L:11:ALA:HB2	7:L:71:ILE:HG21	1.77	0.66
1:B:312:MET:HE2	1:B:316:PHE:HB3	1.78	0.65
1:B:479:LEU:HD13	1:B:496:LYS:HD3	1.78	0.65
6:I:1:VAL:HG23	7:N:40:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ILE:HG12	2:D:398:LEU:HD11	1.79	0.65
1:C:403:PHE:HD2	1:C:405:GLN:H	1.44	0.64
4:G:68:ILE:HB	4:G:105:ILE:HG22	1.78	0.64
7:Q:39:ASN:ND2	7:M:37:ALA:O	2.30	0.64
2:E:298:ILE:HG21	2:E:308:SER:HB2	1.80	0.64
1:A:479:LEU:HD11	1:A:493:THR:HG23	1.80	0.64
7:Q:8:PHE:HB3	7:R:71:ILE:HD11	1.80	0.64
7:N:40:PRO:HG3	7:O:42:LEU:HD11	1.81	0.63
4:G:70:GLY:HA3	4:G:89:ILE:HD11	1.80	0.63
7:N:21:SER:OG	7:N:58:GLU:HA	1.97	0.63
7:Q:49:TYR:HB2	7:M:33:ILE:HD11	1.80	0.63
1:C:210:ARG:HG3	1:C:235:THR:HG21	1.81	0.63
2:F:99:VAL:HG22	2:F:234:VAL:HB	1.80	0.63
4:G:190:MET:SD	4:G:190:MET:N	2.72	0.63
7:P:39:ASN:HD21	7:P:42:LEU:HD23	1.63	0.63
1:C:207:GLY:HA3	1:C:273:LYS:HD3	1.81	0.62
1:A:394:LEU:O	1:A:398:ARG:HG2	1.99	0.62
2:E:268:SER:HA	2:E:284:GLN:HB3	1.80	0.62
1:B:158:PRO:HG2	1:B:375:GLY:HA2	1.81	0.62
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.32	0.62
1:A:423:ARG:HH12	1:A:458:PRO:HG3	1.64	0.62
5:H:16:MET:HA	5:H:88:SER:HB2	1.82	0.62
2:D:224:MET:HA	2:D:231:ARG:HD3	1.82	0.61
2:E:360:MET:HE3	2:E:365:VAL:HG21	1.83	0.61
2:E:336:VAL:HG21	2:E:354:ASP:HB3	1.83	0.61
4:G:136:PRO:HG2	4:G:218:LYS:HE3	1.82	0.61
2:D:186:ALA:HB3	2:D:257:ILE:HG12	1.83	0.61
2:E:239:LEU:HD21	2:E:297:ARG:HB2	1.83	0.61
2:E:246:ARG:HD3	2:E:306:ILE:HG13	1.82	0.60
2:E:259:ASN:H	2:E:311:ALA:HB3	1.65	0.60
2:E:321:ASP:HB3	2:E:324:PRO:HD2	1.82	0.60
4:G:200:VAL:HA	4:G:203:ASN:HD22	1.66	0.60
7:M:55:ALA:HA	7:M:58:GLU:HG2	1.83	0.60
1:A:158:PRO:HB3	1:A:379:GLN:HG3	1.83	0.60
1:C:44:LEU:HB3	1:C:47:VAL:HB	1.83	0.60
2:F:69:GLU:HB2	1:B:94:ILE:HD13	1.82	0.60
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.37	0.60
7:K:56:LEU:HB3	7:R:25:ILE:HD12	1.83	0.60
2:E:198:LEU:HD11	2:E:202:MET:HE3	1.84	0.60
7:N:33:ILE:HG21	7:O:32:LEU:HA	1.83	0.60
4:G:82:HIS:CE1	4:G:111:LYS:HG3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:49:TYR:HB2	7:R:33:ILE:HG12	1.84	0.59
1:A:99:VAL:HG21	1:A:127:ARG:HB3	1.84	0.59
2:D:141:VAL:HG13	2:D:416:LEU:HD22	1.82	0.59
4:G:71:VAL:HA	4:G:108:VAL:HG13	1.85	0.59
2:F:51:VAL:HA	2:F:62:THR:HG22	1.84	0.59
4:G:50:ALA:HA	4:G:53:GLU:HB3	1.85	0.59
7:M:11:ALA:O	7:M:15:THR:OG1	2.21	0.59
7:O:29:PHE:O	7:O:33:ILE:HG12	2.02	0.58
2:F:384:LYS:HA	2:F:387:GLN:HG2	1.85	0.58
1:C:148:THR:HA	1:C:182:THR:HG23	1.85	0.58
1:C:180:ILE:HD12	1:C:216:LEU:HD12	1.86	0.58
6:I:27:LYS:HB2	6:I:30:PHE:HD2	1.67	0.58
4:G:113:ARG:O	4:G:117:HIS:N	2.37	0.58
2:D:222:GLY:HA3	2:D:234:VAL:HG11	1.84	0.58
1:C:411:ASP:HA	1:C:415:GLN:HB2	1.85	0.57
2:D:91:GLU:HB2	2:D:112:THR:HG22	1.85	0.57
7:N:18:VAL:HG13	7:O:60:MET:HE3	1.86	0.57
1:B:390:MET:HE3	1:B:424:LEU:HD22	1.86	0.57
2:F:290:ASP:OD1	2:F:291:MET:N	2.37	0.57
3:J:8:VAL:O	4:G:14:LYS:NZ	2.36	0.57
7:L:12:GLY:HA2	7:N:14:ALA:HB2	1.86	0.57
2:E:87:PRO:HA	2:E:115:PHE:HD1	1.70	0.57
7:P:29:PHE:O	7:P:33:ILE:HG12	2.05	0.57
1:B:208:GLN:NE2	1:B:269:ASP:HB3	2.20	0.57
2:F:346:ILE:HG23	2:F:417:SER:HB3	1.87	0.56
1:C:183:ILE:HD11	1:C:267:ILE:HD13	1.87	0.56
7:P:65:LEU:HD21	7:M:63:PHE:HE2	1.70	0.56
2:D:346:ILE:HG23	2:D:417:SER:HB3	1.87	0.56
2:E:38:LEU:HB2	2:E:49:LEU:HB2	1.85	0.56
1:A:98:PRO:HD2	1:A:112:GLY:HA3	1.86	0.56
1:C:102:GLU:OE1	1:C:102:GLU:N	2.36	0.56
2:E:172:ILE:HG21	2:E:217:VAL:HG22	1.87	0.56
2:E:347:TYR:HB2	2:E:461:MET:HE1	1.85	0.56
1:A:166:LEU:HB2	1:A:346:THR:HG21	1.88	0.56
1:A:456:LEU:HD23	1:A:461:ILE:HD13	1.86	0.56
7:Q:29:PHE:CE2	7:R:56:LEU:HD23	2.40	0.56
1:C:179:ALA:O	1:C:183:ILE:HG12	2.06	0.56
2:F:155:GLY:HA3	2:F:331:LEU:HD13	1.87	0.56
7:K:18:VAL:O	7:K:21:SER:OG	2.21	0.56
7:P:9:ILE:HD12	7:M:9:ILE:HD12	1.87	0.56
1:C:258:ARG:NH1	1:C:308:ARG:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:ILE:HG22	2:D:346:ILE:HB	1.88	0.55
2:F:17:ALA:HB3	2:F:24:ASP:HB3	1.88	0.55
2:F:99:VAL:HG21	2:F:230:ALA:HB1	1.87	0.55
2:D:51:VAL:HA	2:D:62:THR:HG22	1.88	0.55
1:C:182:THR:O	1:C:186:GLN:NE2	2.39	0.55
2:F:31:LEU:HD12	2:F:60:VAL:HG13	1.89	0.55
2:D:89:GLY:HA2	2:D:244:TYR:CE1	2.41	0.55
5:H:76:PHE:HB3	5:H:98:VAL:HG13	1.88	0.55
2:D:188:VAL:HG22	2:D:234:VAL:HG23	1.87	0.55
2:F:159:GLY:O	2:F:164:LYS:NZ	2.40	0.55
1:A:75:VAL:HG12	1:A:77:GLY:H	1.71	0.55
7:K:25:ILE:HD13	7:L:56:LEU:HB3	1.87	0.55
2:E:283:TYR:HD2	2:E:322:PRO:HB2	1.72	0.55
5:H:54:THR:H	5:H:84:VAL:HG13	1.71	0.55
1:B:151:LYS:NZ	1:B:436:MET:SD	2.79	0.55
4:G:181:LEU:HB3	4:G:184:VAL:HG12	1.89	0.55
7:O:18:VAL:HG11	7:O:65:LEU:HD13	1.87	0.55
2:E:372:VAL:HG21	2:E:440:ILE:HG23	1.89	0.55
7:R:31:SER:HA	7:R:34:ILE:HG22	1.89	0.55
1:C:142:VAL:O	1:C:376:SER:OG	2.25	0.54
1:C:397:TYR:CG	1:C:421:GLY:HA3	2.42	0.54
7:O:62:LEU:HD13	7:O:65:LEU:HD23	1.89	0.54
1:B:456:LEU:HD23	1:B:461:ILE:HD13	1.88	0.54
4:G:72:SER:HB3	4:G:82:HIS:CD2	2.41	0.54
5:H:24:THR:OG1	6:I:36:LYS:NZ	2.38	0.54
1:C:267:ILE:HG13	1:C:324:LEU:HB2	1.90	0.54
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.89	0.54
5:H:132:GLN:HA	5:H:135:ILE:HG12	1.89	0.54
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.89	0.54
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.88	0.54
2:E:203:ILE:HD13	2:E:210:LEU:HD11	1.90	0.54
2:F:418:GLN:NE2	2:F:432:LYS:O	2.40	0.54
7:O:25:ILE:HD11	7:P:57:SER:HA	1.89	0.54
2:F:253:VAL:HG23	2:F:306:ILE:HG12	1.90	0.54
4:G:67:LEU:HD11	4:G:148:LEU:HD11	1.89	0.54
1:A:30:ARG:HH21	1:A:42:HIS:HD2	1.56	0.54
1:A:174:GLY:O	1:A:178:ILE:HG12	2.08	0.54
2:E:127:GLU:HA	2:E:302:LYS:HE2	1.90	0.54
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.90	0.54
2:E:88:VAL:HG13	2:E:244:TYR:HB2	1.90	0.54
7:P:18:VAL:HG13	7:M:60:MET:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:MET:HE1	2:F:299:THR:HB	1.91	0.53
1:C:166:LEU:HB2	1:C:346:THR:HG21	1.90	0.53
2:F:110:ILE:HG22	2:F:112:THR:HG23	1.91	0.53
1:B:51:GLU:HA	1:B:94:ILE:HA	1.90	0.53
1:B:166:LEU:HB2	1:B:346:THR:HG21	1.90	0.53
1:A:47:VAL:HA	1:A:90:ARG:HE	1.73	0.53
7:Q:16:VAL:HG22	7:R:13:ALA:O	2.08	0.53
2:D:27:PHE:O	2:D:58:SER:OG	2.23	0.53
1:C:47:VAL:HA	1:C:90:ARG:HE	1.73	0.53
2:D:27:PHE:CD2	2:D:32:PRO:HD3	2.43	0.53
1:B:479:LEU:HD11	1:B:493:THR:HG23	1.91	0.53
1:C:110:ALA:HB3	1:C:242:LEU:HD22	1.91	0.53
2:E:454:LEU:HD21	2:E:469:VAL:HA	1.91	0.53
2:E:470:ALA:O	2:E:474:LYS:HG2	2.08	0.53
4:G:37:ASP:OD2	4:G:218:LYS:NZ	2.42	0.53
2:E:160:ALA:O	2:E:339:ARG:NH2	2.42	0.53
4:G:39:LYS:HB2	4:G:40:PRO:HD3	1.90	0.53
4:G:164:ARG:N	4:G:172:LYS:O	2.42	0.53
5:H:18:PHE:CZ	5:H:20:PHE:HB2	2.44	0.53
5:H:36:VAL:HB	5:H:47:ILE:HB	1.91	0.53
1:A:257:PHE:HB3	1:A:262:LYS:HB2	1.91	0.52
1:A:457:GLU:HG2	1:A:458:PRO:HD2	1.91	0.52
2:E:353:LEU:HD21	2:E:380:LEU:HB2	1.91	0.52
2:F:398:LEU:O	2:F:403:LYS:NZ	2.42	0.52
4:G:195:ASP:HB2	5:H:54:THR:HG23	1.90	0.52
1:A:159:ILE:HD11	1:A:350:ILE:HD11	1.92	0.52
1:C:504:PHE:O	1:C:508:PHE:N	2.42	0.52
2:D:147:PRO:HB2	2:D:359:ILE:HD11	1.92	0.52
2:E:86:ILE:HD11	2:E:240:THR:HB	1.90	0.52
2:F:86:ILE:HD13	2:F:237:THR:HG23	1.92	0.52
1:C:183:ILE:HD12	1:C:201:CYS:HB3	1.92	0.52
2:F:38:LEU:HD12	2:F:62:THR:HG21	1.92	0.52
2:F:376:VAL:HG13	2:F:412:ILE:HG21	1.90	0.52
7:Q:25:ILE:HD11	7:R:57:SER:HA	1.90	0.52
1:B:98:PRO:HD2	1:B:112:GLY:HA3	1.91	0.52
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.44	0.52
1:C:362:ARG:NH2	2:F:374:ARG:HD2	2.25	0.52
2:E:98:ASN:HD21	2:E:100:ILE:HG12	1.73	0.51
4:G:166:ARG:HH11	4:G:172:LYS:HB2	1.75	0.51
2:E:95:ARG:NE	2:E:105:ASP:OD2	2.38	0.51
7:L:65:LEU:HD13	7:N:63:PHE:HZ	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:HIS:NE2	1:B:500:ILE:HG12	2.24	0.51
1:A:407:GLY:HA2	1:A:410:LEU:HD23	1.91	0.51
7:P:54:PHE:CD1	7:M:56:LEU:HD21	2.45	0.51
2:F:392:ILE:HB	3:J:22:PHE:HZ	1.73	0.51
2:E:346:ILE:HG23	2:E:417:SER:HB3	1.93	0.51
7:O:65:LEU:HD21	7:P:63:PHE:CE2	2.45	0.51
1:C:32:LEU:HG	1:C:42:HIS:HB2	1.92	0.51
5:H:48:LEU:HD22	7:Q:39:ASN:HB3	1.93	0.51
5:H:104:ASP:HB3	5:H:107:VAL:HG12	1.93	0.51
7:N:30:GLY:O	7:O:31:SER:OG	2.21	0.51
4:G:148:LEU:HD23	4:G:209:LEU:HD21	1.92	0.51
4:G:164:ARG:HE	4:G:174:GLU:HG3	1.76	0.51
1:A:116:ASP:HA	2:D:126:MET:HE3	1.92	0.51
1:C:109:ASP:OD1	1:C:113:ASN:N	2.41	0.51
7:K:38:ARG:HH12	7:L:38:ARG:HD3	1.76	0.51
1:A:168:ILE:HG23	1:A:351:PHE:HD1	1.76	0.51
2:F:147:PRO:HG2	2:F:359:ILE:HG13	1.93	0.51
4:G:95:ASN:HD22	4:G:96:LEU:HD12	1.76	0.50
6:I:5:ARG:C	6:I:7:ALA:H	2.19	0.50
1:B:394:LEU:O	1:B:398:ARG:HG2	2.10	0.50
7:N:25:ILE:HD11	7:O:57:SER:HA	1.93	0.50
4:G:139:GLY:HA3	6:I:39:GLY:HA3	1.93	0.50
4:G:172:LYS:HG3	4:G:174:GLU:HG2	1.92	0.50
5:H:52:VAL:HG22	7:R:39:ASN:HD22	1.76	0.50
1:A:255:GLU:HG2	1:A:258:ARG:NH1	2.27	0.50
1:C:80:LYS:HD3	2:F:34:ILE:HB	1.92	0.50
1:C:355:GLU:O	1:C:359:LYS:HB2	2.12	0.50
2:E:339:ARG:O	2:E:343:GLU:HG2	2.11	0.50
5:H:78:SER:OG	6:I:18:CYS:SG	2.39	0.50
7:K:19:ALA:HB1	7:L:20:GLY:HA3	1.93	0.50
1:B:255:GLU:HG2	1:B:258:ARG:NH1	2.26	0.50
2:E:138:GLY:HA3	2:E:433:LEU:HD12	1.93	0.50
1:B:27:GLU:OE1	1:B:90:ARG:NH1	2.45	0.50
2:E:154:ILE:HD12	2:E:333:ALA:HB3	1.94	0.50
4:G:121:SER:HA	4:G:124:PHE:HD2	1.76	0.50
7:Q:32:LEU:HA	7:M:33:ILE:HG21	1.94	0.50
1:B:476:HIS:CD2	1:B:500:ILE:HG12	2.47	0.50
1:C:99:VAL:HG23	1:C:253:MET:HA	1.94	0.50
1:C:457:GLU:O	1:C:461:ILE:HG13	2.12	0.50
2:F:27:PHE:HB2	2:F:31:LEU:HD13	1.93	0.50
2:F:392:ILE:HB	3:J:22:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:424:GLU:HG2	2:F:430:LEU:HA	1.94	0.50
2:D:198:LEU:HG	2:D:202:MET:HE2	1.93	0.49
1:C:152:ALA:HB3	1:C:365:ILE:HD12	1.94	0.49
1:C:343:ILE:HG12	1:C:349:GLN:HG2	1.94	0.49
1:C:379:GLN:O	1:C:384:LYS:HE3	2.12	0.49
7:K:8:PHE:CD2	7:L:7:LYS:HG2	2.47	0.49
7:K:22:GLY:O	7:K:25:ILE:HG22	2.12	0.49
1:B:441:GLN:O	1:B:445:ILE:HG12	2.12	0.49
7:K:44:GLN:CD	7:K:44:GLN:H	2.20	0.49
1:C:103:LEU:HG	1:C:121:ILE:HG21	1.94	0.49
4:G:7:THR:HG22	4:G:11:LYS:HE3	1.94	0.49
7:N:65:LEU:HD21	7:O:67:VAL:HG21	1.92	0.49
2:D:143:ASP:HB3	2:D:436:LEU:HD13	1.94	0.49
1:A:52:MET:O	1:A:91:THR:OG1	2.24	0.49
5:H:83:THR:HB	5:H:91:GLN:HB2	1.95	0.49
4:G:156:ASP:N	4:G:156:ASP:OD1	2.44	0.49
1:C:373:ARG:HD2	1:C:375:GLY:N	2.24	0.49
2:E:410:ARG:HA	2:E:413:GLN:HG2	1.95	0.49
2:F:317:ASP:OD1	2:F:317:ASP:N	2.44	0.49
4:G:65:LYS:HB3	4:G:153:TYR:OH	2.13	0.49
5:H:33:VAL:HG11	5:H:65:VAL:HG23	1.95	0.49
6:I:34:ALA:O	6:I:37:THR:OG1	2.23	0.49
1:B:148:THR:HA	1:B:182:THR:HG23	1.95	0.49
1:A:236:ALA:HB1	2:D:292:GLY:HA3	1.95	0.49
2:E:418:GLN:NE2	2:E:432:LYS:O	2.46	0.49
5:H:119:LEU:HD11	5:H:135:ILE:HD13	1.95	0.49
7:Q:18:VAL:HG11	7:R:64:CYS:HB2	1.93	0.49
5:H:58:LEU:HD13	5:H:77:VAL:HG11	1.95	0.48
2:E:33:PRO:HB3	1:B:83:LYS:HD3	1.94	0.48
1:C:200:TYR:HE2	1:C:262:LYS:HD3	1.78	0.48
3:J:36:ALA:HA	3:J:39:ARG:HE	1.78	0.48
7:P:31:SER:HA	7:P:34:ILE:HG22	1.95	0.48
1:C:48:GLN:HB2	1:C:51:GLU:HB2	1.95	0.48
2:E:27:PHE:CD2	2:E:32:PRO:HD3	2.49	0.48
7:L:11:ALA:O	7:L:15:THR:HG23	2.13	0.48
1:B:23:VAL:HG13	1:B:25:LEU:HG	1.95	0.48
1:A:404:ALA:HB2	1:A:418:LEU:HD22	1.95	0.48
2:F:454:LEU:HD11	2:F:469:VAL:HG12	1.95	0.48
4:G:89:ILE:HG12	4:G:161:ILE:HD12	1.95	0.48
5:H:95:GLU:OE1	6:I:15:SER:OG	2.25	0.48
1:B:168:ILE:HG23	1:B:351:PHE:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ILE:HD13	2:D:237:THR:HG23	1.95	0.48
2:D:362:PRO:HD3	2:D:370:TYR:CD1	2.48	0.48
7:P:5:ALA:HA	7:M:6:ALA:CB	2.44	0.48
1:B:356:LEU:HB2	1:B:364:ALA:HB1	1.95	0.48
1:A:217:VAL:HB	1:A:226:MET:HE2	1.94	0.48
2:D:110:ILE:HG22	2:D:112:THR:HG23	1.95	0.48
1:B:255:GLU:HG2	1:B:258:ARG:HH12	1.79	0.48
1:C:474:SER:OG	1:C:475:GLN:OE1	2.23	0.48
4:G:166:ARG:HD3	4:G:172:LYS:HB2	1.95	0.48
7:N:67:VAL:O	7:N:71:ILE:HG12	2.14	0.48
7:O:9:ILE:HB	7:P:9:ILE:HG23	1.94	0.48
1:A:139:ARG:HG2	1:A:310:ALA:HB1	1.96	0.48
1:C:236:ALA:HB1	2:F:292:GLY:HA3	1.96	0.48
2:F:212:ASP:OD1	2:F:212:ASP:N	2.47	0.48
1:B:150:ILE:HD12	1:B:178:ILE:HG23	1.94	0.48
2:F:368:GLU:O	2:F:372:VAL:HG23	2.14	0.47
1:A:390:MET:SD	1:A:445:ILE:HD12	2.54	0.47
2:E:27:PHE:HB2	2:E:31:LEU:HD12	1.95	0.47
2:F:63:ILE:HD11	2:F:274:LEU:HD11	1.97	0.47
2:E:260:ILE:HG21	2:E:327:THR:HG21	1.96	0.47
2:E:398:LEU:HB3	2:E:402:ASP:HB3	1.96	0.47
4:G:196:ILE:HD11	4:G:201:LEU:HD13	1.96	0.47
7:Q:6:ALA:CB	7:M:5:ALA:HA	2.43	0.47
1:B:492:GLU:CD	1:B:492:GLU:H	2.22	0.47
1:A:430:GLN:NE2	1:A:434:ALA:O	2.38	0.47
1:C:139:ARG:NH2	1:C:307:GLU:O	2.46	0.47
2:D:344:LEU:HD21	3:J:16:ARG:HH22	1.80	0.47
4:G:54:LYS:HG2	5:H:85:ASN:HD22	1.79	0.47
7:Q:19:ALA:HB2	7:R:17:GLY:HA2	1.96	0.47
1:A:383:MET:HB2	1:A:438:ILE:HD11	1.95	0.47
1:C:294:TYR:HB3	1:C:298:VAL:HG11	1.96	0.47
2:E:48:VAL:HG22	2:E:65:MET:HB2	1.97	0.47
7:P:19:ALA:HB2	7:M:17:GLY:HA2	1.96	0.47
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.96	0.47
1:B:99:VAL:HG13	1:B:253:MET:HA	1.95	0.47
1:A:183:ILE:HD11	1:A:267:ILE:HD12	1.96	0.47
1:C:190:ASN:O	1:C:198:LYS:NZ	2.48	0.47
1:C:413:ALA:HB2	3:J:39:ARG:NE	2.29	0.47
2:D:159:GLY:O	2:D:164:LYS:NZ	2.37	0.47
4:G:117:HIS:O	4:G:121:SER:HB2	2.15	0.47
7:K:63:PHE:HE2	7:R:65:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:21:SER:OG	7:L:57:SER:O	2.25	0.47
7:N:3:ASP:O	7:N:7:LYS:HG2	2.14	0.47
7:N:25:ILE:HA	7:N:28:VAL:HG12	1.96	0.47
1:B:47:VAL:HG12	1:B:66:LEU:HD21	1.96	0.47
1:A:390:MET:HE3	1:A:424:LEU:HD22	1.97	0.47
1:C:251:CYS:SG	1:C:308:ARG:HD2	2.54	0.47
2:E:96:ILE:HD11	2:E:199:TYR:CD1	2.49	0.47
2:E:167:LEU:HD22	2:E:337:LEU:HD21	1.97	0.47
2:F:319:LEU:HD23	2:F:328:PHE:HZ	1.80	0.47
4:G:30:LYS:HG2	4:G:33:ARG:HH22	1.80	0.47
7:L:17:GLY:HA3	7:L:64:CYS:SG	2.54	0.47
7:L:62:LEU:O	7:L:66:MET:HG3	2.14	0.47
2:E:83:PRO:HB2	2:E:117:ALA:HB1	1.96	0.47
2:E:316:ALA:HA	3:J:6:GLU:HB3	1.97	0.47
2:F:260:ILE:HG22	2:F:312:ILE:HG12	1.96	0.47
5:H:66:HIS:HA	5:H:72:THR:HG22	1.97	0.47
1:A:483:ILE:HD11	1:A:493:THR:HG21	1.97	0.47
1:C:279:ARG:HA	1:C:295:PRO:HD3	1.97	0.47
2:E:53:GLN:NE2	1:B:36:ASP:OD1	2.47	0.47
4:G:125:LEU:HD12	4:G:125:LEU:H	1.80	0.47
5:H:34:ARG:HG3	5:H:68:GLU:HA	1.96	0.47
7:K:24:GLY:O	7:K:28:VAL:HG23	2.15	0.47
7:P:11:ALA:O	7:P:15:THR:OG1	2.31	0.47
1:C:397:TYR:HD1	1:C:418:LEU:HA	1.80	0.47
2:E:43:ARG:NH1	2:E:69:GLU:O	2.42	0.47
2:E:294:MET:HE3	2:E:294:MET:HB3	1.74	0.47
1:A:293:ALA:HB2	4:G:265:ILE:HD13	1.97	0.46
1:C:99:VAL:HG22	1:C:256:TYR:HB2	1.95	0.46
2:E:259:ASN:OD1	2:E:261:PHE:HB3	2.15	0.46
7:N:66:MET:HE2	7:N:70:LEU:HD11	1.97	0.46
1:B:497:LEU:O	1:B:501:VAL:HG23	2.15	0.46
1:C:194:ASP:OD1	1:C:194:ASP:N	2.48	0.46
2:F:31:LEU:HD21	2:F:58:SER:HA	1.97	0.46
5:H:48:LEU:HD11	7:Q:42:LEU:HD23	1.96	0.46
2:E:56:GLY:O	2:E:59:THR:HG22	2.16	0.46
2:F:188:VAL:HG22	2:F:234:VAL:HG13	1.97	0.46
7:N:21:SER:HB3	7:O:60:MET:HE2	1.97	0.46
7:P:38:ARG:HA	7:M:38:ARG:HD3	1.96	0.46
2:F:89:GLY:HA2	2:F:244:TYR:CE2	2.50	0.46
1:A:163:GLN:NE2	1:A:165:GLU:OE1	2.48	0.46
1:C:419:SER:O	1:C:423:ARG:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:128:MET:HE3	1:B:210:ARG:HB2	1.96	0.46
7:P:19:ALA:HB1	7:M:20:GLY:HA3	1.98	0.46
1:A:67:GLU:HG2	2:E:19:ILE:HD11	1.97	0.46
1:C:492:GLU:O	1:C:496:LYS:HG2	2.16	0.46
2:E:259:ASN:C	2:E:261:PHE:N	2.71	0.46
2:F:86:ILE:HG21	2:F:237:THR:HG23	1.96	0.46
7:N:19:ALA:HB2	7:O:17:GLY:HA2	1.97	0.46
7:O:58:GLU:HG3	7:P:60:MET:HE3	1.96	0.46
7:M:36:TYR:CE1	7:M:43:LYS:HD2	2.51	0.46
1:C:80:LYS:HD2	2:F:35:LEU:HG	1.98	0.46
5:H:129:ALA:O	5:H:133:ILE:HG12	2.15	0.46
7:K:28:VAL:O	7:K:31:SER:OG	2.29	0.46
7:Q:6:ALA:HB1	7:M:8:PHE:HB2	1.97	0.46
7:Q:57:SER:HA	7:M:25:ILE:HD11	1.97	0.46
2:E:199:TYR:CZ	2:E:203:ILE:HD11	2.51	0.46
2:F:339:ARG:O	2:F:343:GLU:HG2	2.16	0.46
7:K:38:ARG:NH1	7:L:38:ARG:HD3	2.30	0.46
2:D:63:ILE:HD11	2:D:274:LEU:HD11	1.98	0.46
2:E:313:TYR:OH	3:J:6:GLU:OE2	2.22	0.46
7:N:65:LEU:HD11	7:O:67:VAL:HG21	1.98	0.46
1:A:255:GLU:HG2	1:A:258:ARG:HH12	1.80	0.45
1:C:51:GLU:HA	1:C:94:ILE:HA	1.98	0.45
2:D:162:VAL:N	10:D:501:ADP:O3B	2.49	0.45
2:E:277:ILE:O	2:E:285:PRO:HG3	2.17	0.45
5:H:35:GLN:NE2	5:H:47:ILE:O	2.50	0.45
1:C:423:ARG:HA	1:C:461:ILE:CD1	2.45	0.45
2:D:38:LEU:HD12	2:D:62:THR:HG21	1.98	0.45
2:E:202:MET:HB3	2:E:208:ILE:HG22	1.98	0.45
2:F:98:ASN:HD21	2:F:102:GLU:HB2	1.80	0.45
2:F:170:GLU:HG3	2:F:420:PHE:CG	2.51	0.45
1:A:381:ARG:NH2	1:A:486:ASP:O	2.49	0.45
1:C:209:LYS:NZ	2:F:332:ASP:OD1	2.44	0.45
2:D:188:VAL:HG21	2:D:235:ALA:HB2	1.97	0.45
2:E:361:ASP:O	2:E:365:VAL:HG22	2.17	0.45
2:F:332:ASP:HA	2:F:358:ARG:HE	1.82	0.45
5:H:84:VAL:HA	5:H:90:VAL:HA	1.98	0.45
1:A:101:GLU:HG2	1:A:257:PHE:HE1	1.81	0.45
2:E:105:ASP:OD1	2:E:105:ASP:N	2.48	0.45
2:F:153:LYS:HB3	2:F:331:LEU:HD23	1.98	0.45
4:G:155:PHE:O	4:G:180:SER:OG	2.34	0.45
7:O:3:ASP:O	7:O:7:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:VAL:HG12	2:D:262:ARG:HB2	1.99	0.45
1:A:410:LEU:HD13	1:A:410:LEU:HA	1.87	0.45
1:A:441:GLN:O	1:A:445:ILE:HG12	2.17	0.45
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.81	0.45
2:E:169:MET:HA	2:E:172:ILE:HD12	1.98	0.45
2:E:369:HIS:CD2	2:E:440:ILE:HD11	2.52	0.45
1:B:178:ILE:HA	1:B:181:ASP:OD2	2.17	0.45
1:C:170:ASP:OD2	1:C:332:GLY:N	2.48	0.45
2:E:175:VAL:HG11	2:E:254:LEU:HD12	1.99	0.45
2:E:323:ALA:HB3	2:E:324:PRO:HD3	1.99	0.45
2:F:220:VAL:HG12	2:F:234:VAL:HG23	1.98	0.45
7:P:25:ILE:HG23	7:M:56:LEU:HD23	1.99	0.45
1:C:62:MET:HE3	1:C:64:LEU:HD21	1.99	0.45
2:E:419:PRO:HG2	2:E:432:LYS:HG2	1.99	0.45
1:A:151:LYS:NZ	1:A:436:MET:SD	2.89	0.45
1:C:427:LEU:HD21	1:C:444:VAL:O	2.17	0.45
4:G:96:LEU:C	4:G:98:ALA:H	2.25	0.45
7:N:21:SER:OG	7:O:60:MET:HE2	2.17	0.45
7:R:32:LEU:HD11	7:R:47:PHE:HD1	1.82	0.45
1:B:453:LEU:HD21	1:B:464:PHE:CE1	2.52	0.45
2:E:201:GLU:O	2:E:204:GLU:HG2	2.17	0.45
2:F:98:ASN:OD1	2:F:102:GLU:N	2.49	0.45
7:Q:36:TYR:CE2	7:R:42:LEU:HB3	2.52	0.45
7:M:25:ILE:HG22	7:M:57:SER:HB2	1.99	0.45
1:C:373:ARG:NH1	1:C:375:GLY:HA2	2.32	0.44
4:G:48:SER:HB2	4:G:211:ASN:HD21	1.83	0.44
4:G:190:MET:HA	4:G:193:TYR:CD1	2.52	0.44
7:N:21:SER:CB	7:O:60:MET:HE2	2.47	0.44
1:B:47:VAL:HA	1:B:90:ARG:HE	1.81	0.44
2:E:43:ARG:HD2	2:E:71:LEU:HD21	1.99	0.44
2:F:16:VAL:HG12	1:B:68:PRO:HG3	1.99	0.44
7:L:3:ASP:O	7:L:7:LYS:HG3	2.16	0.44
7:N:16:VAL:HG23	7:O:16:VAL:HB	1.99	0.44
1:A:151:LYS:HG2	1:A:441:GLN:HG2	2.00	0.44
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.52	0.44
2:D:421:GLN:HA	2:D:424:GLU:HG3	1.98	0.44
4:G:47:GLY:HA3	5:H:93:LEU:HD11	2.00	0.44
7:K:62:LEU:O	7:K:66:MET:HG3	2.18	0.44
2:D:376:VAL:HG13	2:D:412:ILE:HG21	1.98	0.44
2:F:246:ARG:NH1	2:F:299:THR:O	2.49	0.44
5:H:48:LEU:HD21	7:Q:41:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:65:LEU:HB2	7:L:63:PHE:HZ	1.81	0.44
7:R:31:SER:O	7:R:32:LEU:C	2.60	0.44
1:C:396:GLN:HB3	1:C:417:LEU:HD21	1.99	0.44
2:D:344:LEU:HD21	3:J:16:ARG:NH2	2.33	0.44
2:E:34:ILE:HB	1:B:80:LYS:HA	2.00	0.44
2:F:165:THR:HG22	10:F:501:ADP:PA	2.57	0.44
4:G:185:ALA:HB1	4:G:201:LEU:HD11	1.99	0.44
7:O:9:ILE:HD12	7:P:9:ILE:HD13	1.99	0.44
1:A:30:ARG:HH21	1:A:42:HIS:CD2	2.35	0.44
1:C:174:GLY:O	1:C:178:ILE:HG12	2.17	0.44
7:O:27:THR:HA	7:P:27:THR:HG21	1.99	0.44
7:Q:17:GLY:HA3	7:Q:64:CYS:SG	2.58	0.44
7:M:6:ALA:HA	7:M:9:ILE:HG12	2.00	0.44
1:B:452:TYR:CD2	1:B:501:VAL:HG11	2.53	0.44
2:D:466:GLU:OE1	2:D:466:GLU:N	2.47	0.44
2:F:86:ILE:HD11	2:F:240:THR:HB	2.00	0.44
2:F:144:LEU:HD22	2:F:443:PHE:CD2	2.52	0.44
2:F:190:GLU:OE2	2:F:259:ASN:ND2	2.50	0.44
2:F:294:MET:HE3	2:F:294:MET:HB3	1.91	0.44
4:G:66:HIS:CE1	4:G:68:ILE:HG12	2.52	0.44
4:G:156:ASP:HB2	4:G:181:LEU:HD22	2.00	0.44
7:K:34:ILE:HG23	7:L:31:SER:OG	2.18	0.44
7:Q:36:TYR:OH	7:R:45:GLN:HB2	2.17	0.44
7:L:36:TYR:CE2	7:N:45:GLN:HB2	2.53	0.44
7:Q:66:MET:O	7:Q:70:LEU:HG	2.18	0.44
1:B:440:GLU:HB3	1:B:469:LEU:HD22	2.00	0.44
2:D:280:ALA:C	2:D:282:GLY:H	2.25	0.43
2:F:165:THR:HA	2:F:168:ILE:HG22	1.99	0.43
7:R:72:LEU:HA	7:R:72:LEU:HD23	1.81	0.43
7:M:3:ASP:N	7:M:3:ASP:OD1	2.51	0.43
1:B:174:GLY:O	1:B:178:ILE:HG12	2.18	0.43
1:A:183:ILE:O	1:A:228:TYR:OH	2.33	0.43
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.74	0.43
1:C:273:LYS:O	1:C:276:VAL:HG22	2.18	0.43
2:E:94:GLY:HA2	2:E:208:ILE:HG13	1.99	0.43
2:E:230:ALA:O	2:E:234:VAL:HG23	2.18	0.43
4:G:148:LEU:O	4:G:151:SER:OG	2.31	0.43
1:B:297:ASP:OD1	1:B:297:ASP:N	2.52	0.43
1:A:152:ALA:HB3	1:A:365:ILE:HD12	2.00	0.43
2:E:86:ILE:HG21	2:E:237:THR:HG23	1.99	0.43
2:E:360:MET:HE1	2:E:369:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:414:ARG:O	2:F:417:SER:OG	2.33	0.43
4:G:126:VAL:HB	6:I:44:ILE:HD11	1.99	0.43
4:G:260:LYS:HE3	4:G:260:LYS:HB3	1.87	0.43
7:N:18:VAL:HG11	7:O:64:CYS:HB2	2.00	0.43
7:Q:29:PHE:HE2	7:R:56:LEU:HD23	1.82	0.43
7:R:56:LEU:HD12	7:R:56:LEU:HA	1.87	0.43
1:B:381:ARG:NH2	1:B:486:ASP:O	2.51	0.43
1:C:174:GLY:O	1:C:177:SER:OG	2.25	0.43
2:E:411:LYS:HE2	2:E:452:ASP:HA	1.99	0.43
7:Q:45:GLN:O	7:Q:48:SER:OG	2.27	0.43
2:D:189:GLY:HA3	2:D:262:ARG:HG3	2.00	0.43
2:D:369:HIS:CE1	2:D:436:LEU:HD11	2.52	0.43
3:J:16:ARG:HH21	3:J:27:GLN:HG3	1.84	0.43
2:F:132:GLN:HB3	2:F:359:ILE:HG22	2.00	0.43
2:F:246:ARG:HD2	2:F:301:THR:HG22	2.01	0.43
1:B:258:ARG:NH1	1:B:308:ARG:O	2.52	0.43
1:A:113:ASN:OD1	1:A:113:ASN:N	2.51	0.43
2:D:383:TYR:CE1	2:D:406:VAL:HG13	2.52	0.43
2:E:369:HIS:HE2	2:E:436:LEU:HD11	1.83	0.43
5:H:127:SER:O	5:H:131:ILE:HG12	2.18	0.43
7:O:25:ILE:HD12	7:P:56:LEU:HG	2.01	0.43
1:A:336:ALA:O	1:A:340:THR:OG1	2.36	0.43
1:C:179:ALA:HB1	1:C:267:ILE:HG12	2.01	0.43
2:D:47:LEU:HD11	2:D:64:ALA:HB1	2.01	0.43
2:D:50:GLU:HG2	2:D:65:MET:HE3	1.99	0.43
4:G:48:SER:HB2	4:G:211:ASN:OD1	2.18	0.43
2:E:222:GLY:CA	2:E:234:VAL:HG21	2.49	0.43
7:Q:64:CYS:HB2	7:M:19:ALA:HB2	2.00	0.43
1:B:211:SER:O	1:B:215:GLN:HG2	2.19	0.43
1:C:358:TYR:O	2:F:378:LYS:HA	2.19	0.43
4:G:37:ASP:HA	4:G:40:PRO:HD2	1.99	0.43
7:O:42:LEU:HB2	7:O:46:LEU:HD13	2.01	0.43
1:A:403:PHE:O	1:A:407:GLY:N	2.52	0.42
2:D:18:VAL:HG13	2:D:23:VAL:HG22	2.00	0.42
2:E:114:GLN:OE1	2:E:114:GLN:N	2.50	0.42
5:H:62:LEU:HD11	5:H:144:ALA:HB2	2.01	0.42
1:B:457:GLU:HG2	1:B:458:PRO:HD2	2.01	0.42
1:C:27:GLU:CD	1:C:27:GLU:H	2.26	0.42
2:E:358:ARG:HD2	1:B:172:GLN:HE22	1.83	0.42
4:G:105:ILE:O	4:G:124:PHE:HA	2.19	0.42
5:H:114:LYS:O	5:H:118:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:30:GLY:O	7:M:31:SER:OG	2.31	0.42
7:R:17:GLY:HA3	7:R:64:CYS:SG	2.60	0.42
1:B:147:GLN:O	1:B:186:GLN:NE2	2.52	0.42
4:G:9:ARG:O	4:G:13:ILE:HG13	2.19	0.42
7:P:58:GLU:O	7:P:62:LEU:HG	2.20	0.42
1:B:414:THR:O	1:B:418:LEU:HG	2.19	0.42
1:A:47:VAL:HG12	1:A:66:LEU:HD21	2.01	0.42
1:C:80:LYS:HD3	1:C:80:LYS:HA	1.84	0.42
2:F:79:ASP:OD1	2:F:80:SER:N	2.52	0.42
2:D:312:ILE:HD11	2:D:331:LEU:HD11	2.01	0.42
2:D:347:TYR:HB3	10:D:501:ADP:N6	2.34	0.42
2:E:153:LYS:HD2	2:E:298:ILE:HB	2.02	0.42
4:G:45:GLY:O	4:G:49:LEU:HG	2.19	0.42
1:A:196:LYS:HE2	1:A:196:LYS:HB2	1.91	0.42
1:A:423:ARG:HH22	1:A:458:PRO:HD3	1.84	0.42
1:C:27:GLU:HG2	1:C:46:ASN:HD22	1.84	0.42
2:D:83:PRO:HB2	2:D:117:ALA:HB1	2.02	0.42
2:F:31:LEU:HD11	2:F:58:SER:C	2.44	0.42
4:G:101:LYS:H	4:G:101:LYS:HG2	1.55	0.42
4:G:186:SER:HA	4:G:190:MET:HG3	2.00	0.42
4:G:262:LEU:HD13	4:G:262:LEU:HA	1.76	0.42
5:H:34:ARG:HG3	5:H:68:GLU:HG2	2.00	0.42
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.77	0.42
1:B:397:TYR:HB2	1:B:421:GLY:HA3	2.02	0.42
1:C:497:LEU:O	1:C:501:VAL:HG23	2.20	0.42
2:E:151:GLY:HA3	2:E:300:THR:OG1	2.20	0.42
4:G:90:LYS:HA	4:G:93:VAL:HG22	2.02	0.42
7:N:3:ASP:OD1	7:N:3:ASP:N	2.51	0.42
1:A:182:THR:O	1:A:186:GLN:HG2	2.20	0.42
1:A:351:PHE:CD2	1:A:369:LEU:HD12	2.55	0.42
1:C:458:PRO:HA	1:C:461:ILE:CD1	2.49	0.42
2:E:459:PHE:HE1	2:E:465:ILE:HD11	1.84	0.42
2:F:314:VAL:HG12	2:F:324:PRO:HB3	2.01	0.42
5:H:36:VAL:HG12	5:H:38:VAL:HG13	2.00	0.42
7:K:6:ALA:HA	7:K:9:ILE:HG22	2.02	0.42
1:B:44:LEU:HB3	1:B:47:VAL:HG23	2.02	0.42
1:A:492:GLU:CD	1:A:492:GLU:H	2.27	0.42
2:D:14:ARG:NH2	2:D:26:GLN:OE1	2.45	0.42
2:E:98:ASN:ND2	2:E:100:ILE:HG12	2.35	0.42
2:E:358:ARG:HH22	8:B:601:ATP:PG	2.42	0.42
1:A:59:LEU:HD11	1:A:81:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LEU:HD13	1:C:414:THR:HG21	2.02	0.42
2:D:243:GLU:OE2	2:D:297:ARG:HB3	2.20	0.42
2:F:17:ALA:HA	1:B:66:LEU:O	2.19	0.42
2:F:254:LEU:HD22	2:F:307:THR:HB	2.02	0.42
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.02	0.42
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.49	0.42
1:A:208:GLN:NE2	1:A:269:ASP:HB3	2.35	0.41
1:C:351:PHE:HD1	1:C:370:SER:HA	1.85	0.41
1:C:353:GLU:OE2	1:C:366:ASN:ND2	2.53	0.41
2:E:99:VAL:HG11	2:E:230:ALA:HB1	2.02	0.41
2:F:26:GLN:HA	2:F:59:THR:HA	2.01	0.41
6:I:33:ASN:O	6:I:37:THR:HG23	2.20	0.41
7:L:19:ALA:HB2	7:N:17:GLY:HA2	2.01	0.41
1:A:140:ILE:HG12	1:A:143:ARG:HH22	1.85	0.41
2:E:153:LYS:HG2	2:E:295:GLN:OE1	2.20	0.41
7:K:56:LEU:HD13	7:K:56:LEU:HA	1.82	0.41
7:L:5:ALA:O	7:L:9:ILE:HG13	2.19	0.41
1:B:140:ILE:HD13	1:B:143:ARG:HH12	1.85	0.41
1:C:476:HIS:CE1	1:C:500:ILE:HG12	2.56	0.41
2:D:259:ASN:H	2:D:311:ALA:HB3	1.85	0.41
2:E:168:ILE:O	2:E:172:ILE:HG13	2.20	0.41
2:F:203:ILE:HD13	2:F:210:LEU:HD11	2.02	0.41
5:H:18:PHE:HD1	5:H:90:VAL:HG13	1.84	0.41
7:R:62:LEU:O	7:R:66:MET:HG2	2.20	0.41
1:B:163:GLN:HG3	1:B:347:ASP:HB2	2.03	0.41
1:C:201:CYS:O	1:C:229:THR:HA	2.19	0.41
1:C:249:SER:O	1:C:253:MET:HG3	2.21	0.41
2:D:14:ARG:NH1	2:D:28:ASP:OD1	2.52	0.41
2:D:441:LYS:HE3	2:D:441:LYS:HB3	1.91	0.41
2:E:280:ALA:C	2:E:282:GLY:H	2.28	0.41
4:G:242:MET:HE3	4:G:242:MET:HB2	1.89	0.41
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.92	0.41
1:B:291:ARG:HH22	1:B:336:ALA:HA	1.85	0.41
2:D:31:LEU:HD12	2:D:32:PRO:HD2	2.03	0.41
7:P:3:ASP:OD1	7:P:3:ASP:N	2.53	0.41
7:R:25:ILE:HD13	7:R:58:GLU:OE2	2.21	0.41
1:C:415:GLN:HA	1:C:418:LEU:HG	2.01	0.41
2:D:27:PHE:HB2	2:D:31:LEU:HD12	2.02	0.41
2:F:222:GLY:HA3	2:F:234:VAL:HG11	2.01	0.41
4:G:192:ILE:HG13	7:R:40:PRO:HD2	2.02	0.41
5:H:40:THR:HG21	5:H:56:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:43:LYS:HE3	7:P:43:LYS:HB2	1.90	0.41
1:A:148:THR:HG23	1:A:182:THR:OG1	2.21	0.41
2:F:33:PRO:O	2:F:36:ASN:HB2	2.20	0.41
2:F:170:GLU:HG3	2:F:420:PHE:CD2	2.56	0.41
6:I:27:LYS:O	6:I:31:LYS:N	2.53	0.41
1:A:408:SER:O	1:A:415:GLN:NE2	2.54	0.41
1:C:373:ARG:HE	1:C:373:ARG:HB3	1.62	0.41
2:D:332:ASP:HA	2:D:358:ARG:HE	1.86	0.41
4:G:259:THR:O	4:G:263:ILE:HG13	2.21	0.41
7:L:18:VAL:O	7:L:21:SER:HB3	2.21	0.41
7:M:44:GLN:H	7:M:44:GLN:HG2	1.65	0.41
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.90	0.41
1:A:101:GLU:HG3	1:A:256:TYR:HE2	1.86	0.41
1:C:28:THR:OG1	1:C:87:ILE:HG23	2.20	0.41
1:C:452:TYR:HD2	1:C:501:VAL:HG11	1.86	0.41
2:D:185:PHE:HA	2:D:256:PHE:O	2.20	0.41
2:D:257:ILE:HG21	2:D:260:ILE:HD13	2.03	0.41
2:D:398:LEU:HB3	2:D:402:ASP:HB2	2.01	0.41
2:F:260:ILE:HD12	2:F:260:ILE:HA	1.92	0.41
5:H:133:ILE:HD12	6:I:14:TYR:CE1	2.56	0.41
7:N:36:TYR:CZ	7:O:42:LEU:HD13	2.56	0.41
7:P:54:PHE:CE1	7:M:56:LEU:HD11	2.56	0.41
1:B:182:THR:O	1:B:186:GLN:HG2	2.21	0.41
1:B:271:LEU:HD23	1:B:271:LEU:HA	1.80	0.41
1:B:356:LEU:HD22	1:B:361:ILE:HD12	2.01	0.41
1:B:450:ARG:HB2	1:B:452:TYR:CE2	2.56	0.41
1:C:366:ASN:HD21	1:C:369:LEU:HD13	1.86	0.41
2:E:47:LEU:HD11	2:E:64:ALA:HB1	2.03	0.41
2:E:222:GLY:HA3	2:E:234:VAL:HG21	2.03	0.41
2:F:224:MET:HG3	1:B:307:GLU:HG3	2.03	0.41
10:F:501:ADP:O3'	1:B:373:ARG:HD3	2.21	0.41
5:H:57:VAL:HB	6:I:11:TYR:CZ	2.55	0.41
7:L:8:PHE:CE2	7:N:7:LYS:HE3	2.56	0.41
1:C:59:LEU:HD13	1:C:59:LEU:HA	1.90	0.40
2:D:144:LEU:HD22	2:D:443:PHE:CD2	2.56	0.40
2:F:252:ASP:OD1	2:F:252:ASP:N	2.54	0.40
2:F:314:VAL:HG12	2:F:324:PRO:CB	2.51	0.40
4:G:67:LEU:HD23	4:G:104:LYS:O	2.21	0.40
6:I:2:ALA:HB3	6:I:4:TRP:NE1	2.35	0.40
7:O:18:VAL:HB	7:O:61:GLY:O	2.21	0.40
7:O:60:MET:HE3	7:O:60:MET:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:65:LEU:HG	7:R:63:PHE:CE2	2.57	0.40
1:A:174:GLY:H	8:A:601:ATP:PB	2.44	0.40
1:C:104:LEU:HD23	1:C:230:ILE:HG13	2.04	0.40
2:D:236:LEU:HA	2:D:239:LEU:HG	2.03	0.40
2:D:294:MET:HE2	2:D:294:MET:HB3	1.92	0.40
2:D:387:GLN:HG2	3:J:30:GLU:OE2	2.21	0.40
2:D:391:ALA:O	3:J:25:LYS:NZ	2.47	0.40
2:F:423:ALA:O	2:F:427:THR:HG22	2.21	0.40
2:F:435:PRO:O	2:F:439:THR:HG23	2.21	0.40
6:I:4:TRP:H	6:I:4:TRP:CD1	2.39	0.40
7:L:47:PHE:O	7:L:51:ILE:HG12	2.20	0.40
7:O:7:LYS:HD2	7:O:72:LEU:O	2.22	0.40
7:P:43:LYS:HD3	7:P:44:GLN:N	2.36	0.40
1:B:476:HIS:CE1	1:B:500:ILE:HG12	2.56	0.40
1:A:175:LYS:HE3	1:A:175:LYS:HB2	1.85	0.40
1:C:427:LEU:HG	1:C:444:VAL:HG22	2.03	0.40
2:D:165:THR:O	2:D:168:ILE:HG22	2.22	0.40
2:D:386:LEU:O	2:D:390:ILE:HG13	2.22	0.40
2:E:69:GLU:H	2:E:69:GLU:CD	2.29	0.40
2:E:454:LEU:HG	2:E:455:PRO:HD2	2.03	0.40
2:F:412:ILE:O	2:F:416:LEU:HG	2.21	0.40
5:H:112:LEU:HB2	5:H:138:ASN:HB3	2.03	0.40
7:L:4:THR:O	7:L:7:LYS:HB2	2.22	0.40
1:B:96:ASP:N	1:B:96:ASP:OD1	2.55	0.40
1:A:140:ILE:HG22	1:A:311:LYS:HG3	2.02	0.40
1:C:291:ARG:HG2	2:D:281:VAL:O	2.21	0.40
2:E:379:ILE:HD12	2:E:379:ILE:HA	1.88	0.40
2:F:158:GLY:C	2:F:314:VAL:HG22	2.46	0.40
4:G:128:PHE:CE2	4:G:144:ILE:HA	2.57	0.40
1:A:386:VAL:HB	1:A:445:ILE:HG22	2.03	0.40
1:A:454:ASP:OD1	1:A:455:LYS:N	2.54	0.40
1:C:453:LEU:HD21	1:C:464:PHE:CE1	2.56	0.40
2:D:260:ILE:HD11	2:D:294:MET:SD	2.61	0.40
2:E:157:PHE:HB2	2:E:336:VAL:HG12	2.03	0.40
7:L:25:ILE:HG21	7:N:56:LEU:HB3	2.03	0.40
1:B:422:VAL:O	1:B:426:GLU:HG2	2.21	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	487/550 (88%)	482 (99%)	5 (1%)	0	100	100
1	B	487/550 (88%)	478 (98%)	9 (2%)	0	100	100
1	C	480/550 (87%)	469 (98%)	11 (2%)	0	100	100
2	D	468/570 (82%)	454 (97%)	13 (3%)	1 (0%)	43	71
2	E	465/570 (82%)	452 (97%)	12 (3%)	1 (0%)	43	71
2	F	465/570 (82%)	451 (97%)	14 (3%)	0	100	100
3	J	51/108 (47%)	51 (100%)	0	0	100	100
4	G	270/273 (99%)	261 (97%)	8 (3%)	1 (0%)	30	60
5	H	130/168 (77%)	124 (95%)	6 (5%)	0	100	100
6	I	46/136 (34%)	44 (96%)	2 (4%)	0	100	100
7	K	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
7	L	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
7	M	70/141 (50%)	70 (100%)	0	0	100	100
7	N	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
7	O	70/141 (50%)	70 (100%)	0	0	100	100
7	P	70/141 (50%)	70 (100%)	0	0	100	100
7	Q	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
7	R	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
All	All	3909/5173 (76%)	3819 (98%)	87 (2%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	281	VAL
4	G	60	PRO
2	D	281	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	394/443 (89%)	380 (96%)	14 (4%)	31	59
1	B	394/443 (89%)	380 (96%)	14 (4%)	31	59
1	C	388/443 (88%)	371 (96%)	17 (4%)	25	54
2	D	378/452 (84%)	367 (97%)	11 (3%)	37	63
2	E	375/452 (83%)	351 (94%)	24 (6%)	16	42
2	F	375/452 (83%)	362 (96%)	13 (4%)	32	60
3	J	35/85 (41%)	35 (100%)	0	100	100
4	G	230/231 (100%)	214 (93%)	16 (7%)	14	39
5	H	105/127 (83%)	100 (95%)	5 (5%)	23	52
6	I	38/109 (35%)	37 (97%)	1 (3%)	40	66
7	K	49/103 (48%)	43 (88%)	6 (12%)	5	19
7	L	49/103 (48%)	45 (92%)	4 (8%)	10	34
7	M	48/103 (47%)	45 (94%)	3 (6%)	16	43
7	N	48/103 (47%)	43 (90%)	5 (10%)	7	25
7	O	48/103 (47%)	42 (88%)	6 (12%)	4	18
7	P	49/103 (48%)	45 (92%)	4 (8%)	10	34
7	Q	49/103 (48%)	46 (94%)	3 (6%)	17	44
7	R	48/103 (47%)	45 (94%)	3 (6%)	16	43
All	All	3100/4061 (76%)	2951 (95%)	149 (5%)	24	52

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	47	VAL
1	A	71	VAL
1	A	73	VAL
1	A	95	VAL
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	173	THR
1	A	206	ILE
1	A	216	LEU
1	A	226	MET
1	A	301	LEU
1	A	334	VAL
1	A	410	LEU
1	A	462	THR
1	C	59	LEU
1	C	95	VAL
1	C	99	VAL
1	C	108	VAL
1	C	157	VAL
1	C	206	ILE
1	C	297	ASP
1	C	301	LEU
1	C	389	THR
1	C	410	LEU
1	C	426	GLU
1	C	427	LEU
1	C	454	ASP
1	C	456	LEU
1	C	489	ILE
1	C	492	GLU
1	C	497	LEU
2	D	72	VAL
2	D	130	VAL
2	D	136	VAL
2	D	141	VAL
2	D	207	VAL
2	D	217	VAL
2	D	253	VAL
2	D	264	THR
2	D	281	VAL
2	D	300	THR
2	D	327	THR
2	E	12	THR
2	E	14	ARG
2	E	23	VAL
2	E	28	ASP
2	E	36	ASN
2	E	48	VAL

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Mol	Chain	Res	Type
2	E	60	VAL
2	E	65	MET
2	E	68	THR
2	E	77	VAL
2	E	88	VAL
2	E	91	GLU
2	E	134	ILE
2	E	136	VAL
2	E	141	VAL
2	E	208	ILE
2	E	214	THR
2	E	217	VAL
2	E	253	VAL
2	E	281	VAL
2	E	336	VAL
2	E	377	GLN
2	E	397	GLU
2	E	454	LEU
2	F	88	VAL
2	F	126	MET
2	F	141	VAL
2	F	207	VAL
2	F	212	ASP
2	F	217	VAL
2	F	234	VAL
2	F	253	VAL
2	F	258	ASP
2	F	264	THR
2	F	317	ASP
2	F	365	VAL
2	F	396	ASP
4	G	56	ASP
4	G	59	VAL
4	G	65	LYS
4	G	67	LEU
4	G	71	VAL
4	G	74	ASP
4	G	106	VAL
4	G	108	VAL
4	G	125	LEU
4	G	137	THR
4	G	169	ILE

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Mol	Chain	Res	Type
4	G	190	MET
4	G	196	ILE
4	G	200	VAL
4	G	211	ASN
4	G	262	LEU
5	H	25	GLN
5	H	48	LEU
5	H	65	VAL
5	H	84	VAL
5	H	90	VAL
6	I	1	VAL
7	K	16	VAL
7	K	18	VAL
7	K	42	LEU
7	K	54	PHE
7	K	56	LEU
7	K	64	CYS
7	L	34	ILE
7	L	42	LEU
7	L	64	CYS
7	L	71	ILE
7	N	18	VAL
7	N	56	LEU
7	N	58	GLU
7	N	65	LEU
7	N	66	MET
7	O	9	ILE
7	O	18	VAL
7	O	29	PHE
7	O	43	LYS
7	O	44	GLN
7	O	46	LEU
7	P	25	ILE
7	P	43	LYS
7	P	52	LEU
7	P	60	MET
7	Q	18	VAL
7	Q	45	GLN
7	Q	65	LEU
7	R	18	VAL
7	R	43	LYS
7	R	46	LEU

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Mol	Chain	Res	Type
7	M	15	THR
7	M	18	VAL
7	M	62	LEU
1	B	47	VAL
1	B	71	VAL
1	B	73	VAL
1	B	113	ASN
1	B	180	ILE
1	B	206	ILE
1	B	209	LYS
1	B	216	LEU
1	B	226	MET
1	B	245	LEU
1	B	301	LEU
1	B	410	LEU
1	B	462	THR
1	B	483	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	46	ASN
1	A	416	GLN
1	C	46	ASN
1	C	48	GLN
1	C	186	GLN
1	C	330	GLN
1	C	341	ASN
1	C	366	ASN
1	C	441	GLN
1	C	466	ASN
1	C	476	HIS
2	D	173	ASN
2	D	196	ASN
2	D	200	HIS
2	D	209	ASN
2	D	251	GLN
2	D	259	ASN
2	D	381	GLN
2	D	479	HIS
2	E	36	ASN

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Mol	Chain	Res	Type
2	E	330	HIS
2	E	363	ASN
2	F	173	ASN
2	F	225	ASN
2	F	295	GLN
4	G	66	HIS
4	G	82	HIS
4	G	95	ASN
4	G	150	ASN
4	G	163	ASN
4	G	211	ASN
4	G	234	ASN
5	H	32	ASN
5	H	138	ASN
6	I	6	GLN
6	I	41	ASN
7	K	44	GLN
7	L	44	GLN
7	N	44	GLN
7	P	39	ASN
7	P	45	GLN
7	Q	39	ASN
1	B	476	HIS
1	B	503	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
8	ATP	B	601	-	32,33,33	0.41	0	48,52,52	0.30	0
8	ATP	A	601	9	32,33,33	0.37	0	48,52,52	0.41	0
10	ADP	F	501	9	28,29,29	1.38	5 (17%)	43,45,45	1.76	8 (18%)
10	ADP	D	501	9	28,29,29	1.39	4 (14%)	43,45,45	1.84	10 (23%)
8	ATP	C	601	9	32,33,33	0.57	1 (3%)	48,52,52	0.34	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
8	ATP	B	601	-	-	0/22/38/38	0/3/3/3
8	ATP	A	601	9	-	5/22/38/38	0/3/3/3
10	ADP	F	501	9	-	6/16/32/32	0/3/3/3
10	ADP	D	501	9	-	6/16/32/32	0/3/3/3
8	ATP	C	601	9	-	1/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	501	ADP	C5-C4	4.49	1.47	1.39
10	D	501	ADP	C5-C4	4.48	1.47	1.39
10	D	501	ADP	C5-C6	2.68	1.48	1.41
8	C	601	ATP	PB-O3B	-2.62	1.56	1.59
10	F	501	ADP	C5-C6	2.53	1.48	1.41
10	D	501	ADP	C8-N7	2.49	1.36	1.31
10	F	501	ADP	C5-N7	-2.36	1.34	1.39
10	F	501	ADP	C8-N7	2.24	1.36	1.31
10	D	501	ADP	C5-N7	-2.20	1.35	1.39
10	F	501	ADP	C4-N9	-2.03	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	501	ADP	C5-C4-N3	-5.90	118.59	126.72
10	F	501	ADP	C5-C4-N3	-5.76	118.79	126.72
10	F	501	ADP	N3-C4-N9	4.57	134.94	127.17
10	D	501	ADP	N3-C4-N9	4.33	134.53	127.17
10	D	501	ADP	C2-N3-C4	3.70	120.86	111.83
10	D	501	ADP	C4-C5-N7	-3.64	106.42	110.58
10	F	501	ADP	C2-N3-C4	3.50	120.38	111.83
10	D	501	ADP	N3-C2-N1	-3.12	123.86	128.58
10	F	501	ADP	C4-C5-N7	-3.06	107.08	110.58
10	F	501	ADP	N3-C2-N1	-2.94	124.14	128.58
10	F	501	ADP	C2'-C1'-N9	-2.60	106.85	113.30
10	D	501	ADP	C2'-C1'-N9	-2.53	107.01	113.30
10	D	501	ADP	C5-N7-C8	2.46	107.31	103.45
10	F	501	ADP	C4-N9-C8	2.39	108.25	105.74
10	D	501	ADP	C4-N9-C8	2.25	108.10	105.74
10	D	501	ADP	C3'-C2'-C1'	2.17	105.57	101.46
10	D	501	ADP	C6-C5-N7	2.16	136.26	132.09
10	F	501	ADP	C5-N7-C8	2.10	106.75	103.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

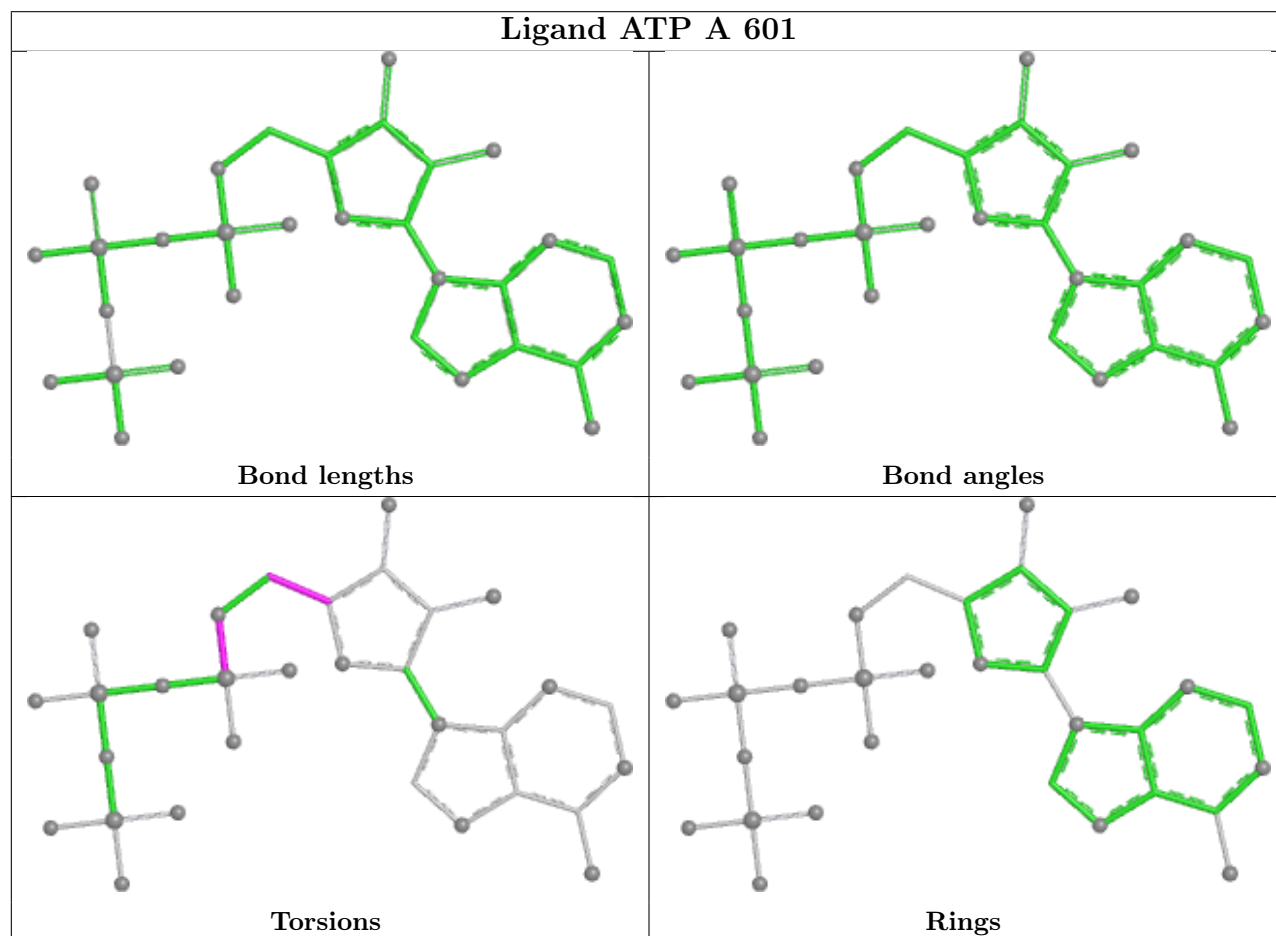
Mol	Chain	Res	Type	Atoms
8	A	601	ATP	C5'-O5'-PA-O1A
8	A	601	ATP	C5'-O5'-PA-O3A
10	D	501	ADP	C5'-O5'-PA-O1A
10	D	501	ADP	C5'-O5'-PA-O2A
10	D	501	ADP	C5'-O5'-PA-O3A
10	F	501	ADP	PA-O3A-PB-O3B
10	F	501	ADP	C5'-O5'-PA-O1A
10	F	501	ADP	C5'-O5'-PA-O2A
10	F	501	ADP	C5'-O5'-PA-O3A
10	D	501	ADP	O4'-C1'-N9-C8
8	A	601	ATP	O4'-C4'-C5'-O5'
10	D	501	ADP	O4'-C1'-N9-C4
8	A	601	ATP	C3'-C4'-C5'-O5'
8	A	601	ATP	C5'-O5'-PA-O2A
8	C	601	ATP	C5'-O5'-PA-O1A
10	D	501	ADP	PB-O3A-PA-O2A
10	F	501	ADP	PA-O3A-PB-O2B
10	F	501	ADP	O4'-C4'-C5'-O5'

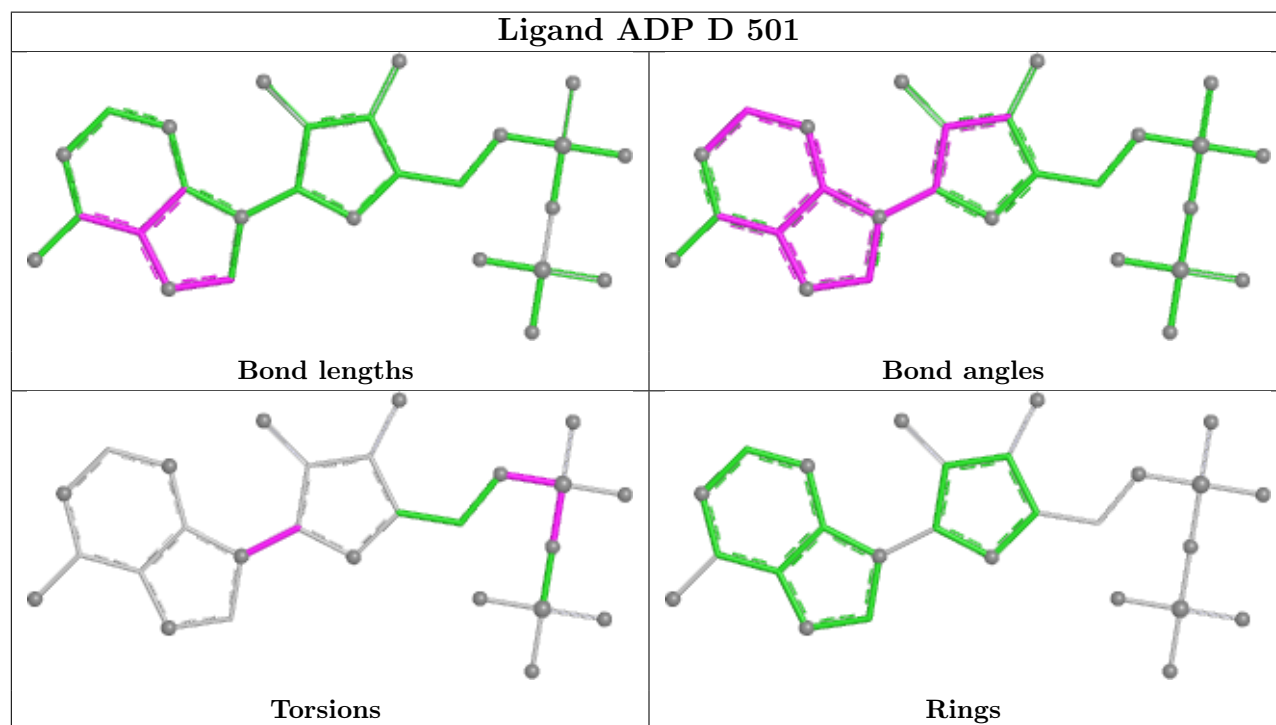
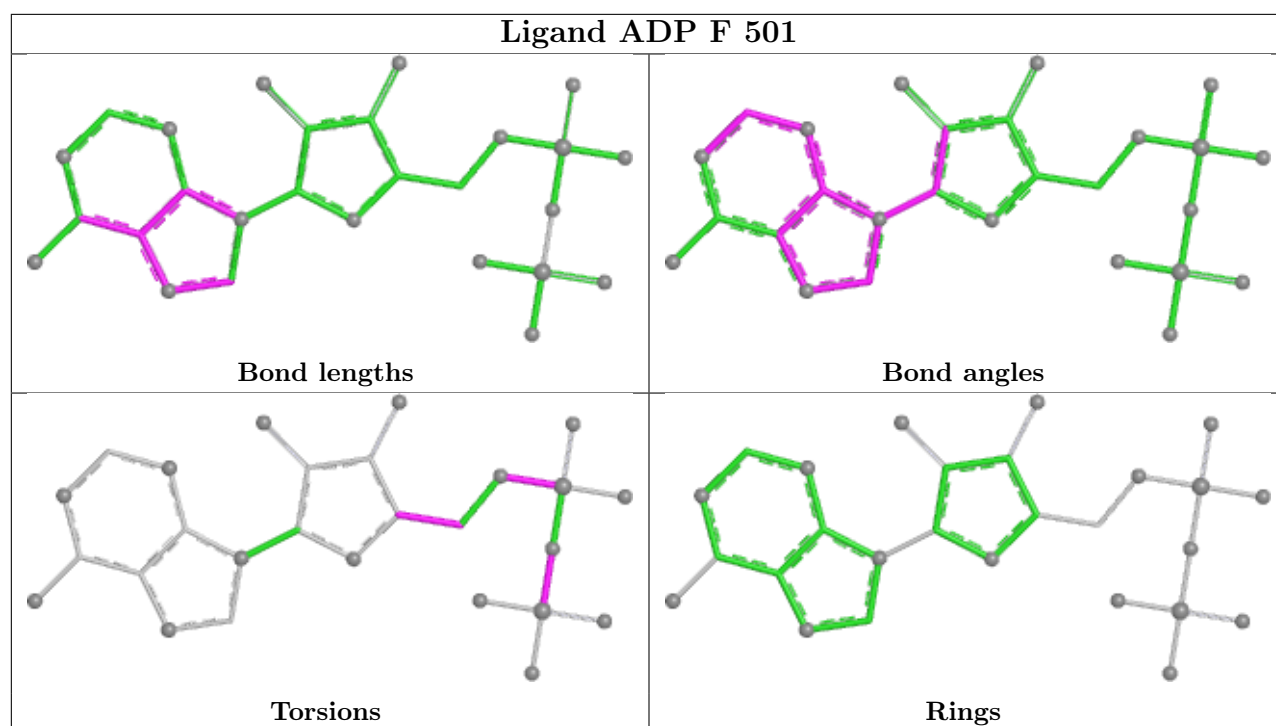
There are no ring outliers.

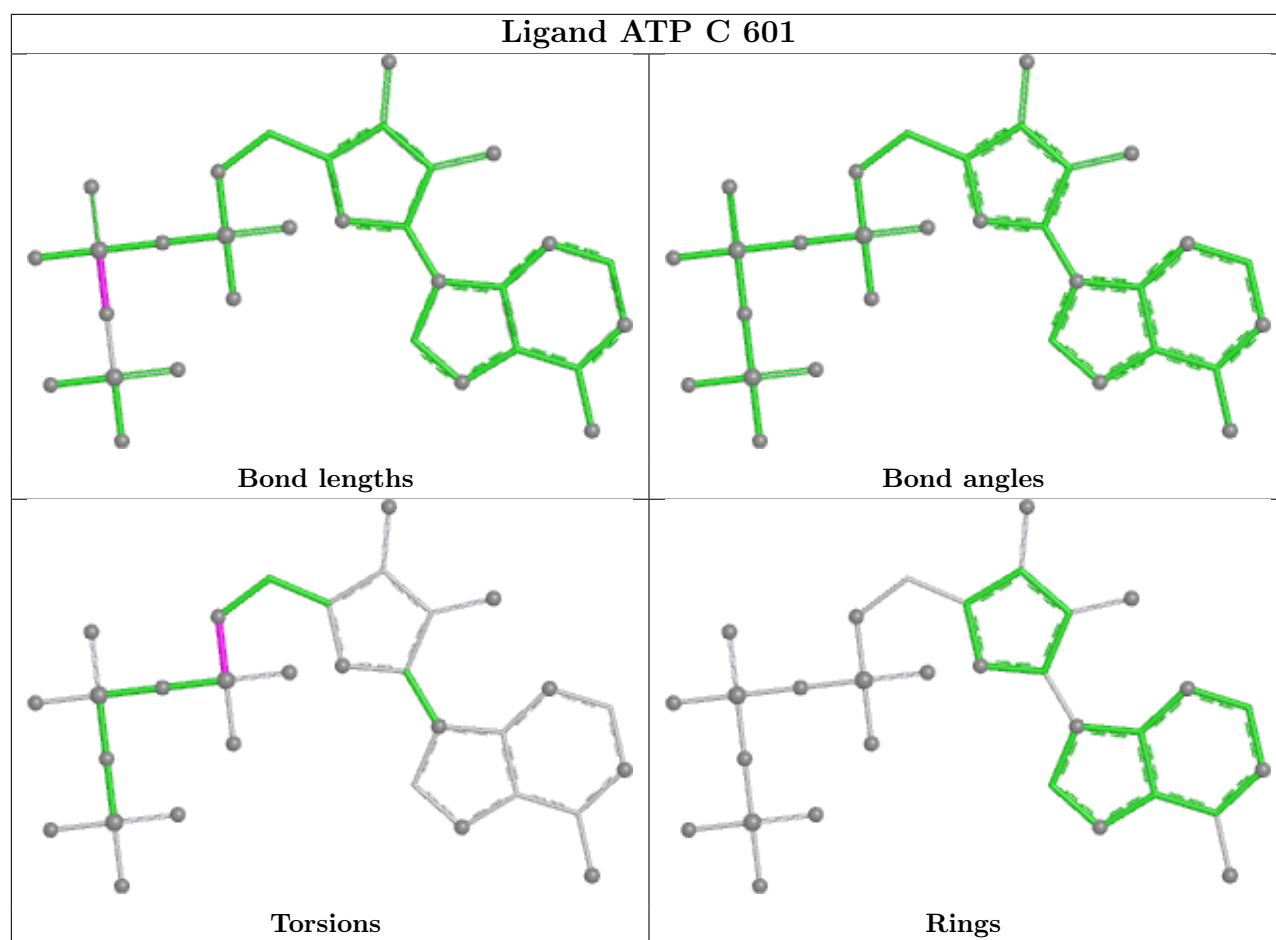
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	601	ATP	1	0
8	A	601	ATP	1	0
10	F	501	ADP	3	0
10	D	501	ADP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

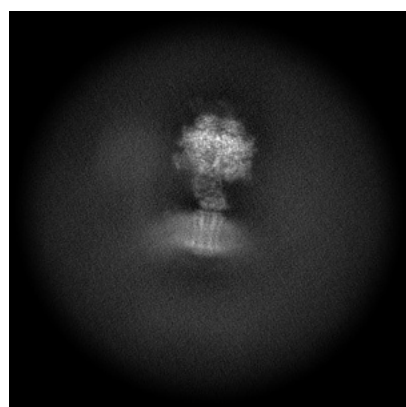
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45038. These allow visual inspection of the internal detail of the map and identification of artifacts.

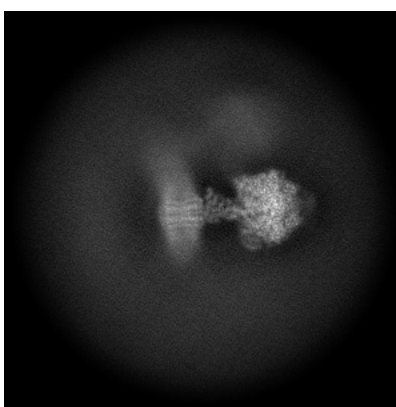
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

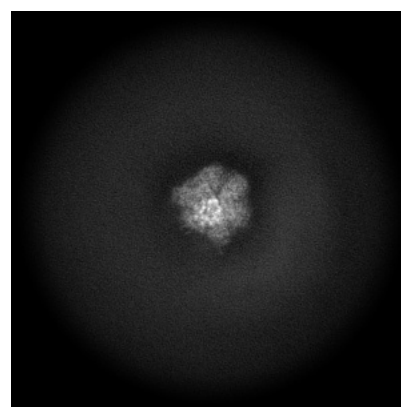
6.1.1 Primary map



X



Y

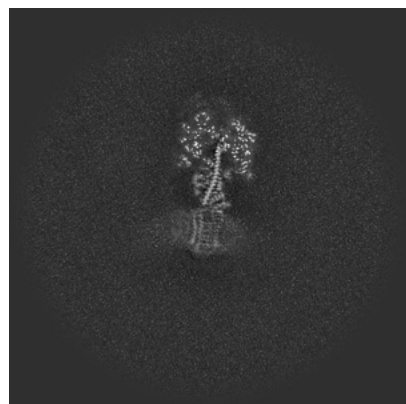


Z

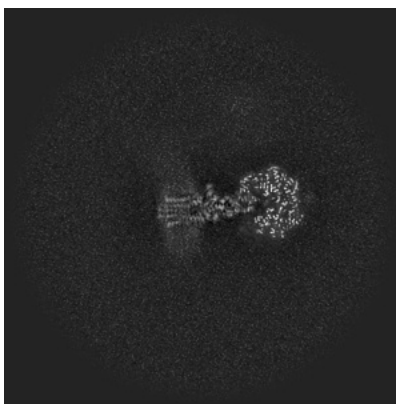
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

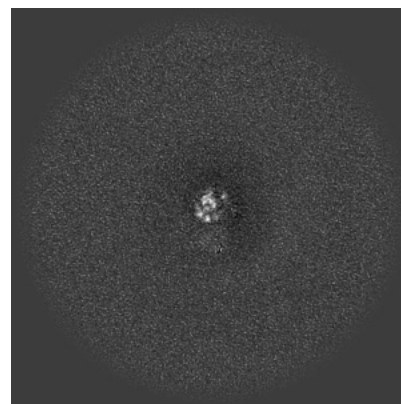
6.2.1 Primary map



X Index: 256



Y Index: 256

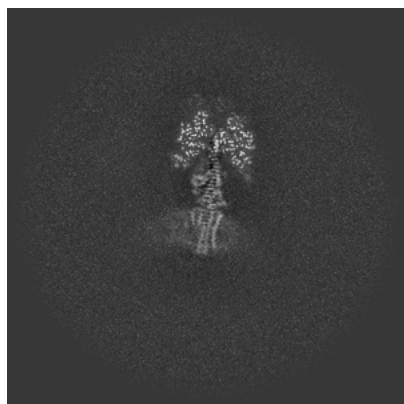


Z Index: 256

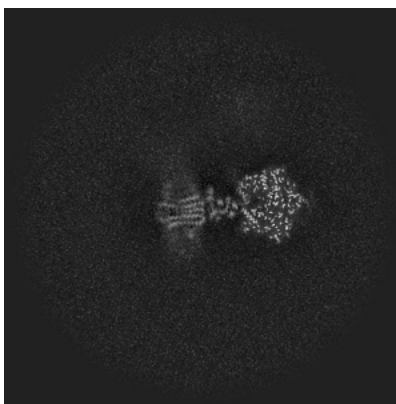
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

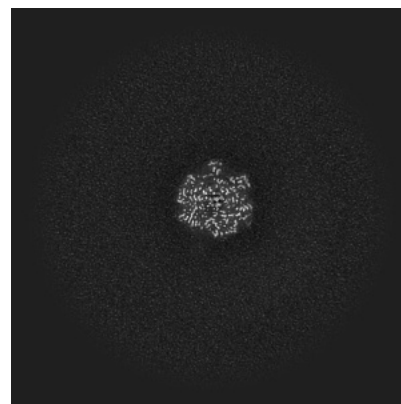
6.3.1 Primary map



X Index: 259



Y Index: 246

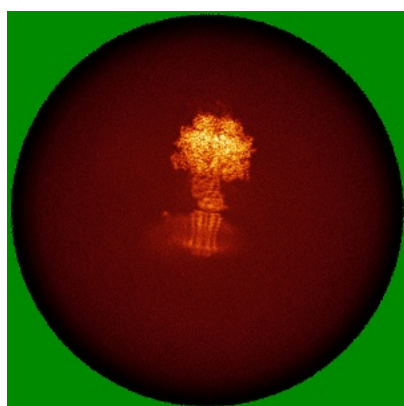


Z Index: 348

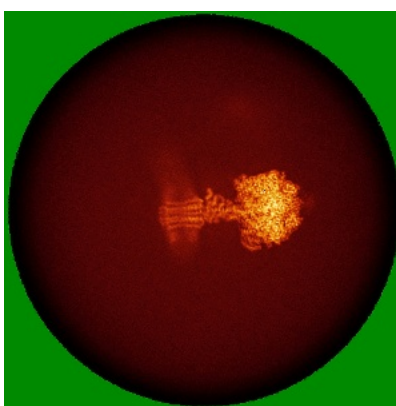
The images above show the largest variance slices of the map in three orthogonal directions.

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

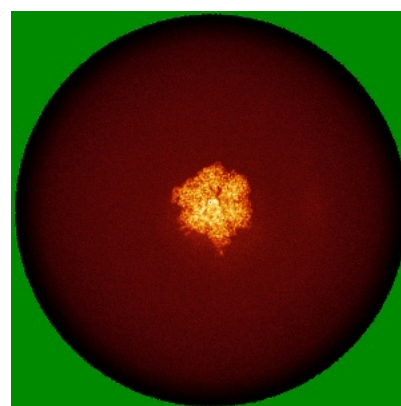
6.4.1 Primary map



X



Y

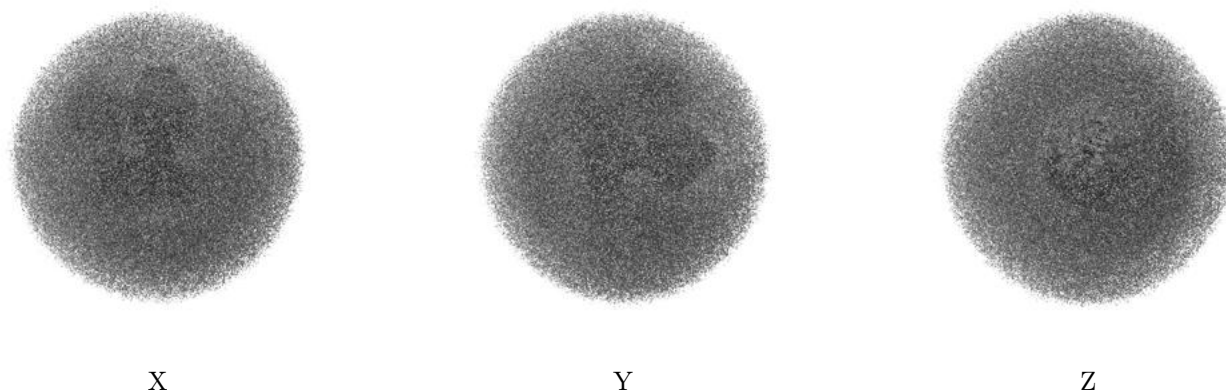


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

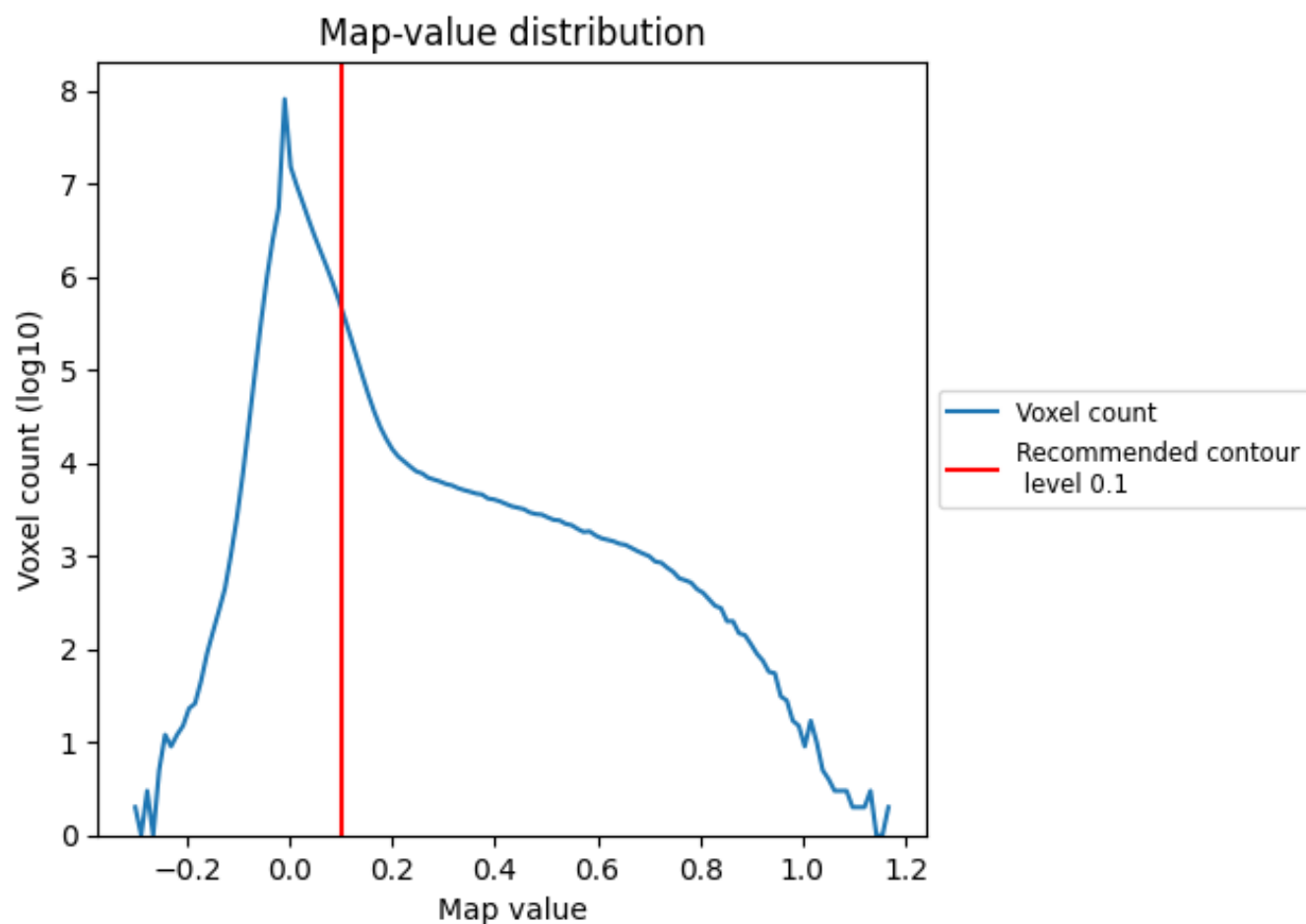
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

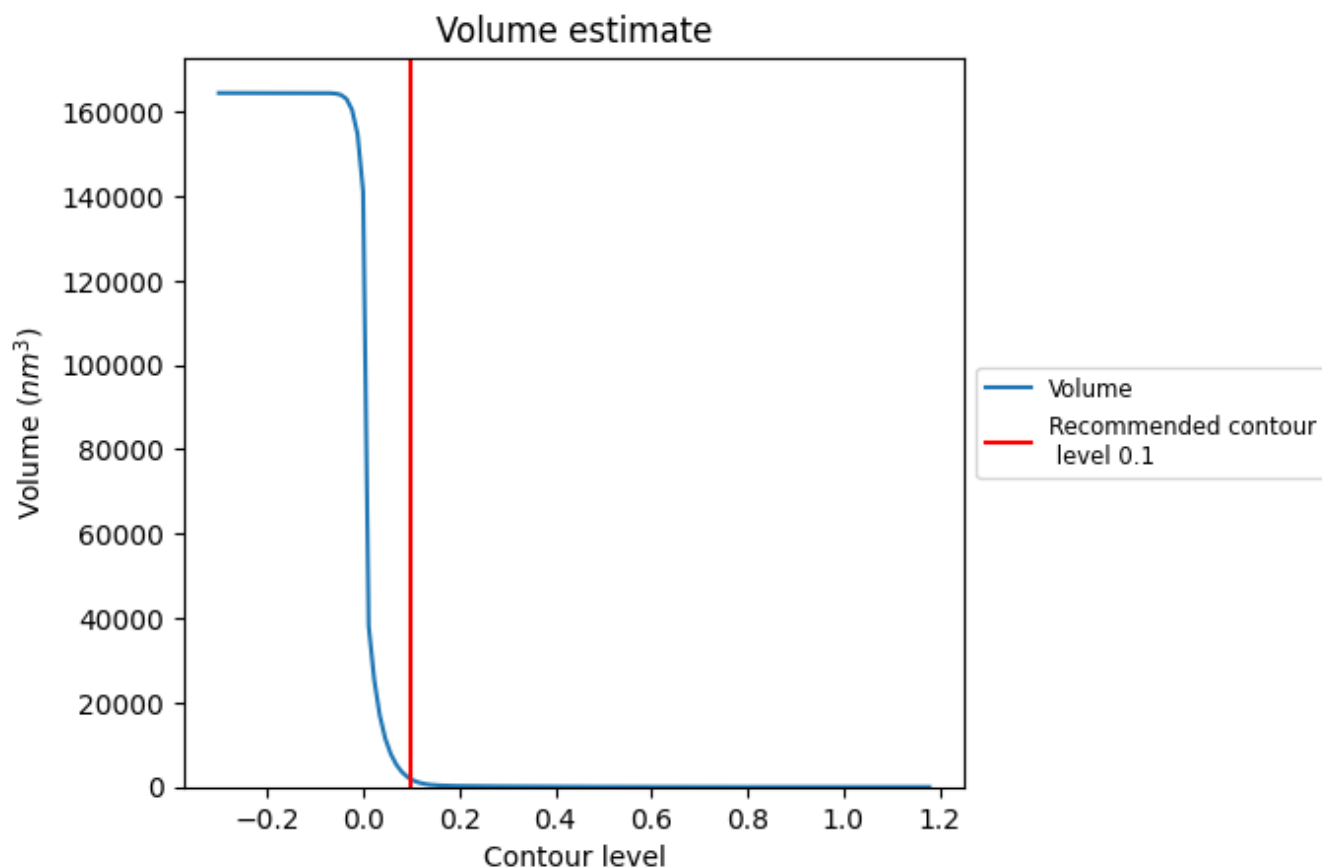
This section contains the results of statistical analysis of the map.

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.

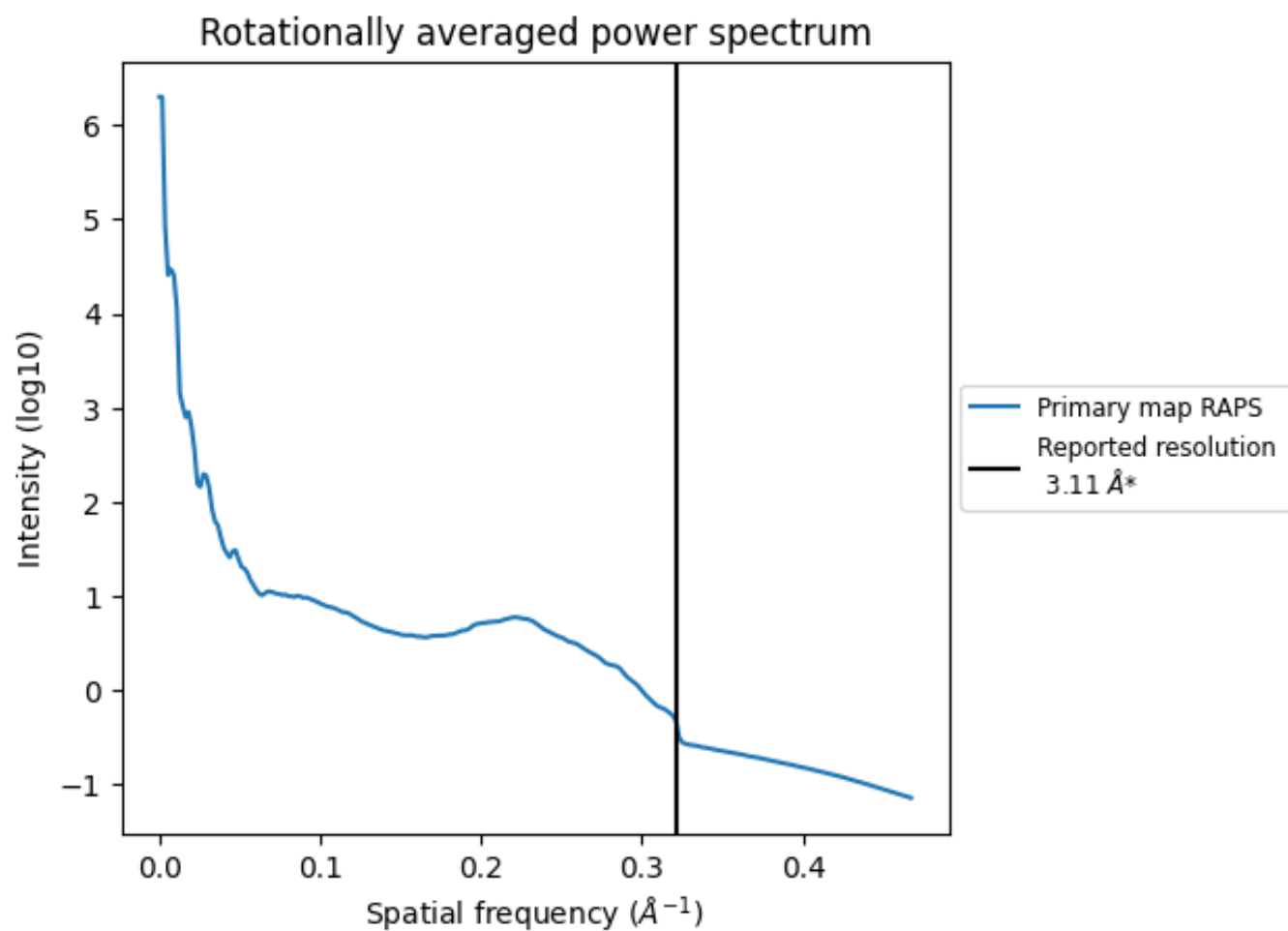
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1822 nm³; this corresponds to an approximate mass of 1646 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 0.322 Å⁻¹

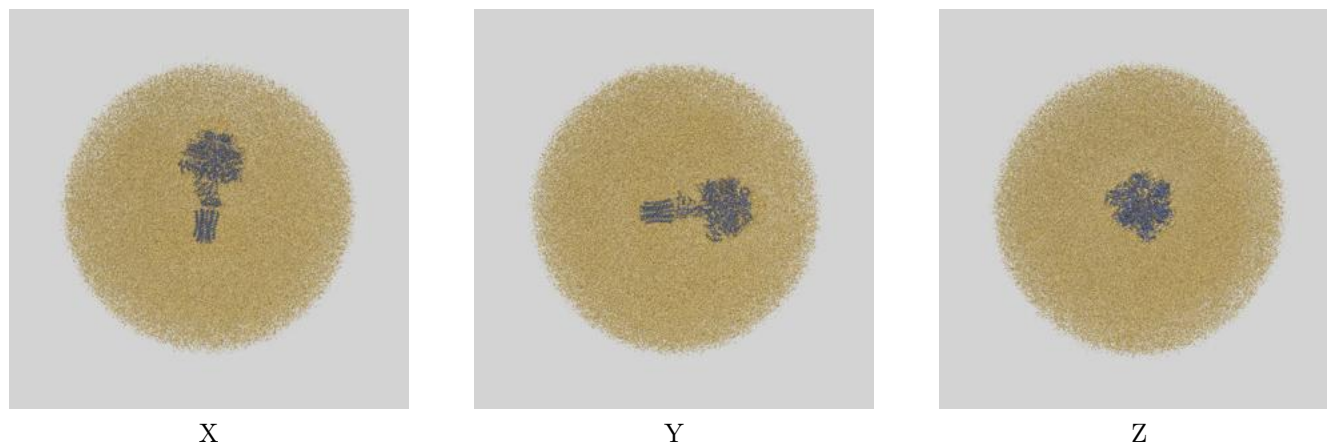
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

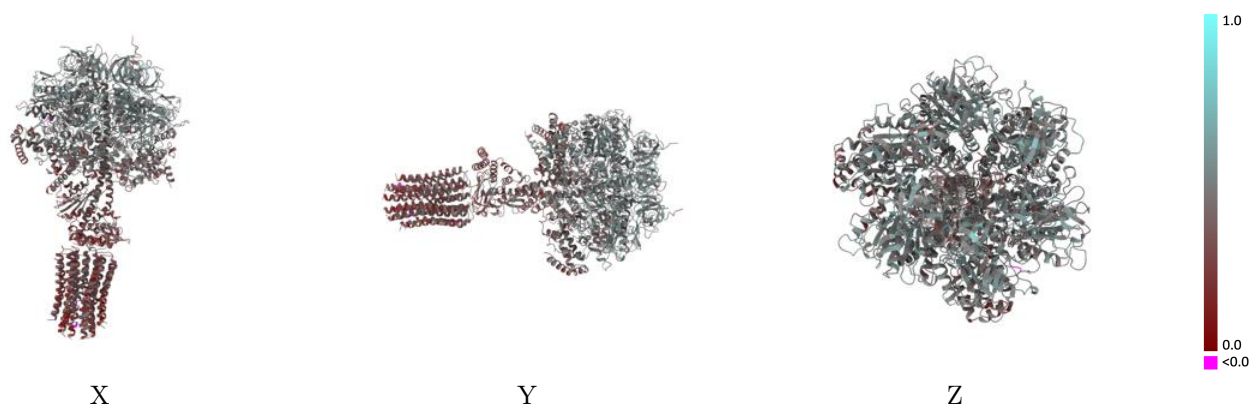
This section contains information regarding the fit between EMDB map EMD-45038 and PDB model 9BYM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



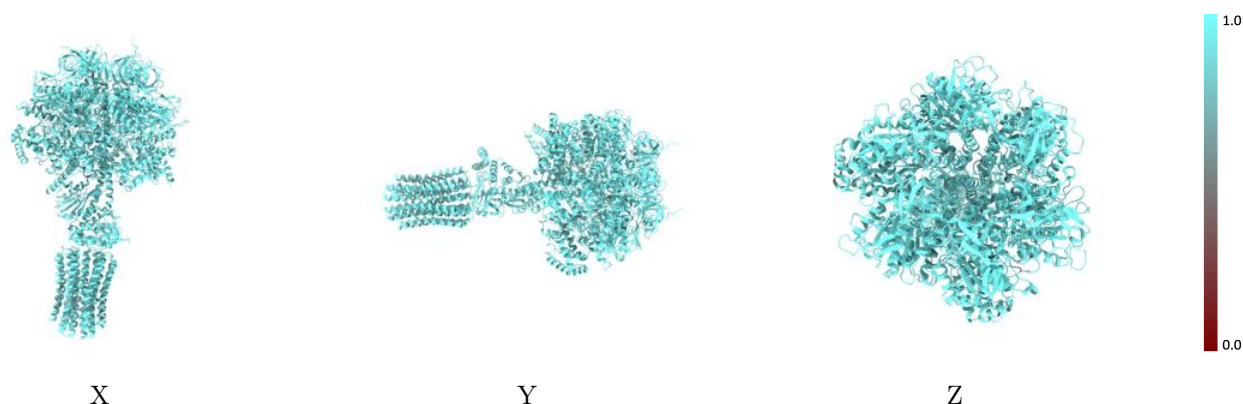
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



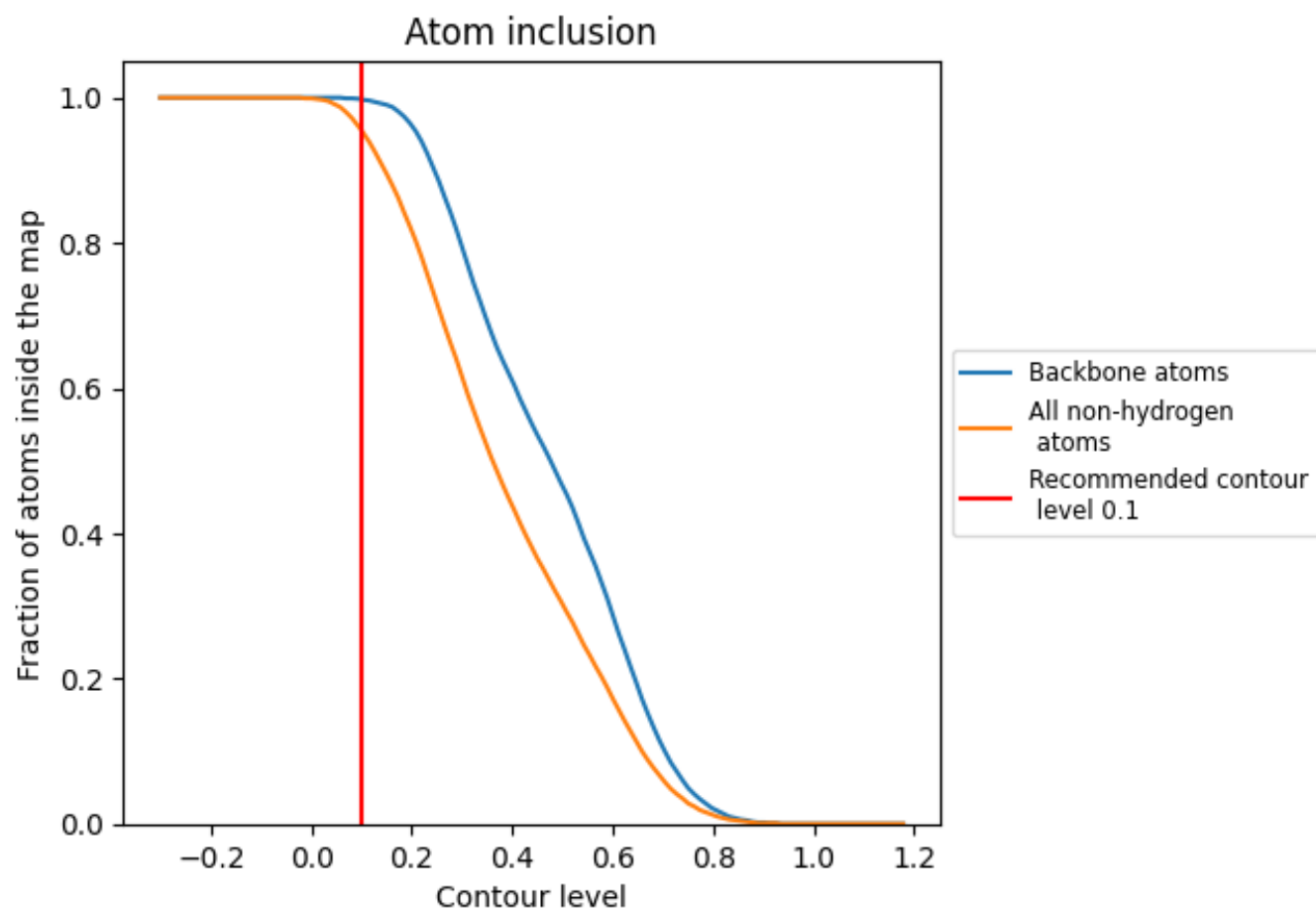
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.4360
A	 0.9690	 0.4790
B	 0.9610	 0.4600
C	 0.9630	 0.4640
D	 0.9620	 0.4830
E	 0.9670	 0.4780
F	 0.9720	 0.4900
G	 0.9370	 0.3650
H	 0.9380	 0.3320
I	 0.9050	 0.3080
J	 0.9200	 0.4290
K	 0.9230	 0.2930
L	 0.9120	 0.2760
M	 0.9310	 0.3030
N	 0.9190	 0.2800
O	 0.9110	 0.2960
P	 0.9060	 0.3130
Q	 0.9210	 0.2900
R	 0.9410	 0.3090

