



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:05 AM UTC

PDB ID : 6EF0 / pdb_00006ef0
EMDB ID : EMD-9042
Title : Yeast 26S proteasome bound to ubiquitinated substrate (1D* motor state)
Authors : de la Pena, A.H.; Goodall, E.A.; Gates, S.N.; Lander, G.C.; Martin, A.
Deposited on : 2018-08-15
Resolution : 4.43 Å(reported)
Based on initial model : 5MPC

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

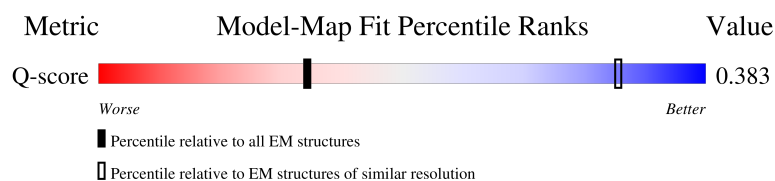
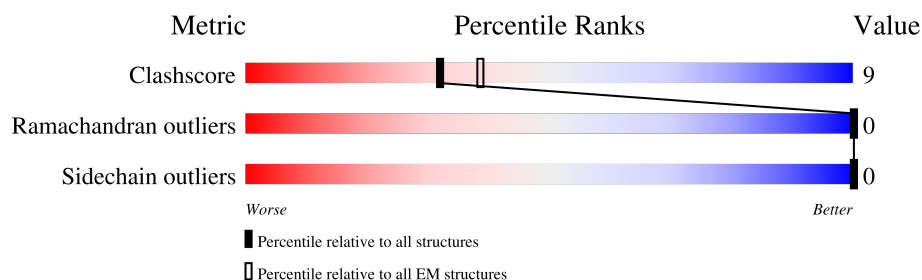
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.43 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	3083 (3.93 - 4.93)

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	238	
2	B	250	
3	C	244	
4	D	242	

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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	234	
7	G	246	
8	H	257	
9	I	271	
10	J	276	
11	K	272	
12	L	273	
13	M	258	
14	s	12	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 24748 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	238	Total	C	N	O	S	0	0
			1864	1187	314	356	7		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	250	Total	C	N	O	S	0	0
			1859	1186	312	358	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	244	Total	C	N	O	S	0	0
			1834	1163	311	356	4		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1856	1163	325	364	4		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	249	Total	C	N	O	S	0	0
			1885	1182	321	375	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	234	Total	C	N	O	S	0	0
			1783	1122	313	344	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	246	Total	C	N	O	S	0	0
			1868	1191	325	348	4		

- Molecule 8 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	257	Total	C	N	O	S	0	0
			1831	1158	320	345	8		

- Molecule 9 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	271	Total	C	N	O	S	0	0
			1913	1198	317	388	10		

- Molecule 10 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	272	Total	C	N	O	S	0	0
			2005	1257	362	371	15		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	272	Total	C	N	O	S	0	0
			2016	1264	358	386	8		

- Molecule 12 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	273	Total	C	N	O	S	0	0
			2057	1310	352	385	10		

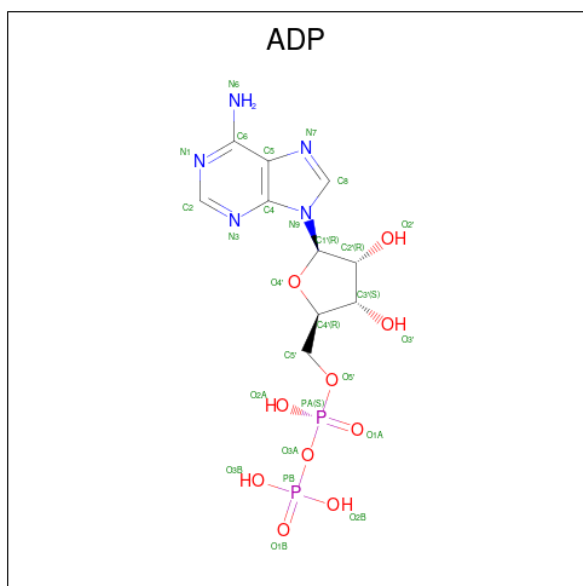
- Molecule 13 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	258	Total	C	N	O	S	0	0
			1737	1086	319	328	4		

- Molecule 14 is a protein called model substrate polypeptide.

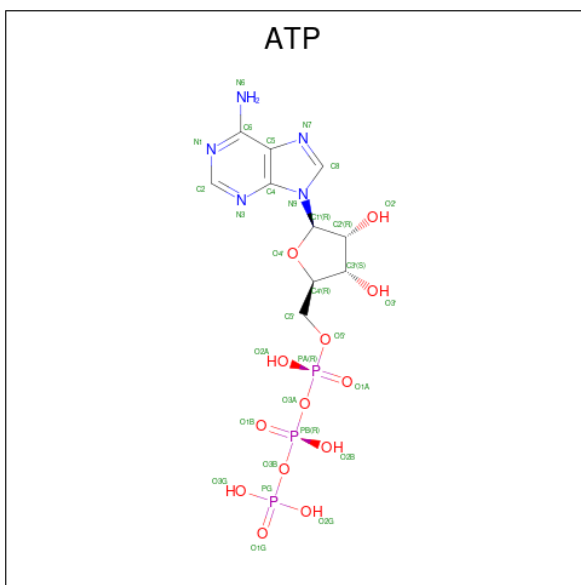
Mol	Chain	Residues	Atoms				AltConf	Trace
14	s	12	Total	C	N	O	0	0
			66	38	13	15		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

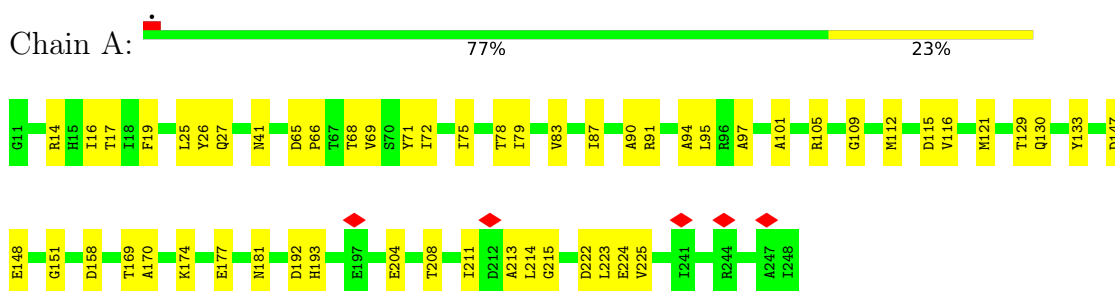


Mol	Chain	Residues	Atoms					AltConf
16	I	1	Total 31	C 10	N 5	O 13	P 3	0
16	J	1	Total 31	C 10	N 5	O 13	P 3	0
16	K	1	Total 31	C 10	N 5	O 13	P 3	0

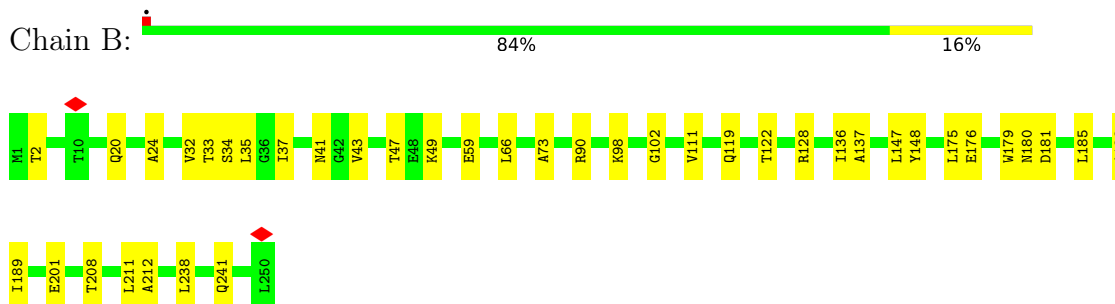
3 Residue-property plots

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

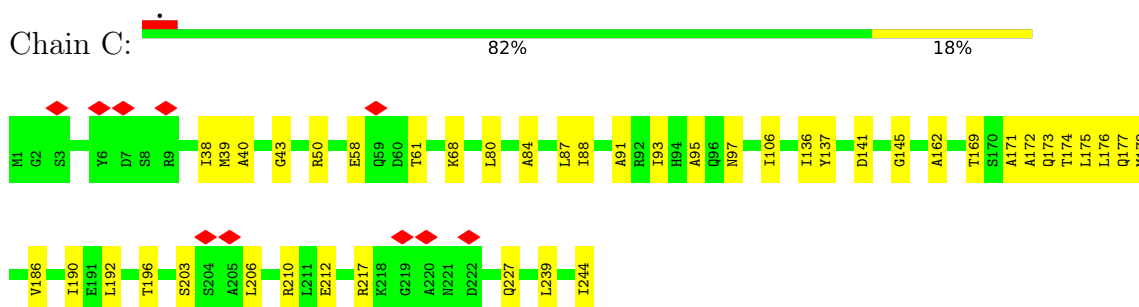
- Molecule 1: Proteasome subunit alpha type-1



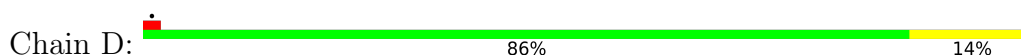
- Molecule 2: Proteasome subunit alpha type-2

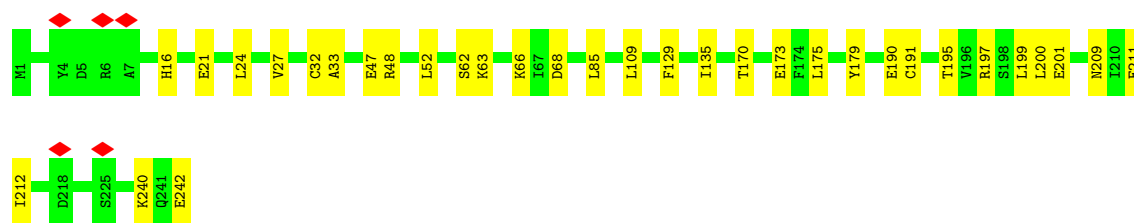


- Molecule 3: Proteasome subunit alpha type-3

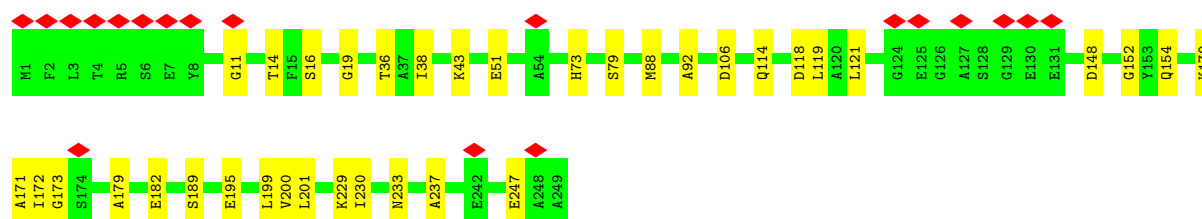
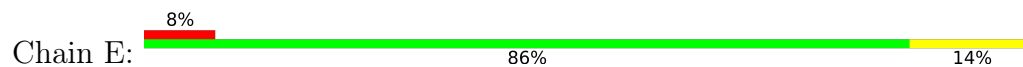


- Molecule 4: Proteasome subunit alpha type-4

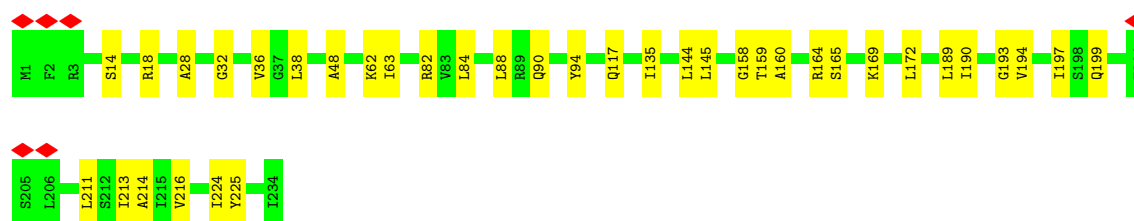
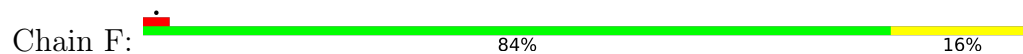




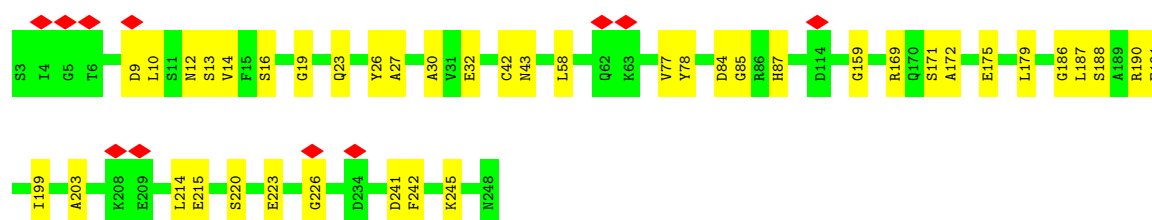
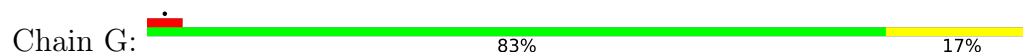
- Molecule 5: Proteasome subunit alpha type-5



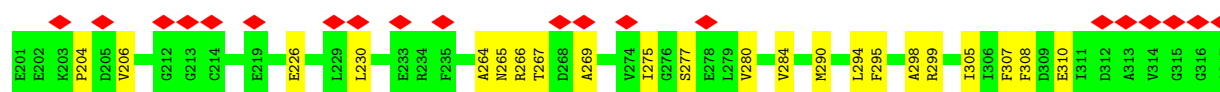
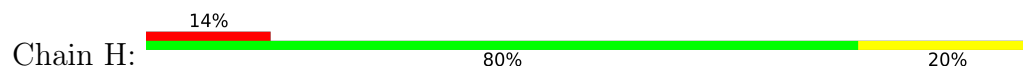
- Molecule 6: Proteasome subunit alpha type-6

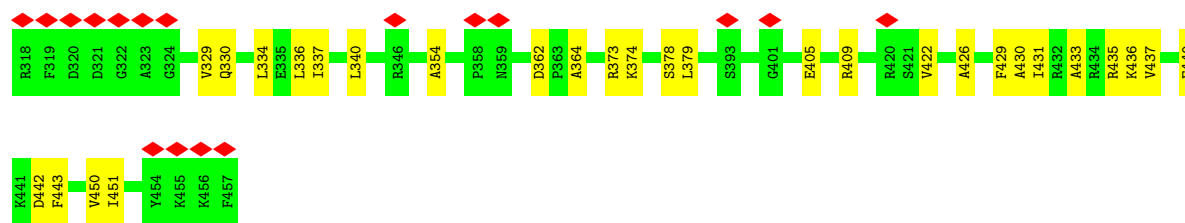


- Molecule 7: Probable proteasome subunit alpha type-7

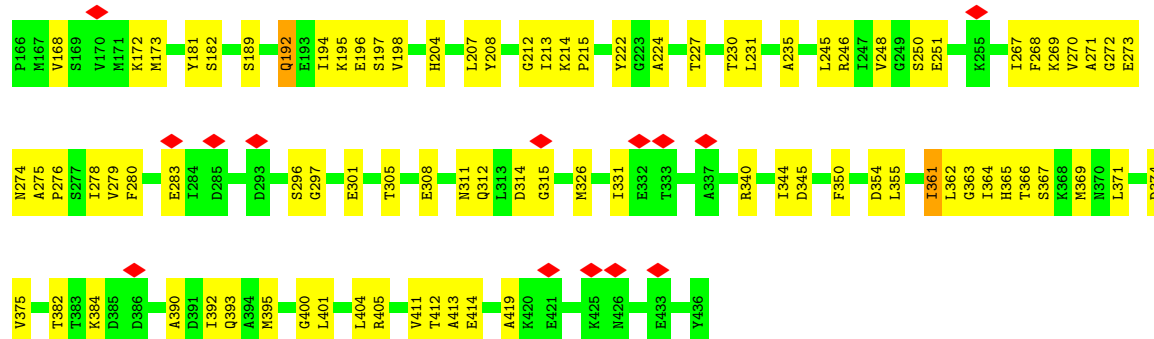


- Molecule 8: 26S proteasome regulatory subunit 7 homolog

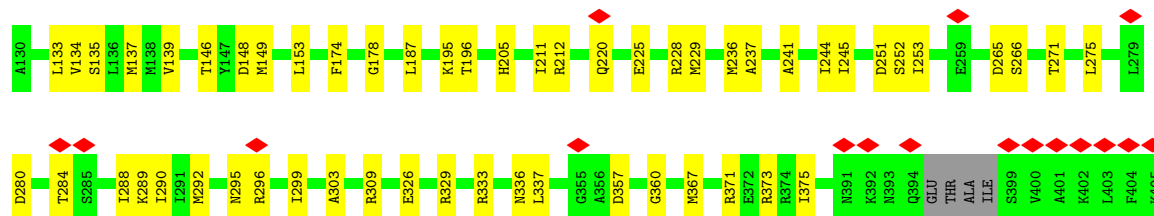
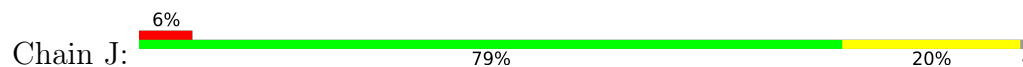




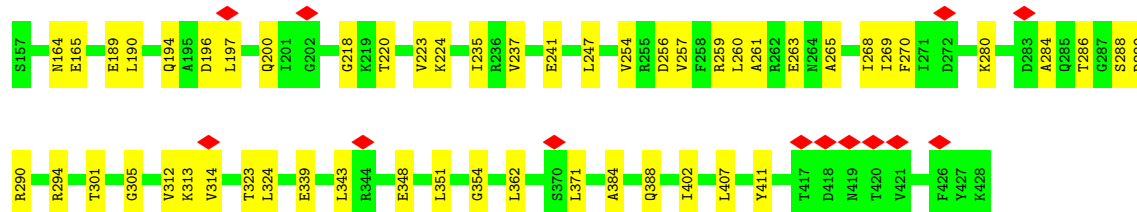
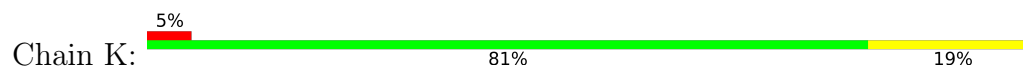
- Molecule 9: 26S proteasome regulatory subunit 4 homolog



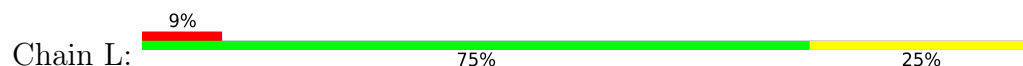
- Molecule 10: 26S proteasome regulatory subunit 8 homolog

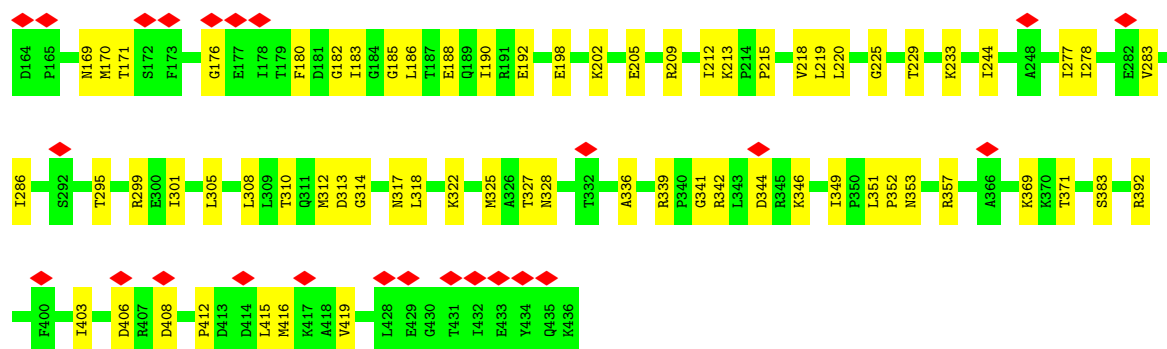


- Molecule 11: 26S proteasome regulatory subunit 6B homolog

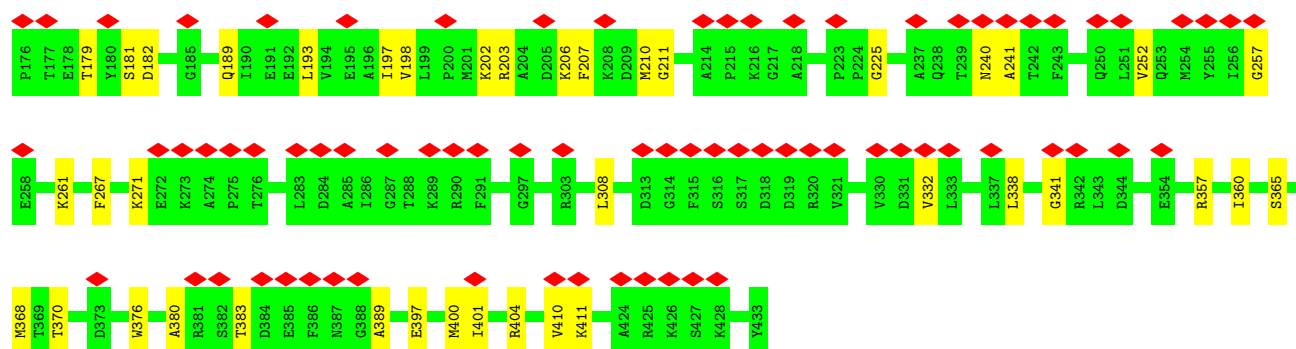
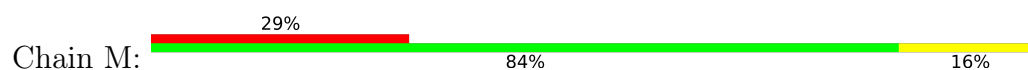


- Molecule 12: 26S proteasome subunit RPT4

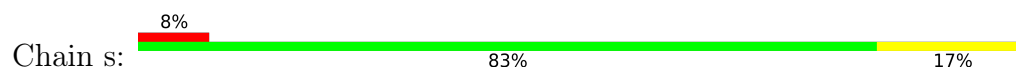




- Molecule 13: 26S proteasome regulatory subunit 6A



- Molecule 14: model substrate polypeptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34701	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed by Relion during reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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

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	0.49	0/1901	0.57	0/2576
2	B	0.52	0/1895	0.54	0/2570
3	C	0.46	0/1863	0.55	0/2526
4	D	0.50	0/1885	0.54	0/2556
5	E	0.48	0/1911	0.51	0/2578
6	F	0.46	0/1810	0.57	0/2447
7	G	0.46	0/1908	0.50	0/2582
8	H	0.35	0/1860	0.56	0/2527
9	I	0.46	0/1936	0.60	0/2633
10	J	0.48	0/2030	0.62	0/2739
11	K	0.52	0/2042	0.60	0/2767
12	L	0.45	0/2093	0.57	0/2831
13	M	0.30	0/1756	0.54	0/2396
14	s	0.30	0/65	0.53	0/87
All	All	0.46	0/24955	0.56	0/33815

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	GLN	Peptide
9	I	215	PRO	Peptide
9	I	361	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1864	0	1849	36	0
2	B	1859	0	1829	31	0
3	C	1834	0	1791	26	0
4	D	1856	0	1832	20	0
5	E	1885	0	1834	25	0
6	F	1783	0	1778	24	0
7	G	1868	0	1819	25	0
8	H	1831	0	1749	34	0
9	I	1913	0	1786	57	0
10	J	2005	0	2013	41	0
11	K	2016	0	1961	36	0
12	L	2057	0	2032	49	0
13	M	1737	0	1601	30	0
14	s	66	0	53	1	0
15	H	27	0	12	0	0
15	L	27	0	12	2	0
15	M	27	0	12	0	0
16	I	31	0	12	2	0
16	J	31	0	12	3	0
16	K	31	0	12	4	0
All	All	24748	0	23999	421	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 9.

All (421) 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)
6:F:38:LEU:HD11	6:F:189:LEU:HD13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:295:PHE:O	8:H:299:ARG:N	2.18	0.76
8:H:430:ALA:O	8:H:435:ARG:N	2.17	0.76
12:L:313:ASP:OD2	12:L:339:ARG:NH2	2.20	0.75
10:J:280:ASP:O	10:J:284:THR:N	2.20	0.75
12:L:336:ALA:O	12:L:342:ARG:NH1	2.20	0.75
5:E:43:LYS:NZ	5:E:189:SER:O	2.19	0.74
9:I:390:ALA:HB1	9:I:393:GLN:HE22	1.52	0.74
12:L:357:ARG:NE	12:L:383:SER:O	2.23	0.72
12:L:352:PRO:O	12:L:357:ARG:NH1	2.23	0.71
12:L:215:PRO:O	12:L:322:LYS:NZ	2.24	0.71
9:I:208:TYR:O	9:I:212:GLY:N	2.24	0.70
10:J:146:THR:HG1	10:J:205:HIS:HE2	1.40	0.70
1:A:97:ALA:HB2	1:A:121:MET:HE3	1.73	0.69
12:L:170:MET:HB3	12:L:244:ILE:HD11	1.74	0.68
10:J:326:GLU:OE1	10:J:329:ARG:NH2	2.25	0.68
9:I:230:THR:OG1	16:I:501:ATP:O1B	2.10	0.67
9:I:308:GLU:O	9:I:312:GLN:N	2.27	0.67
12:L:205:GLU:O	12:L:209:ARG:N	2.27	0.67
8:H:405:GLU:N	8:H:405:GLU:OE1	2.27	0.67
11:K:220:THR:OG1	16:K:501:ATP:O3B	2.09	0.67
13:M:207:PHE:O	13:M:211:GLY:N	2.27	0.67
1:A:41:ASN:OD1	1:A:174:LYS:NZ	2.28	0.67
4:D:32:CYS:SG	4:D:33:ALA:N	2.68	0.67
2:B:185:LEU:O	2:B:188:ALA:N	2.28	0.66
10:J:329:ARG:O	10:J:333:ARG:NH1	2.28	0.66
8:H:277:SER:N	8:H:310:GLU:OE1	2.29	0.66
9:I:168:VAL:O	9:I:172:LYS:N	2.28	0.66
10:J:195:LYS:NZ	16:J:501:ATP:O1G	2.26	0.66
4:D:16:HIS:ND1	4:D:21:GLU:OE2	2.29	0.66
1:A:147:ASP:OD1	1:A:151:GLY:N	2.29	0.66
10:J:237:ALA:O	10:J:241:ALA:N	2.28	0.66
1:A:14:ARG:O	1:A:27:GLN:NE2	2.28	0.65
7:G:188:SER:N	7:G:191:GLU:OE2	2.29	0.65
9:I:270:VAL:O	9:I:274:ASN:N	2.27	0.65
7:G:43:ASN:ND2	7:G:186:GLY:O	2.29	0.65
4:D:32:CYS:N	4:D:47:GLU:OE2	2.29	0.64
8:H:206:VAL:O	8:H:265:ASN:ND2	2.29	0.64
11:K:261:ALA:O	11:K:265:ALA:N	2.30	0.64
6:F:172:LEU:HD22	7:G:58:LEU:HD21	1.80	0.64
9:I:308:GLU:N	9:I:308:GLU:OE1	2.31	0.64
1:A:158:ASP:OD1	1:A:158:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:363:GLY:O	9:I:367:SER:N	2.32	0.64
2:B:176:GLU:OE1	2:B:176:GLU:N	2.31	0.63
3:C:171:ALA:O	3:C:175:LEU:N	2.31	0.63
9:I:251:GLU:N	9:I:251:GLU:OE1	2.31	0.63
6:F:28:ALA:O	6:F:32:GLY:N	2.30	0.63
12:L:188:GLU:N	12:L:188:GLU:OE1	2.31	0.63
12:L:225:GLY:N	15:L:501:ADP:O1B	2.32	0.63
11:K:286:THR:HG22	11:K:288:SER:H	1.62	0.63
2:B:43:VAL:HG11	2:B:137:ALA:HB1	1.81	0.63
7:G:16:SER:O	7:G:19:GLY:N	2.32	0.63
4:D:48:ARG:N	4:D:209:ASN:O	2.32	0.62
8:H:226:GLU:O	8:H:230:LEU:N	2.31	0.62
8:H:290:MET:O	8:H:294:LEU:N	2.33	0.62
12:L:310:THR:O	12:L:314:GLY:N	2.33	0.62
5:E:148:ASP:OD1	5:E:152:GLY:N	2.32	0.62
8:H:430:ALA:HB1	8:H:435:ARG:C	2.25	0.61
10:J:236:MET:SD	10:J:237:ALA:N	2.73	0.61
10:J:133:LEU:HD13	10:J:134:VAL:N	2.16	0.61
6:F:84:LEU:O	6:F:88:LEU:N	2.33	0.61
1:A:181:ASN:O	1:A:181:ASN:ND2	2.32	0.60
10:J:245:ILE:HD11	10:J:290:ILE:HG22	1.82	0.60
9:I:194:ILE:O	9:I:198:VAL:N	2.34	0.60
13:M:206:LYS:O	13:M:210:MET:N	2.33	0.60
11:K:343:LEU:O	11:K:343:LEU:HD13	2.02	0.60
1:A:224:GLU:OE1	1:A:225:VAL:N	2.35	0.60
13:M:267:PHE:O	13:M:271:LYS:N	2.34	0.59
3:C:58:GLU:OE2	3:C:61:THR:N	2.36	0.59
11:K:241:GLU:N	11:K:241:GLU:OE1	2.35	0.59
1:A:211:ILE:O	1:A:215:GLY:N	2.35	0.59
9:I:301:GLU:O	9:I:305:THR:N	2.35	0.59
11:K:268:ILE:HD13	11:K:312:VAL:HG23	1.84	0.59
3:C:50:ARG:NE	3:C:212:GLU:OE2	2.34	0.59
5:E:16:SER:OG	5:E:19:GLY:N	2.33	0.59
12:L:341:GLY:N	12:L:344:ASP:OD1	2.34	0.59
14:s:117:SER:OG	14:s:118:ALA:N	2.36	0.59
9:I:245:LEU:HD13	9:I:246:ARG:N	2.18	0.58
9:I:393:GLN:N	9:I:393:GLN:OE1	2.35	0.58
12:L:313:ASP:OD2	12:L:342:ARG:NE	2.36	0.58
5:E:36:THR:N	5:E:51:GLU:OE2	2.36	0.57
12:L:229:THR:N	15:L:501:ADP:O2A	2.37	0.57
1:A:105:ARG:NH1	1:A:109:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:268:PHE:O	9:I:272:GLY:N	2.35	0.57
9:I:400:GLY:O	9:I:404:LEU:N	2.33	0.57
2:B:20:GLN:O	2:B:24:ALA:N	2.36	0.57
2:B:98:LYS:O	2:B:102:GLY:N	2.38	0.57
5:E:171:ALA:O	5:E:172:ILE:HD13	2.04	0.57
5:E:121:LEU:HD13	5:E:121:LEU:O	2.05	0.57
11:K:384:ALA:O	11:K:388:GLN:N	2.37	0.57
1:A:192:ASP:OD1	1:A:193:HIS:N	2.37	0.56
10:J:265:ASP:OD2	11:K:294:ARG:NH2	2.38	0.56
1:A:115:ASP:OD1	1:A:116:VAL:N	2.38	0.56
3:C:95:ALA:HA	3:C:106:ILE:HD11	1.85	0.56
9:I:189:SER:O	9:I:192:GLN:NE2	2.36	0.56
16:K:501:ATP:O1B	12:L:339:ARG:NE	2.38	0.56
3:C:203:SER:O	3:C:210:ARG:NH2	2.38	0.56
9:I:248:VAL:HG13	9:I:251:GLU:OE1	2.04	0.56
11:K:324:LEU:HD23	11:K:324:LEU:H	1.70	0.56
8:H:429:PHE:O	8:H:433:ALA:N	2.37	0.56
1:A:133:TYR:HB3	2:B:2:THR:HG23	1.88	0.56
9:I:231:LEU:O	9:I:235:ALA:N	2.38	0.56
2:B:201:GLU:N	2:B:201:GLU:OE1	2.39	0.56
11:K:348:GLU:N	11:K:348:GLU:OE1	2.38	0.56
12:L:403:ILE:O	12:L:406:ASP:N	2.37	0.56
7:G:190:ARG:NH2	7:G:223:GLU:OE1	2.38	0.55
11:K:196:ASP:O	11:K:200:GLN:N	2.40	0.55
5:E:172:ILE:HG22	5:E:173:GLY:H	1.72	0.55
1:A:75:ILE:HD11	1:A:79:ILE:HG21	1.88	0.55
9:I:326:MET:N	9:I:326:MET:SD	2.80	0.55
13:M:198:VAL:O	13:M:202:LYS:N	2.37	0.55
3:C:177:GLN:NE2	4:D:52:LEU:O	2.40	0.54
9:I:364:ILE:O	9:I:367:SER:OG	2.22	0.54
6:F:90:GLN:O	6:F:94:TYR:N	2.39	0.54
1:A:148:GLU:OE1	1:A:148:GLU:N	2.40	0.54
6:F:213:ILE:O	6:F:225:TYR:N	2.40	0.54
7:G:12:ASN:OD1	7:G:13:SER:N	2.40	0.54
13:M:189:GLN:O	13:M:193:LEU:N	2.39	0.54
13:M:225:GLY:O	13:M:389:ALA:N	2.40	0.54
13:M:397:GLU:O	13:M:400:MET:N	2.40	0.54
9:I:250:SER:N	9:I:283:GLU:OE1	2.41	0.54
4:D:109:LEU:HD12	4:D:135:ILE:HD13	1.90	0.54
6:F:214:ALA:HB2	6:F:224:ILE:HG13	1.88	0.54
8:H:436:LYS:HB3	8:H:437:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:169:ASN:OD1	12:L:170:MET:N	2.40	0.54
12:L:180:PHE:HA	12:L:183:ILE:HD13	1.90	0.54
7:G:77:VAL:HG22	7:G:78:TYR:H	1.72	0.53
7:G:9:ASP:OD2	7:G:26:TYR:OH	2.23	0.53
1:A:65:ASP:N	7:G:159:GLY:O	2.41	0.53
5:E:11:GLY:O	5:E:14:THR:OG1	2.22	0.53
10:J:148:ASP:OD1	10:J:149:MET:N	2.40	0.53
12:L:170:MET:CB	12:L:244:ILE:HD11	2.39	0.53
7:G:175:GLU:O	7:G:179:LEU:N	2.41	0.53
2:B:180:ASN:HD22	2:B:181:ASP:H	1.56	0.53
1:A:94:ALA:O	1:A:97:ALA:HB3	2.08	0.53
1:A:97:ALA:HB2	1:A:121:MET:CE	2.38	0.53
13:M:357:ARG:HA	13:M:360:ILE:HD13	1.91	0.53
4:D:211:GLU:C	4:D:212:ILE:HD12	2.34	0.53
8:H:430:ALA:HB1	8:H:436:LYS:N	2.23	0.52
3:C:206:LEU:HD23	3:C:206:LEU:O	2.09	0.52
1:A:16:ILE:HD12	1:A:129:THR:HA	1.90	0.52
8:H:329:VAL:HG13	8:H:330:GLN:HG3	1.90	0.52
9:I:361:ILE:O	9:I:365:HIS:ND1	2.41	0.52
2:B:211:LEU:HD11	2:B:238:LEU:HD12	1.92	0.52
9:I:194:ILE:O	9:I:197:SER:N	2.43	0.52
12:L:171:THR:OG1	12:L:244:ILE:HD13	2.09	0.52
12:L:406:ASP:OD1	13:M:203:ARG:NH2	2.43	0.52
13:M:181:SER:OG	13:M:182:ASP:N	2.43	0.52
5:E:229:LYS:NZ	5:E:230:ILE:O	2.42	0.52
8:H:269:ALA:HB1	8:H:305:ILE:CD1	2.39	0.52
12:L:182:GLY:C	12:L:183:ILE:HD12	2.35	0.52
1:A:177:GLU:OE1	1:A:177:GLU:N	2.43	0.51
5:E:36:THR:OG1	5:E:51:GLU:OE1	2.27	0.51
5:E:118:ASP:OD1	5:E:119:LEU:N	2.42	0.51
7:G:32:GLU:OE1	7:G:169:ARG:NE	2.36	0.51
5:E:200:VAL:HG13	5:E:201:LEU:HD22	1.92	0.51
10:J:244:ILE:HG22	10:J:289:LYS:HB2	1.93	0.51
6:F:189:LEU:O	6:F:193:GLY:N	2.42	0.51
9:I:214:LYS:NZ	9:I:345:ASP:OD2	2.43	0.51
5:E:179:ALA:O	5:E:182:GLU:N	2.44	0.51
1:A:71:TYR:CE1	1:A:87:ILE:HD11	2.46	0.51
2:B:59:GLU:N	2:B:59:GLU:OE1	2.44	0.51
8:H:431:ILE:HD12	8:H:431:ILE:H	1.76	0.51
13:M:370:THR:HG1	13:M:410:VAL:C	2.14	0.51
2:B:111:VAL:HB	2:B:136:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:LYS:NZ	4:D:68:ASP:O	2.41	0.50
8:H:442:ASP:OD1	8:H:443:PHE:N	2.45	0.50
10:J:336:ASN:ND2	10:J:375:ILE:O	2.44	0.50
16:K:501:ATP:O1G	12:L:342:ARG:NH2	2.43	0.50
4:D:85:LEU:HD21	4:D:129:PHE:CE2	2.46	0.50
9:I:245:LEU:HD13	9:I:246:ARG:C	2.36	0.50
3:C:141:ASP:OD1	3:C:145:GLY:N	2.44	0.50
7:G:187:LEU:HD12	7:G:191:GLU:HG3	1.93	0.50
10:J:271:THR:O	10:J:275:LEU:N	2.42	0.50
9:I:375:VAL:HB	9:I:413:ALA:HB2	1.94	0.50
9:I:340:ARG:O	9:I:344:ILE:N	2.40	0.50
10:J:195:LYS:NZ	16:J:501:ATP:O1B	2.43	0.50
11:K:164:ASN:OD1	11:K:165:GLU:N	2.45	0.50
11:K:339:GLU:N	11:K:339:GLU:OE1	2.42	0.50
13:M:338:LEU:HD13	13:M:338:LEU:O	2.12	0.50
11:K:196:ASP:OD1	11:K:197:LEU:N	2.44	0.50
4:D:190:GLU:OE1	4:D:190:GLU:N	2.42	0.50
11:K:189:GLU:OE1	11:K:189:GLU:N	2.43	0.50
11:K:268:ILE:CD1	11:K:312:VAL:HG23	2.41	0.50
2:B:66:LEU:O	2:B:90:ARG:NH2	2.45	0.50
2:B:119:GLN:HA	2:B:122:THR:HG22	1.94	0.50
2:B:185:LEU:O	2:B:189:ILE:HD12	2.12	0.49
9:I:362:LEU:HD23	9:I:362:LEU:H	1.77	0.49
1:A:17:THR:OG1	2:B:128:ARG:N	2.45	0.49
10:J:135:SER:HA	10:J:137:MET:HE1	1.94	0.49
13:M:376:TRP:O	13:M:380:ALA:N	2.46	0.49
10:J:336:ASN:OD1	10:J:337:LEU:N	2.45	0.49
13:M:357:ARG:NE	13:M:383:THR:HG21	2.28	0.49
2:B:34:SER:OG	2:B:35:LEU:N	2.46	0.49
9:I:401:LEU:O	9:I:405:ARG:N	2.45	0.49
10:J:251:ASP:OD1	10:J:299:ILE:HD11	2.12	0.49
10:J:211:ILE:HD12	10:J:212:ARG:N	2.27	0.49
3:C:95:ALA:CA	3:C:106:ILE:HD11	2.43	0.49
6:F:194:VAL:O	6:F:197:ILE:N	2.45	0.49
6:F:144:LEU:C	6:F:145:LEU:HD12	2.38	0.49
12:L:198:GLU:O	12:L:202:LYS:N	2.45	0.49
12:L:349:ILE:HD12	12:L:349:ILE:O	2.12	0.49
5:E:152:GLY:O	5:E:154:GLN:NE2	2.46	0.48
10:J:225:GLU:OE1	10:J:228:ARG:NE	2.36	0.48
8:H:373:ARG:NH1	8:H:374:LYS:O	2.46	0.48
10:J:133:LEU:HD13	10:J:134:VAL:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:353:ASN:O	12:L:357:ARG:N	2.44	0.48
1:A:204:GLU:O	1:A:208:THR:HG22	2.14	0.48
2:B:33:THR:O	2:B:47:THR:OG1	2.27	0.48
1:A:83:VAL:HG11	1:A:90:ALA:HB1	1.95	0.48
2:B:147:LEU:HD13	2:B:148:TYR:N	2.29	0.48
9:I:192:GLN:OE1	9:I:192:GLN:N	2.42	0.48
9:I:371:LEU:HA	9:I:411:VAL:HG11	1.95	0.48
12:L:295:THR:O	12:L:299:ARG:NH1	2.47	0.48
3:C:38:ILE:HG22	3:C:162:ALA:HB1	1.95	0.48
6:F:158:GLY:O	6:F:159:THR:OG1	2.31	0.48
8:H:295:PHE:HA	8:H:298:ALA:HB3	1.94	0.48
9:I:269:LYS:O	9:I:273:GLU:N	2.39	0.48
9:I:412:THR:HG22	9:I:414:GLU:H	1.78	0.48
12:L:369:LYS:NZ	12:L:371:THR:HG22	2.29	0.48
1:A:66:PRO:HA	1:A:69:VAL:HG12	1.96	0.48
11:K:190:LEU:O	11:K:194:GLN:N	2.46	0.48
4:D:197:ARG:HA	4:D:200:LEU:HD23	1.96	0.47
8:H:275:ILE:HG23	8:H:308:PHE:HA	1.96	0.47
8:H:334:LEU:HA	8:H:337:ILE:HD12	1.95	0.47
10:J:245:ILE:HD11	10:J:290:ILE:CG2	2.43	0.47
8:H:226:GLU:N	8:H:226:GLU:OE1	2.47	0.47
8:H:269:ALA:HB1	8:H:305:ILE:HD13	1.95	0.47
8:H:336:LEU:O	8:H:340:LEU:N	2.47	0.47
10:J:252:SER:OG	10:J:253:ILE:HD12	2.13	0.47
6:F:117:GLN:OE1	7:G:87:HIS:ND1	2.47	0.47
9:I:224:ALA:HB2	9:I:350:PHE:O	2.15	0.47
13:M:198:VAL:HG13	13:M:202:LYS:NZ	2.29	0.47
9:I:181:TYR:O	9:I:182:SER:OG	2.21	0.47
12:L:327:THR:OG1	12:L:328:ASN:N	2.47	0.47
3:C:40:ALA:HB3	3:C:43:GLY:O	2.15	0.47
12:L:186:LEU:O	12:L:190:ILE:HG22	2.15	0.47
6:F:164:ARG:O	6:F:199:GLN:NE2	2.43	0.47
1:A:222:ASP:C	1:A:223:LEU:HD12	2.39	0.47
8:H:266:ARG:O	8:H:267:THR:OG1	2.29	0.47
9:I:382:THR:HG21	9:I:384:LYS:NZ	2.30	0.47
9:I:267:ILE:HD12	9:I:268:PHE:CD1	2.50	0.47
11:K:288:SER:OG	11:K:289:ASP:N	2.47	0.47
3:C:80:LEU:HD23	3:C:80:LEU:H	1.79	0.47
12:L:176:GLY:O	12:L:233:LYS:NZ	2.48	0.47
2:B:241:GLN:OE1	2:B:241:GLN:N	2.47	0.46
4:D:199:LEU:O	4:D:201:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:361:ILE:HG21	9:I:392:ILE:CD1	2.45	0.46
11:K:371:LEU:HD23	11:K:371:LEU:H	1.80	0.46
11:K:407:LEU:O	11:K:411:TYR:N	2.49	0.46
2:B:211:LEU:HD12	2:B:212:ALA:N	2.31	0.46
4:D:62:SER:OG	4:D:63:LYS:N	2.47	0.46
11:K:256:ASP:O	11:K:260:LEU:N	2.41	0.46
5:E:36:THR:HG22	5:E:173:GLY:HA3	1.97	0.46
10:J:196:THR:HG23	16:J:501:ATP:O1B	2.15	0.46
1:A:101:ALA:HA	1:A:112:MET:HE2	1.97	0.46
1:A:130:GLN:NE2	2:B:128:ARG:O	2.47	0.46
7:G:27:ALA:O	7:G:30:ALA:N	2.48	0.46
10:J:153:LEU:HD23	10:J:153:LEU:H	1.81	0.46
12:L:351:LEU:HD11	12:L:357:ARG:HD3	1.97	0.46
12:L:416:MET:HA	12:L:419:VAL:HG12	1.97	0.46
8:H:378:SER:OG	8:H:379:LEU:N	2.49	0.46
10:J:367:MET:O	10:J:371:ARG:N	2.46	0.46
13:M:240:ASN:OD1	13:M:241:ALA:N	2.47	0.46
3:C:87:LEU:O	3:C:91:ALA:N	2.48	0.46
11:K:259:ARG:O	11:K:263:GLU:N	2.40	0.46
10:J:295:ASN:OD1	10:J:296:ARG:N	2.48	0.46
5:E:114:GLN:OE1	6:F:82:ARG:NE	2.49	0.46
8:H:204:PRO:HG3	8:H:264:ALA:HB3	1.98	0.46
10:J:174:PHE:O	10:J:178:GLY:N	2.49	0.46
10:J:220:GLN:CB	11:K:247:LEU:HD22	2.46	0.46
9:I:192:GLN:O	9:I:195:LYS:N	2.49	0.45
13:M:400:MET:O	13:M:404:ARG:N	2.45	0.45
3:C:192:LEU:O	3:C:196:THR:N	2.48	0.45
6:F:62:LYS:C	6:F:63:ILE:HD12	2.42	0.45
9:I:196:GLU:N	9:I:196:GLU:OE1	2.49	0.45
13:M:267:PHE:CE2	13:M:308:LEU:HD13	2.51	0.45
12:L:218:VAL:HG12	12:L:219:LEU:N	2.31	0.45
12:L:412:PRO:HA	12:L:415:LEU:HD22	1.98	0.45
4:D:173:GLU:OE1	4:D:173:GLU:N	2.43	0.45
6:F:62:LYS:HB3	6:F:63:ILE:HD12	1.98	0.45
7:G:42:CYS:SG	7:G:43:ASN:N	2.89	0.45
11:K:254:VAL:O	11:K:257:VAL:HG22	2.17	0.45
9:I:227:THR:N	16:I:501:ATP:O1A	2.44	0.45
10:J:265:ASP:OD1	10:J:266:SER:N	2.50	0.45
5:E:88:MET:O	5:E:92:ALA:N	2.45	0.45
9:I:395:MET:SD	9:I:419:ALA:HB3	2.56	0.45
11:K:269:ILE:HD11	11:K:314:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:257:GLY:O	13:M:261:LYS:N	2.47	0.45
10:J:139:VAL:HG22	10:J:211:ILE:HG22	1.99	0.45
13:M:179:THR:HG23	13:M:181:SER:H	1.81	0.45
2:B:189:ILE:HD12	2:B:189:ILE:H	1.82	0.44
8:H:265:ASN:OD1	8:H:266:ARG:N	2.50	0.44
9:I:311:ASN:O	9:I:315:GLY:N	2.43	0.44
2:B:41:ASN:OD1	2:B:41:ASN:N	2.50	0.44
9:I:275:ALA:HB3	9:I:276:PRO:HD3	1.98	0.44
2:B:32:VAL:HG22	2:B:33:THR:H	1.82	0.44
9:I:173:MET:HG3	9:I:245:LEU:HD22	1.99	0.44
12:L:283:VAL:HG21	12:L:325:MET:HB2	1.99	0.44
12:L:317:ASN:OD1	12:L:318:LEU:N	2.49	0.44
1:A:91:ARG:O	1:A:95:LEU:N	2.47	0.44
5:E:38:ILE:HD12	5:E:170:LYS:O	2.17	0.44
11:K:268:ILE:HD11	11:K:313:LYS:O	2.17	0.44
12:L:392:ARG:NH1	13:M:341:GLY:O	2.50	0.44
9:I:279:VAL:HG22	9:I:280:PHE:O	2.18	0.44
11:K:362:LEU:HD22	11:K:402:ILE:HD11	2.00	0.44
12:L:219:LEU:C	12:L:220:LEU:HD22	2.43	0.44
1:A:19:PHE:N	2:B:20:GLN:OE1	2.48	0.44
10:J:357:ASP:O	10:J:360:GLY:N	2.49	0.44
10:J:288:ILE:HD12	10:J:290:ILE:HG23	2.00	0.43
13:M:252:VAL:O	13:M:252:VAL:HG23	2.18	0.43
10:J:245:ILE:CD1	10:J:290:ILE:HG22	2.48	0.43
12:L:185:GLY:C	12:L:186:LEU:HD22	2.43	0.43
12:L:212:ILE:HG22	12:L:213:LYS:C	2.43	0.43
5:E:172:ILE:HG22	5:E:173:GLY:N	2.32	0.43
11:K:301:THR:O	11:K:305:GLY:N	2.52	0.43
7:G:84:ASP:OD1	7:G:85:GLY:N	2.48	0.43
8:H:405:GLU:O	8:H:409:ARG:N	2.42	0.43
13:M:179:THR:HG23	13:M:181:SER:N	2.33	0.43
6:F:36:VAL:HG12	6:F:160:ALA:HA	2.01	0.43
6:F:48:ALA:HB3	6:F:63:ILE:HD11	2.00	0.43
11:K:351:LEU:O	11:K:354:GLY:N	2.52	0.43
3:C:68:LYS:NZ	3:C:227:GLN:OE1	2.47	0.43
3:C:93:ILE:O	3:C:97:ASN:N	2.52	0.43
6:F:199:GLN:OE1	6:F:199:GLN:N	2.45	0.43
9:I:204:HIS:HB3	9:I:207:LEU:HD23	2.01	0.43
12:L:305:LEU:O	12:L:308:LEU:N	2.51	0.43
3:C:136:ILE:HG22	3:C:137:TYR:N	2.34	0.43
7:G:171:SER:OG	7:G:172:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:198:VAL:HG13	13:M:202:LYS:HZ3	1.84	0.43
13:M:397:GLU:O	13:M:401:ILE:N	2.47	0.43
2:B:73:ALA:HB2	2:B:136:ILE:HG22	2.00	0.43
9:I:268:PHE:HA	9:I:271:ALA:HB3	2.00	0.43
10:J:133:LEU:HD13	10:J:135:SER:H	1.83	0.43
10:J:187:LEU:HD23	10:J:292:MET:O	2.18	0.43
13:M:332:VAL:HG23	13:M:332:VAL:O	2.18	0.43
10:J:371:ARG:O	10:J:373:ARG:NH1	2.51	0.42
12:L:286:ILE:HG22	12:L:286:ILE:O	2.19	0.42
2:B:49:LYS:NZ	2:B:208:THR:O	2.52	0.42
9:I:314:ASP:OD1	9:I:315:GLY:N	2.52	0.42
11:K:269:ILE:HD12	11:K:270:PHE:N	2.35	0.42
8:H:362:ASP:OD2	8:H:364:ALA:HB3	2.18	0.42
11:K:223:VAL:HG23	11:K:224:LYS:HG3	2.01	0.42
12:L:219:LEU:HD21	12:L:346:LYS:HG3	2.02	0.42
6:F:190:ILE:O	6:F:194:VAL:HG23	2.20	0.42
10:J:225:GLU:O	10:J:229:MET:N	2.49	0.42
11:K:235:ILE:HD13	11:K:237:VAL:HB	2.01	0.42
5:E:247:GLU:OE1	5:E:247:GLU:N	2.53	0.42
12:L:408:ASP:OD2	13:M:203:ARG:NH1	2.52	0.42
2:B:175:LEU:O	2:B:179:TRP:N	2.48	0.42
3:C:176:LEU:HD12	3:C:176:LEU:C	2.45	0.42
9:I:296:SER:OG	9:I:297:GLY:N	2.53	0.42
11:K:284:ALA:O	11:K:290:ARG:NH2	2.53	0.42
1:A:78:THR:HG22	1:A:78:THR:O	2.20	0.42
3:C:174:THR:O	3:C:178:MET:HE1	2.20	0.42
7:G:10:LEU:O	7:G:23:GLN:NE2	2.53	0.42
8:H:450:VAL:HG23	8:H:451:ILE:HG12	2.02	0.42
1:A:213:ALA:C	1:A:214:LEU:HD22	2.45	0.42
2:B:35:LEU:C	2:B:35:LEU:HD12	2.44	0.42
4:D:85:LEU:HD21	4:D:129:PHE:HE2	1.85	0.42
7:G:14:VAL:HG23	7:G:14:VAL:O	2.19	0.42
8:H:422:VAL:O	8:H:426:ALA:N	2.50	0.42
13:M:197:ILE:HG22	13:M:197:ILE:O	2.20	0.42
3:C:186:VAL:HG11	3:C:217:ARG:NH1	2.35	0.42
4:D:170:THR:O	4:D:170:THR:HG22	2.20	0.42
8:H:264:ALA:HA	8:H:269:ALA:HB3	2.01	0.42
11:K:280:LYS:N	11:K:323:THR:O	2.53	0.42
3:C:190:ILE:HD12	3:C:190:ILE:H	1.85	0.41
9:I:374:ASP:OD1	9:I:374:ASP:N	2.44	0.41
1:A:72:ILE:N	1:A:72:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:301:ILE:O	12:L:305:LEU:N	2.46	0.41
1:A:25:LEU:HD12	1:A:26:TYR:N	2.35	0.41
10:J:146:THR:HG1	10:J:205:HIS:CE1	2.38	0.41
10:J:146:THR:OG1	10:J:205:HIS:NE2	2.41	0.41
1:A:101:ALA:CA	1:A:112:MET:HE2	2.50	0.41
6:F:211:LEU:HD21	6:F:213:ILE:HD11	2.01	0.41
7:G:199:ILE:O	7:G:203:ALA:N	2.46	0.41
11:K:268:ILE:HD13	11:K:312:VAL:C	2.45	0.41
12:L:198:GLU:OE1	12:L:198:GLU:N	2.46	0.41
3:C:169:THR:O	3:C:172:ALA:N	2.54	0.41
4:D:191:CYS:O	4:D:195:THR:N	2.45	0.41
4:D:240:LYS:O	4:D:242:GLU:N	2.54	0.41
7:G:241:ASP:O	7:G:245:LYS:N	2.52	0.41
7:G:241:ASP:OD1	7:G:242:PHE:N	2.54	0.41
12:L:308:LEU:HD23	12:L:312:MET:HE3	2.01	0.41
2:B:37:ILE:HD12	2:B:37:ILE:C	2.45	0.41
3:C:84:ALA:O	3:C:88:ILE:HD12	2.19	0.41
7:G:220:SER:O	7:G:226:GLY:N	2.50	0.41
8:H:440:GLU:OE1	8:H:440:GLU:N	2.49	0.41
9:I:222:TYR:CD1	9:I:331:ILE:HD11	2.56	0.41
9:I:354:ASP:OD1	9:I:355:LEU:N	2.51	0.41
7:G:214:LEU:HD12	7:G:215:GLU:N	2.36	0.41
8:H:280:VAL:O	8:H:284:VAL:HG12	2.20	0.41
10:J:303:ALA:O	10:J:309:ARG:NH2	2.48	0.41
13:M:365:SER:OG	13:M:368:MET:O	2.37	0.41
3:C:173:GLN:O	3:C:177:GLN:N	2.53	0.41
1:A:169:THR:OG1	1:A:170:ALA:N	2.54	0.41
9:I:208:TYR:O	9:I:213:ILE:N	2.50	0.41
12:L:277:ILE:HD12	12:L:278:ILE:N	2.36	0.41
13:M:410:VAL:HG12	13:M:411:LYS:O	2.21	0.41
4:D:175:LEU:O	4:D:179:TYR:N	2.54	0.41
6:F:135:ILE:HD13	6:F:216:VAL:CG2	2.51	0.41
1:A:65:ASP:O	1:A:68:THR:OG1	2.30	0.40
3:C:38:ILE:HD12	3:C:39:MET:N	2.36	0.40
4:D:24:LEU:O	4:D:27:VAL:HG12	2.21	0.40
5:E:79:SER:CB	5:E:172:ILE:HG21	2.52	0.40
12:L:188:GLU:O	12:L:192:GLU:N	2.48	0.40
5:E:195:GLU:O	5:E:199:LEU:N	2.52	0.40
6:F:14:SER:OG	6:F:18:ARG:N	2.54	0.40
6:F:165:SER:OG	6:F:169:LYS:NZ	2.54	0.40
9:I:245:LEU:N	9:I:278:ILE:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:366:THR:HA	9:I:369:MET:HB3	2.03	0.40
2:B:180:ASN:HD22	2:B:181:ASP:N	2.18	0.40
5:E:73:HIS:NE2	5:E:106:ASP:OD2	2.54	0.40
5:E:233:ASN:O	5:E:237:ALA:N	2.49	0.40
7:G:27:ALA:O	7:G:30:ALA:HB3	2.22	0.40
9:I:362:LEU:HD23	9:I:362:LEU:N	2.36	0.40
3:C:239:LEU:HD13	3:C:244:ILE:HD11	2.03	0.40
5:E:38:ILE:HD13	5:E:171:ALA:HB2	2.03	0.40
8:H:307:PHE:CZ	8:H:354:ALA:HB2	2.57	0.40
11:K:218:GLY:N	16:K:501:ATP:O1A	2.52	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	236/238 (99%)	198 (84%)	38 (16%)	0	100	100
2	B	248/250 (99%)	211 (85%)	37 (15%)	0	100	100
3	C	242/244 (99%)	200 (83%)	42 (17%)	0	100	100
4	D	240/242 (99%)	206 (86%)	34 (14%)	0	100	100
5	E	247/249 (99%)	199 (81%)	48 (19%)	0	100	100
6	F	232/234 (99%)	198 (85%)	34 (15%)	0	100	100
7	G	244/246 (99%)	206 (84%)	38 (16%)	0	100	100
8	H	255/257 (99%)	210 (82%)	45 (18%)	0	100	100
9	I	269/271 (99%)	224 (83%)	45 (17%)	0	100	100
10	J	268/276 (97%)	216 (81%)	52 (19%)	0	100	100
11	K	270/272 (99%)	211 (78%)	59 (22%)	0	100	100
12	L	271/273 (99%)	239 (88%)	32 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	256/258 (99%)	211 (82%)	45 (18%)	0	100	100
14	s	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
All	All	3288/3322 (99%)	2737 (83%)	551 (17%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/204 (98%)	199 (100%)	0	100	100
2	B	190/209 (91%)	190 (100%)	0	100	100
3	C	183/203 (90%)	183 (100%)	0	100	100
4	D	201/214 (94%)	201 (100%)	0	100	100
5	E	192/205 (94%)	192 (100%)	0	100	100
6	F	186/193 (96%)	186 (100%)	0	100	100
7	G	189/203 (93%)	189 (100%)	0	100	100
8	H	174/214 (81%)	174 (100%)	0	100	100
9	I	187/234 (80%)	187 (100%)	0	100	100
10	J	205/233 (88%)	205 (100%)	0	100	100
11	K	199/231 (86%)	199 (100%)	0	100	100
12	L	207/226 (92%)	207 (100%)	0	100	100
13	M	146/214 (68%)	146 (100%)	0	100	100
14	s	4/7 (57%)	4 (100%)	0	100	100
All	All	2462/2790 (88%)	2462 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	180	ASN
3	C	120	GLN
3	C	156	ASN
4	D	19	GLN
4	D	96	HIS
5	E	180	GLN
7	G	237	GLN
9	I	311	ASN
11	K	375	ASN
12	L	409	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	ADP	M	501	-	28,29,29	1.32	5 (17%)	43,45,45	1.82	9 (20%)
15	ADP	L	501	-	28,29,29	1.30	4 (14%)	43,45,45	1.85	9 (20%)
16	ATP	K	501	-	32,33,33	1.28	5 (15%)	48,52,52	1.80	12 (25%)
16	ATP	I	501	-	32,33,33	1.30	4 (12%)	48,52,52	1.95	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	ADP	H	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.87	9 (20%)
16	ATP	J	501	-	32,33,33	1.26	4 (12%)	48,52,52	1.77	10 (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
15	ADP	M	501	-	-	2/16/32/32	0/3/3/3
15	ADP	L	501	-	-	7/16/32/32	0/3/3/3
16	ATP	K	501	-	-	4/22/38/38	0/3/3/3
16	ATP	I	501	-	-	7/22/38/38	0/3/3/3
15	ADP	H	501	-	-	7/16/32/32	0/3/3/3
16	ATP	J	501	-	-	4/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	501	ADP	C5-C4	4.38	1.46	1.39
16	I	501	ATP	C5-C4	4.17	1.46	1.39
15	M	501	ADP	C5-C4	4.06	1.46	1.39
16	J	501	ATP	C5-C4	3.94	1.46	1.39
16	K	501	ATP	C5-C4	3.89	1.46	1.39
15	L	501	ADP	C5-C4	3.83	1.45	1.39
15	L	501	ADP	C5-N7	-3.17	1.33	1.39
16	I	501	ATP	C5-N7	-3.03	1.33	1.39
16	J	501	ATP	C5-N7	-2.87	1.33	1.39
16	K	501	ATP	C5-N7	-2.71	1.34	1.39
15	H	501	ADP	C5-N7	-2.63	1.34	1.39
15	M	501	ADP	C5-N7	-2.51	1.34	1.39
16	K	501	ATP	C4-N9	-2.46	1.32	1.37
15	H	501	ADP	C5-C6	2.43	1.47	1.41
16	I	501	ATP	C8-N9	-2.40	1.33	1.37
15	M	501	ADP	C5-C6	2.37	1.47	1.41
16	J	501	ATP	C4-N9	-2.33	1.32	1.37
16	K	501	ATP	C5-C6	2.19	1.47	1.41
15	M	501	ADP	C4-N9	-2.15	1.33	1.37
16	I	501	ATP	C5-C6	2.13	1.46	1.41
16	K	501	ATP	C8-N7	2.09	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	501	ADP	C4-N9	-2.09	1.33	1.37
15	M	501	ADP	C8-N7	2.07	1.35	1.31
15	H	501	ADP	C8-N7	2.04	1.35	1.31
16	J	501	ATP	C8-N7	2.04	1.35	1.31
15	L	501	ADP	C5-C6	2.02	1.46	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	501	ATP	C5-C4-N3	-6.46	117.82	126.72
15	H	501	ADP	C5-C4-N3	-6.00	118.45	126.72
15	L	501	ADP	C5-C4-N3	-5.82	118.70	126.72
16	J	501	ATP	C5-C4-N3	-5.70	118.88	126.72
15	M	501	ADP	C5-C4-N3	-5.53	119.11	126.72
16	I	501	ATP	N3-C4-N9	5.43	136.41	127.17
16	K	501	ATP	C5-C4-N3	-5.19	119.57	126.72
15	H	501	ADP	N3-C4-N9	5.03	135.72	127.17
15	L	501	ADP	N3-C4-N9	4.78	135.29	127.17
16	J	501	ATP	N3-C4-N9	4.67	135.10	127.17
15	M	501	ADP	N3-C4-N9	4.62	135.02	127.17
16	I	501	ATP	C2-N3-C4	4.09	121.81	111.83
16	K	501	ATP	N3-C4-N9	3.98	133.94	127.17
15	H	501	ADP	C2-N3-C4	3.90	121.36	111.83
16	I	501	ATP	N3-C2-N1	-3.76	122.88	128.58
15	M	501	ADP	C2-N3-C4	3.72	120.92	111.83
15	L	501	ADP	C2-N3-C4	3.68	120.81	111.83
15	H	501	ADP	N3-C2-N1	-3.67	123.03	128.58
15	M	501	ADP	N3-C2-N1	-3.62	123.10	128.58
16	K	501	ATP	C2-N3-C4	3.61	120.64	111.83
16	J	501	ATP	C2-N3-C4	3.58	120.57	111.83
16	K	501	ATP	N3-C2-N1	-3.57	123.17	128.58
15	L	501	ADP	N3-C2-N1	-3.44	123.38	128.58
16	K	501	ATP	C4-C5-N7	-3.33	106.78	110.58
16	I	501	ATP	C1'-N9-C8	-3.32	119.73	127.09
15	M	501	ADP	C4-N9-C8	3.31	109.22	105.74
16	J	501	ATP	N3-C2-N1	-3.29	123.61	128.58
15	M	501	ADP	C4-C5-N7	-3.23	106.89	110.58
15	H	501	ADP	C4-C5-N7	-2.97	107.18	110.58
16	J	501	ATP	C4-C5-N7	-2.92	107.24	110.58
15	L	501	ADP	C4-C5-N7	-2.89	107.28	110.58
16	I	501	ATP	C4-C5-N7	-2.86	107.32	110.58
16	J	501	ATP	C4-N9-C8	2.82	108.70	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	501	ATP	C4-N9-C8	2.79	108.66	105.74
15	H	501	ADP	C4-N9-C8	2.68	108.56	105.74
16	K	501	ATP	C3'-C2'-C1'	2.64	106.46	101.46
15	M	501	ADP	C5-N7-C8	2.58	107.51	103.45
16	K	501	ATP	C5-N7-C8	2.48	107.35	103.45
15	L	501	ADP	C4-N9-C8	2.45	108.31	105.74
15	M	501	ADP	N9-C8-N7	-2.42	110.51	113.94
16	I	501	ATP	C4-N9-C8	2.37	108.23	105.74
15	L	501	ADP	C5-N7-C8	2.37	107.18	103.45
15	L	501	ADP	C3'-C2'-C1'	2.37	105.95	101.46
15	L	501	ADP	N6-C6-N1	2.36	123.63	118.38
16	K	501	ATP	C6-C5-N7	2.32	136.56	132.09
15	H	501	ADP	C1'-N9-C8	-2.30	121.98	127.09
16	I	501	ATP	C4-N9-C1'	2.30	132.02	126.63
15	H	501	ADP	C5-N7-C8	2.30	107.07	103.45
16	K	501	ATP	N9-C8-N7	-2.26	110.73	113.94
16	J	501	ATP	C5-N7-C8	2.25	106.98	103.45
16	J	501	ATP	C3'-C2'-C1'	2.23	105.68	101.46
15	H	501	ADP	C3'-C2'-C1'	2.17	105.57	101.46
15	M	501	ADP	C6-C5-N7	2.11	136.16	132.09
16	I	501	ATP	C5-N7-C8	2.11	106.77	103.45
16	K	501	ATP	O3G-PG-O2G	2.11	115.70	107.80
16	J	501	ATP	O2B-PB-O1B	2.06	122.03	112.44
16	K	501	ATP	O4'-C4'-C3'	2.04	109.20	105.15
16	J	501	ATP	N9-C8-N7	-2.02	111.07	113.94
16	I	501	ATP	O2B-PB-O1B	2.01	121.77	112.44

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	501	ADP	C5'-O5'-PA-O1A
15	H	501	ADP	C5'-O5'-PA-O2A
15	H	501	ADP	C5'-O5'-PA-O3A
15	L	501	ADP	C5'-O5'-PA-O1A
15	L	501	ADP	C5'-O5'-PA-O2A
15	L	501	ADP	C5'-O5'-PA-O3A
15	L	501	ADP	O4'-C4'-C5'-O5'
16	I	501	ATP	C5'-O5'-PA-O1A
16	I	501	ATP	C5'-O5'-PA-O2A
16	I	501	ATP	C5'-O5'-PA-O3A
16	I	501	ATP	C2'-C1'-N9-C8

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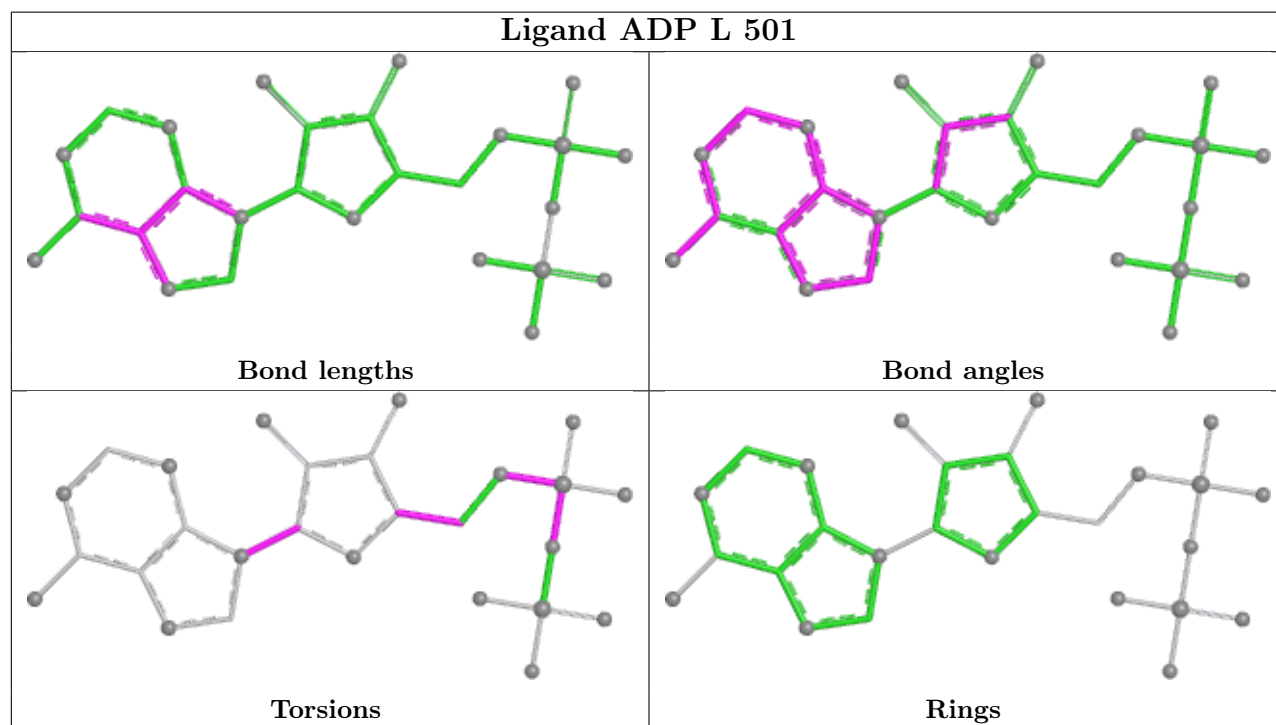
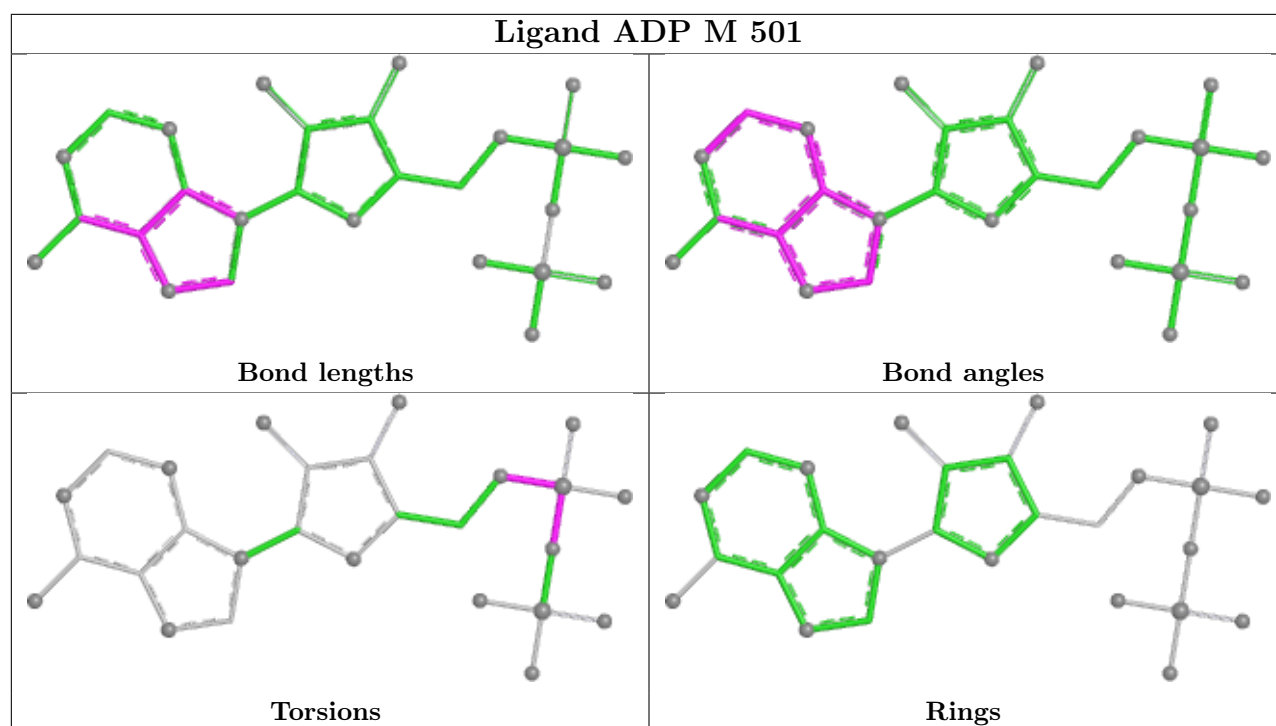
Mol	Chain	Res	Type	Atoms
16	I	501	ATP	C2'-C1'-N9-C4
16	J	501	ATP	C5'-O5'-PA-O3A
16	K	501	ATP	C5'-O5'-PA-O1A
16	K	501	ATP	C5'-O5'-PA-O2A
16	K	501	ATP	C5'-O5'-PA-O3A
15	L	501	ADP	C3'-C4'-C5'-O5'
15	H	501	ADP	O4'-C4'-C5'-O5'
15	H	501	ADP	C3'-C4'-C5'-O5'
15	H	501	ADP	C2'-C1'-N9-C4
16	I	501	ATP	PB-O3B-PG-O1G
15	H	501	ADP	C2'-C1'-N9-C8
15	M	501	ADP	C5'-O5'-PA-O1A
16	J	501	ATP	C5'-O5'-PA-O1A
16	I	501	ATP	PB-O3A-PA-O2A
16	J	501	ATP	PB-O3A-PA-O2A
15	L	501	ADP	C2'-C1'-N9-C8
15	L	501	ADP	PB-O3A-PA-O2A
15	M	501	ADP	PB-O3A-PA-O2A
16	J	501	ATP	PB-O3A-PA-O1A
16	K	501	ATP	PA-O3A-PB-O1B

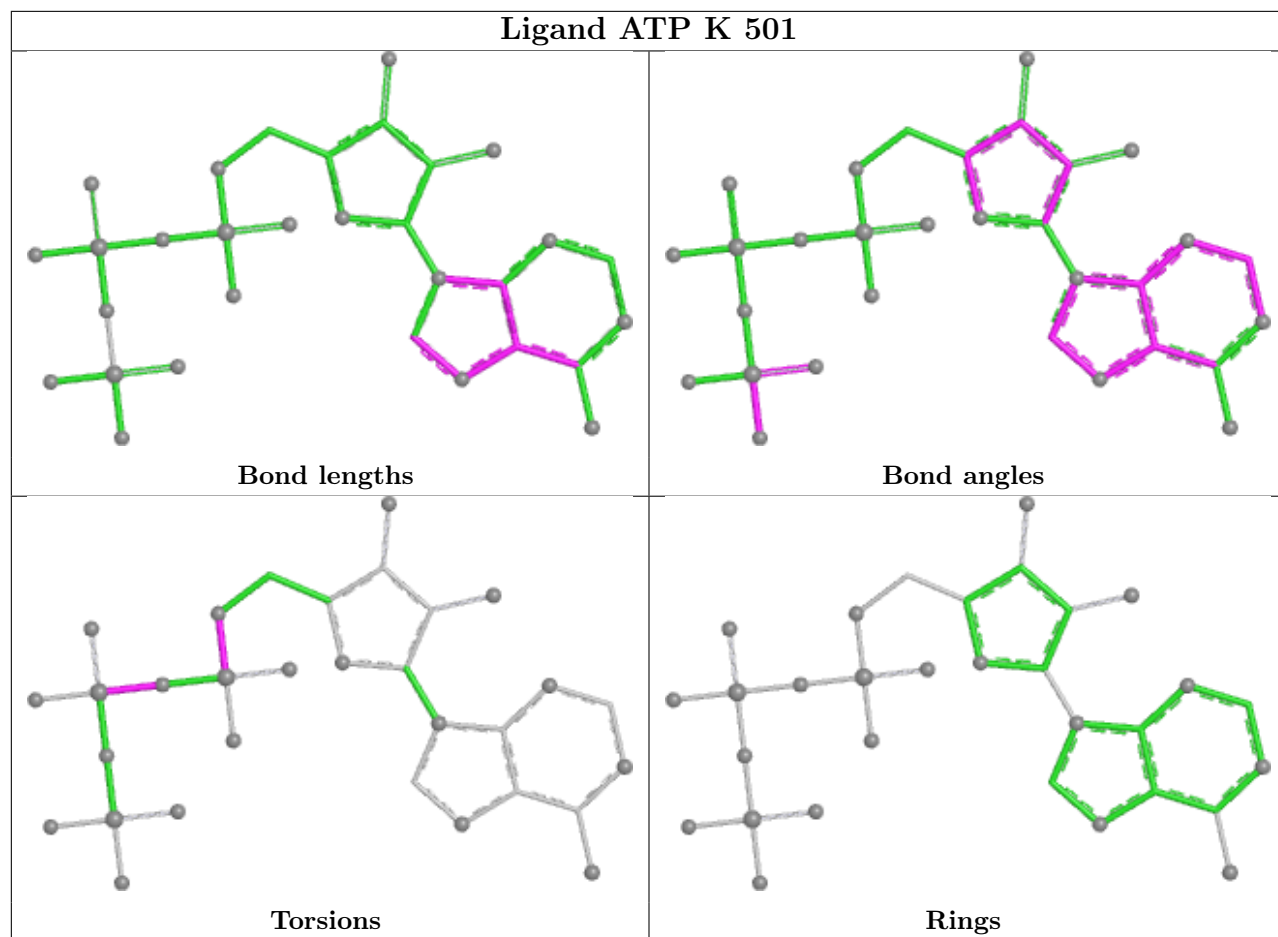
There are no ring outliers.

4 monomers are involved in 11 short contacts:

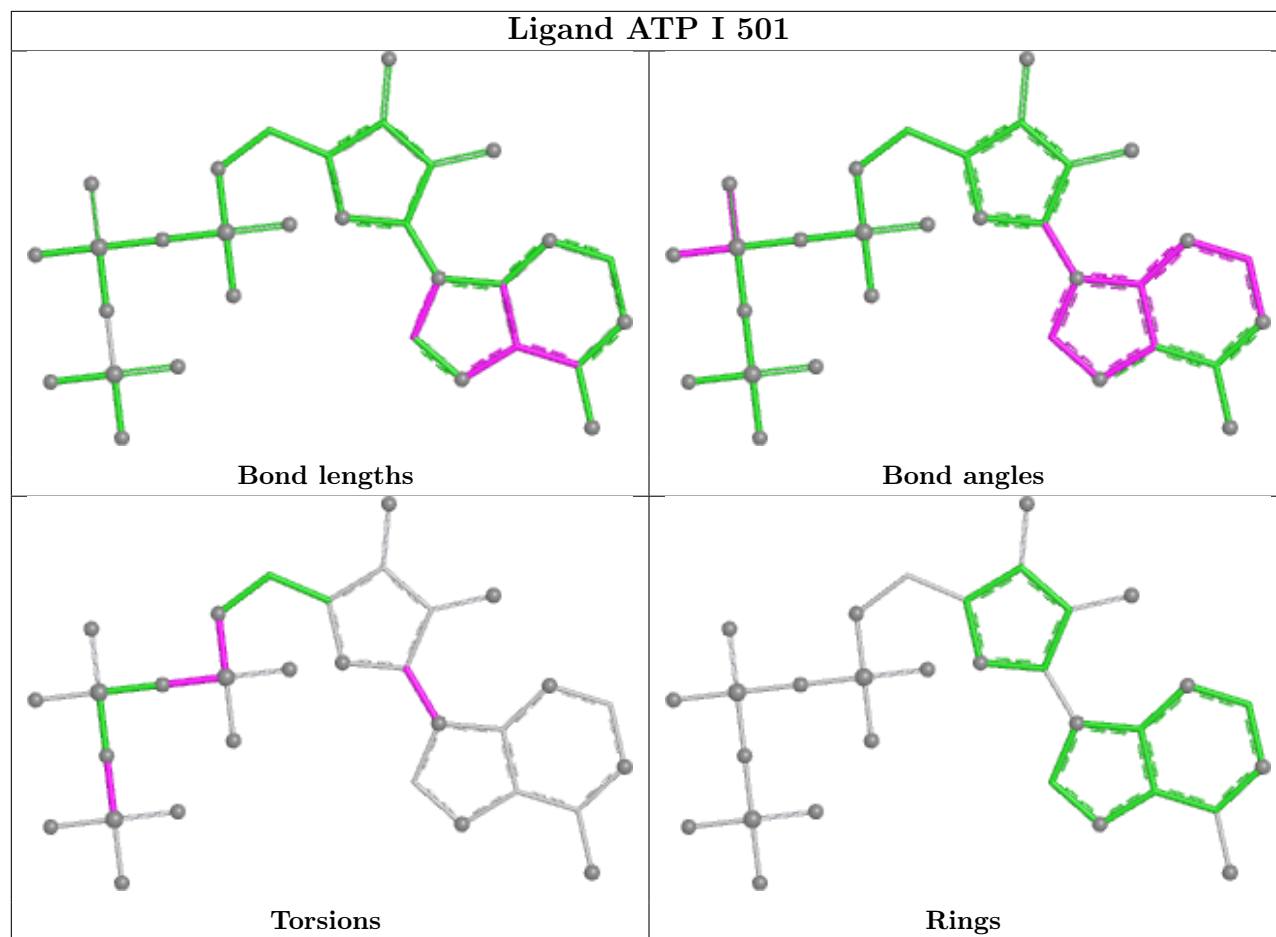
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	501	ADP	2	0
16	K	501	ATP	4	0
16	I	501	ATP	2	0
16	J	501	ATP	3	0

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

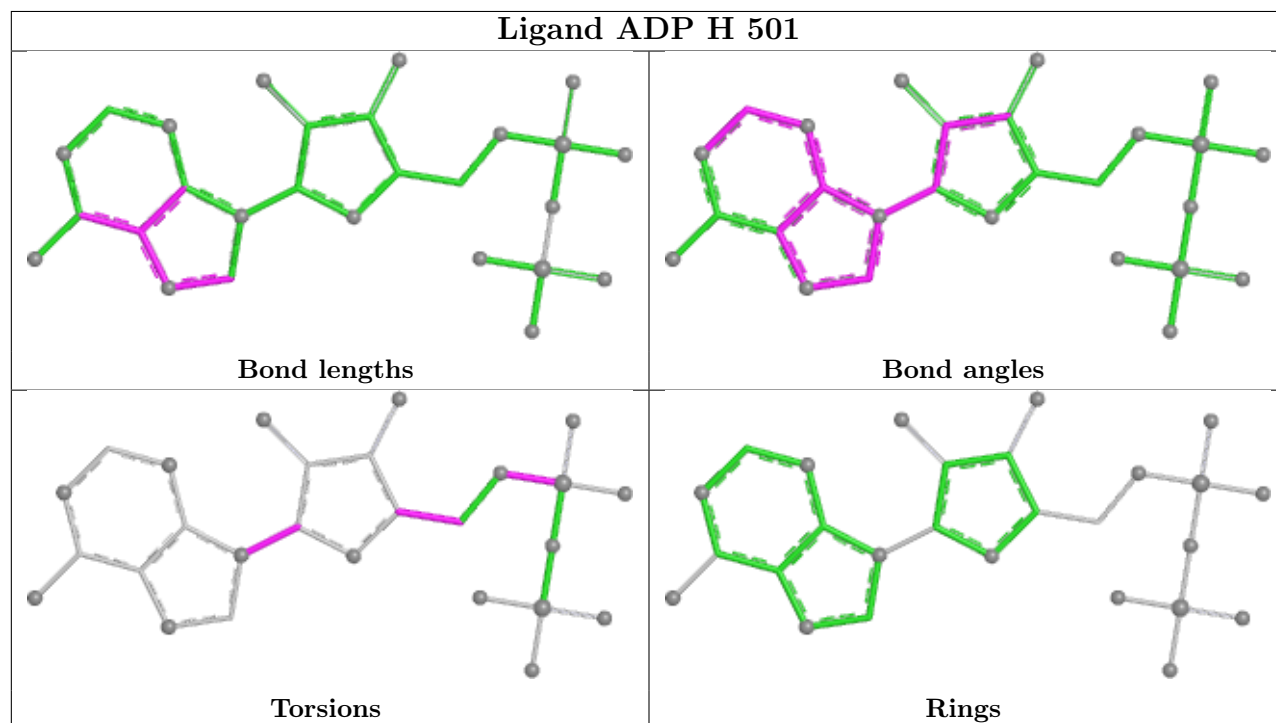


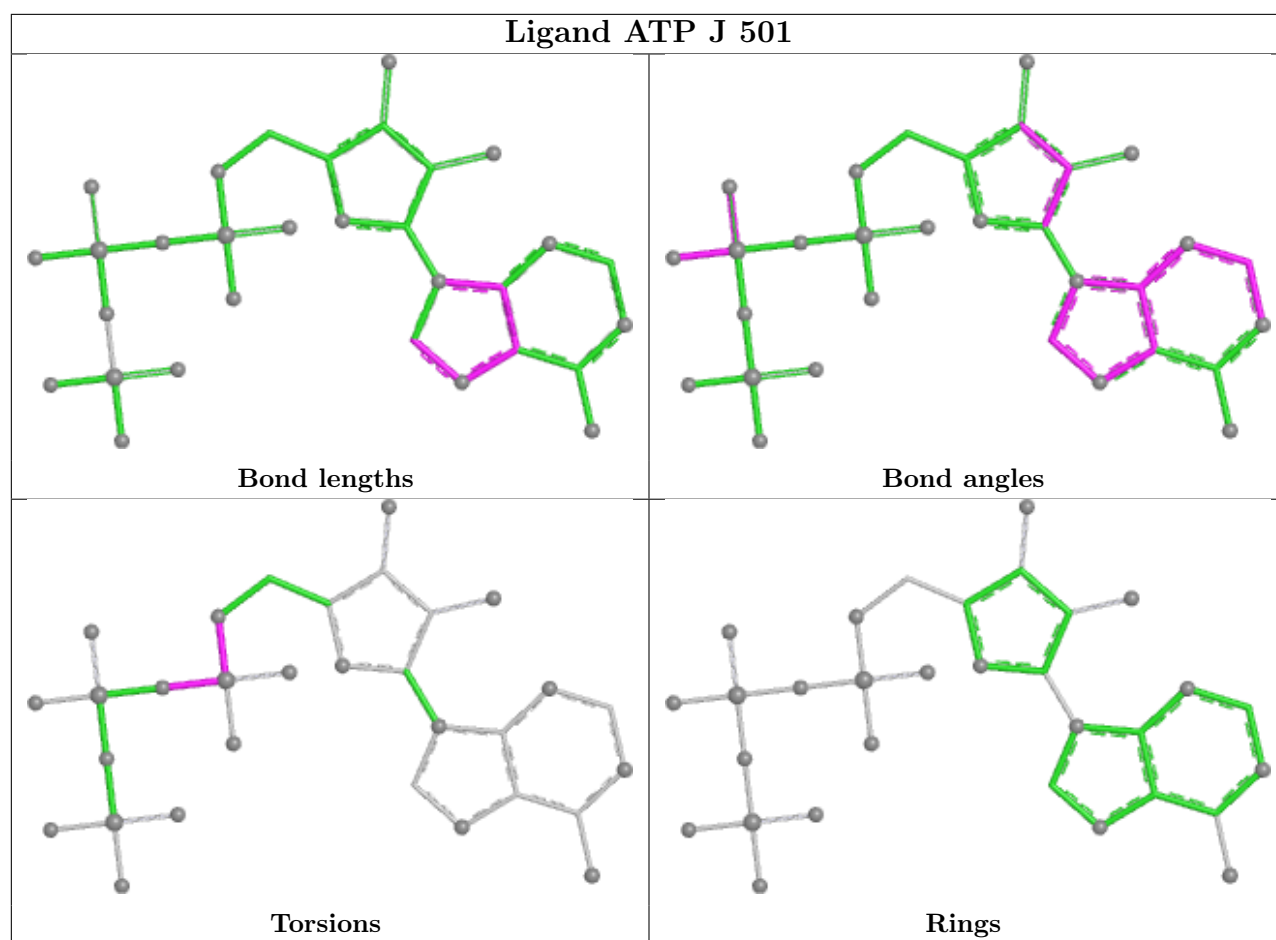


Ligand ATP I 501



Ligand ADP H 501





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.

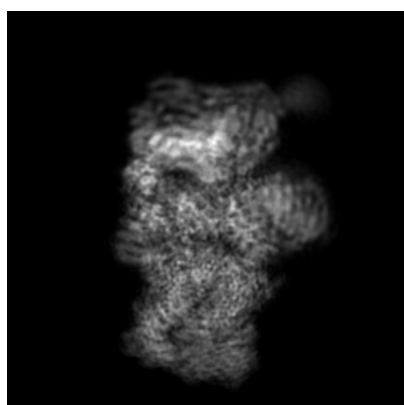
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9042. These allow visual inspection of the internal detail of the map and identification of artifacts.

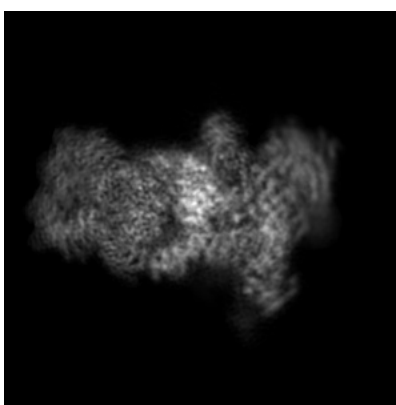
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

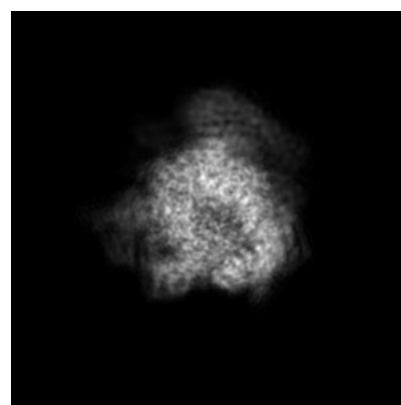
6.1.1 Primary map



X



Y

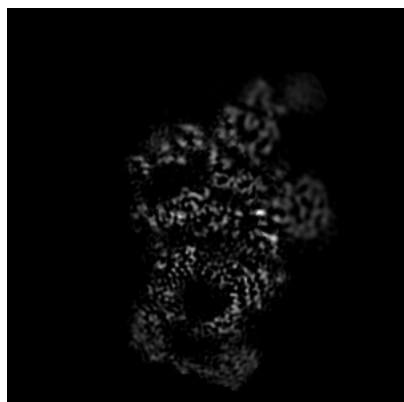


Z

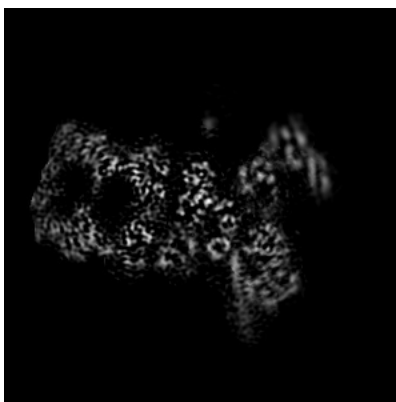
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

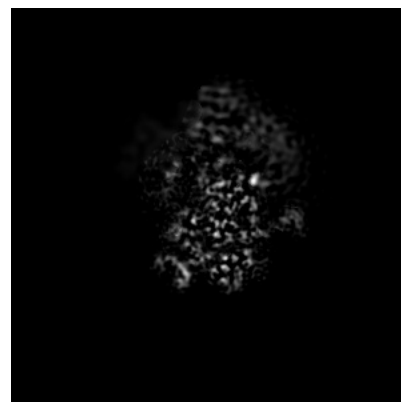
6.2.1 Primary map



X Index: 170



Y Index: 170

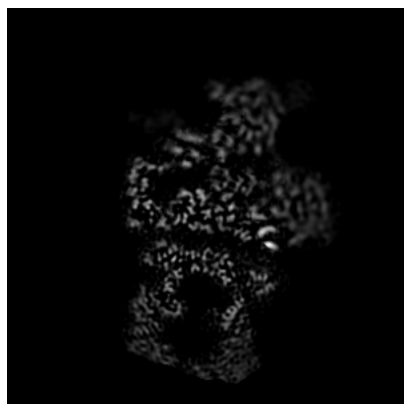


Z Index: 170

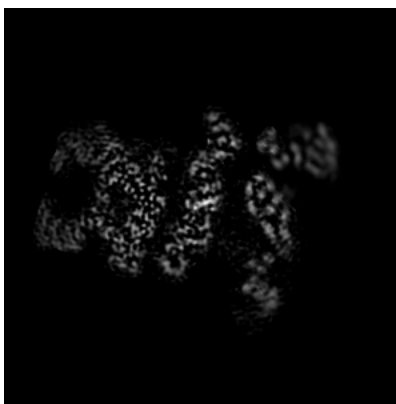
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

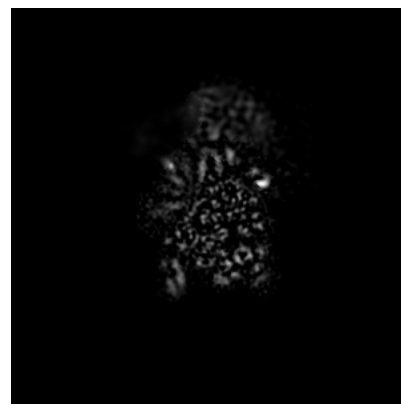
6.3.1 Primary map



X Index: 179



Y Index: 147

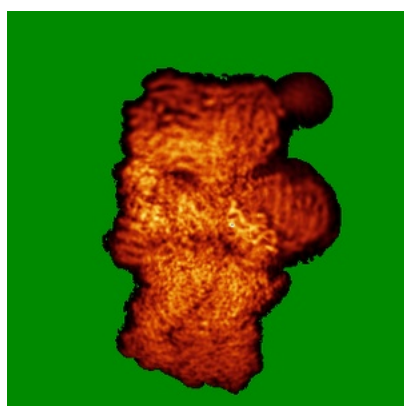


Z Index: 158

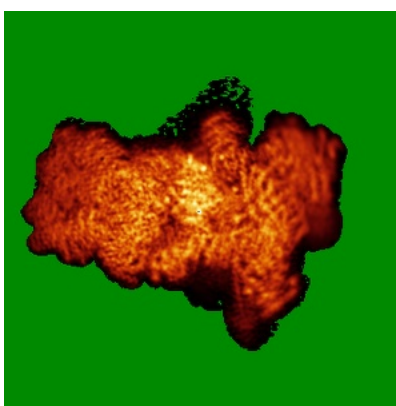
The images above show the largest variance slices of the map in three orthogonal directions.

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

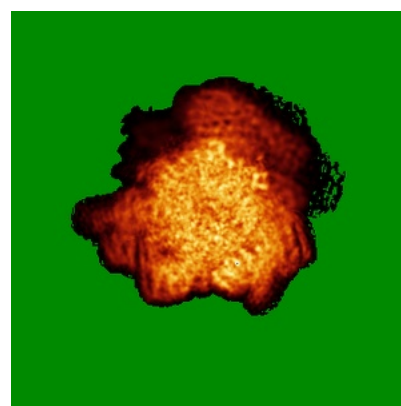
6.4.1 Primary map



X



Y



Z

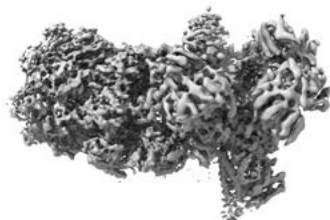
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

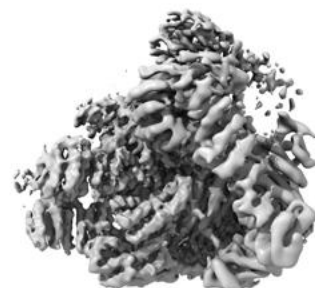
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

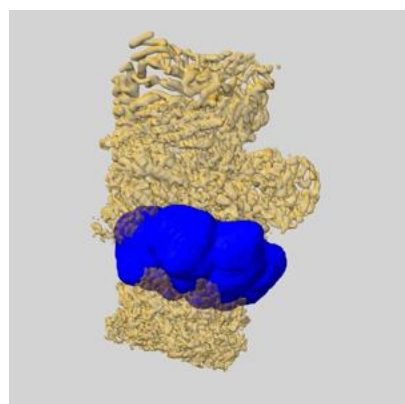
6.6 Mask visualisation [i](#)

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

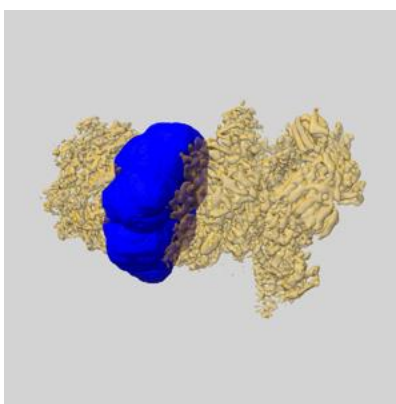
A mask typically either:

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

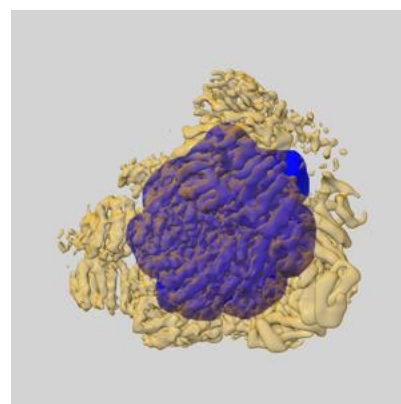
6.6.1 emd_9042_msk_3.map [i](#)



X

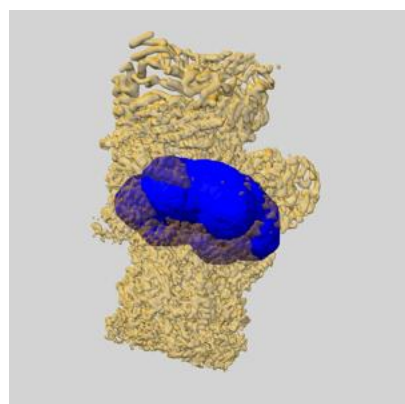


Y

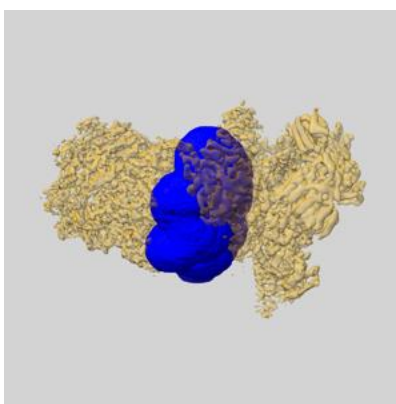


Z

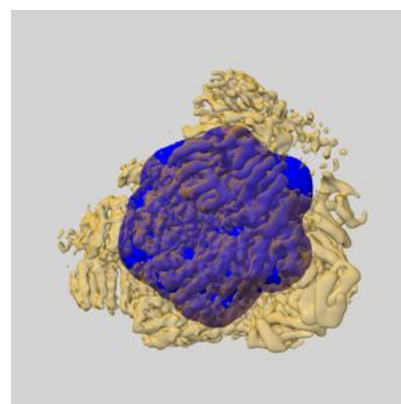
6.6.2 emd_9042_msk_2.map [i](#)



X

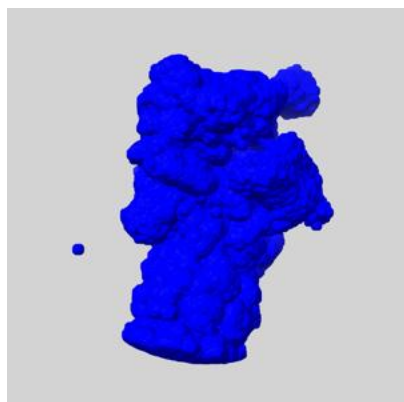


Y

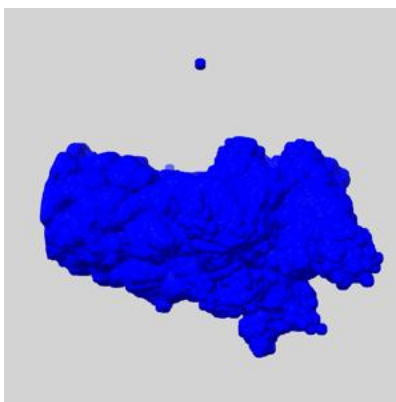


Z

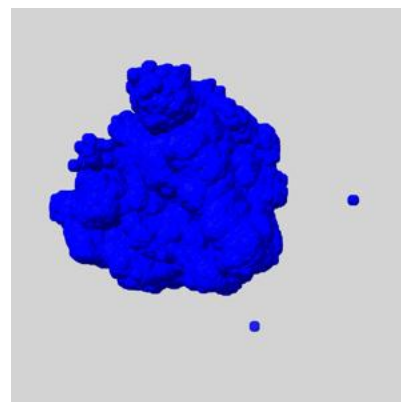
6.6.3 emd_9042_msk_1.map ⓘ



X



Y

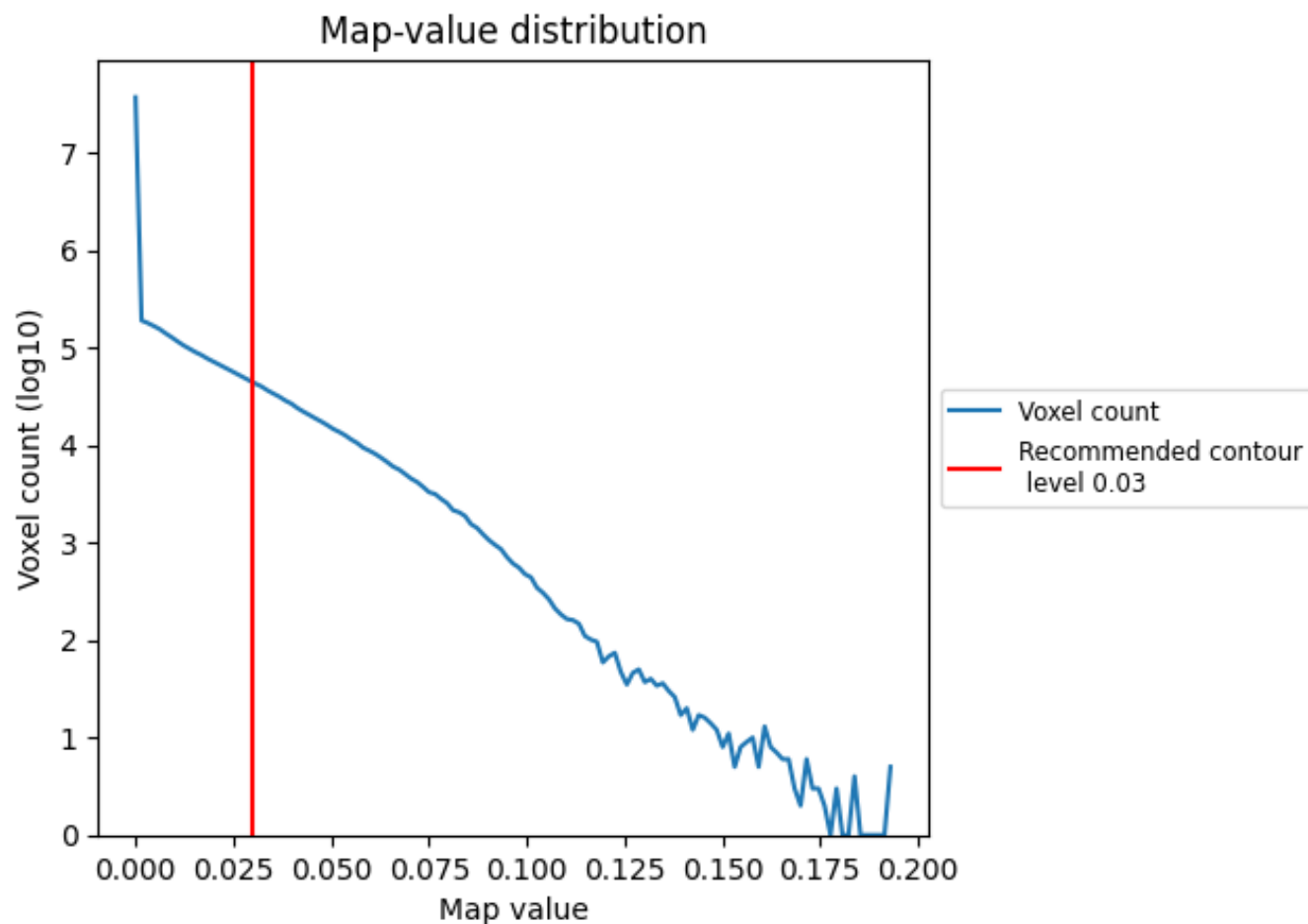


Z

7 Map analysis [i](#)

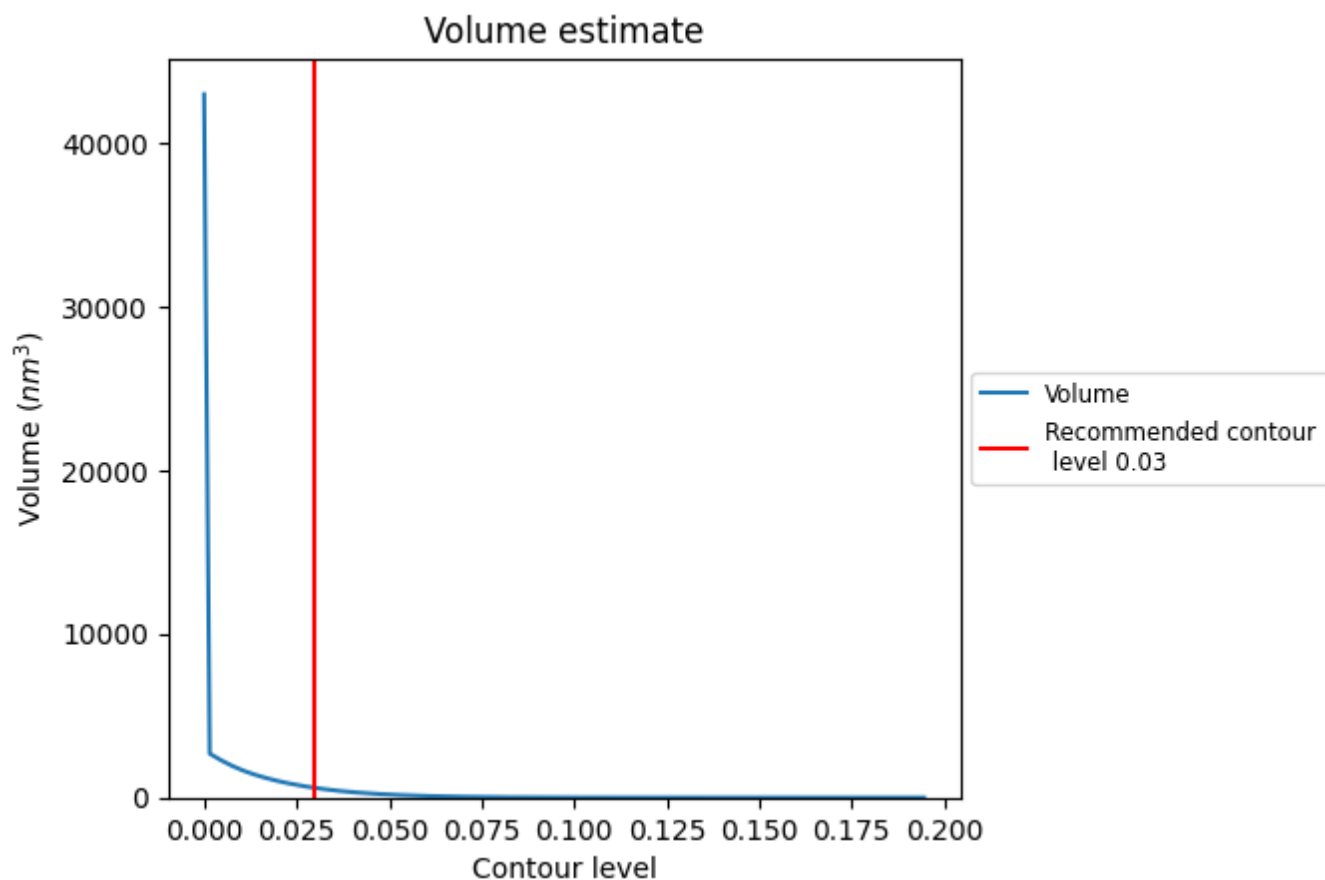
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

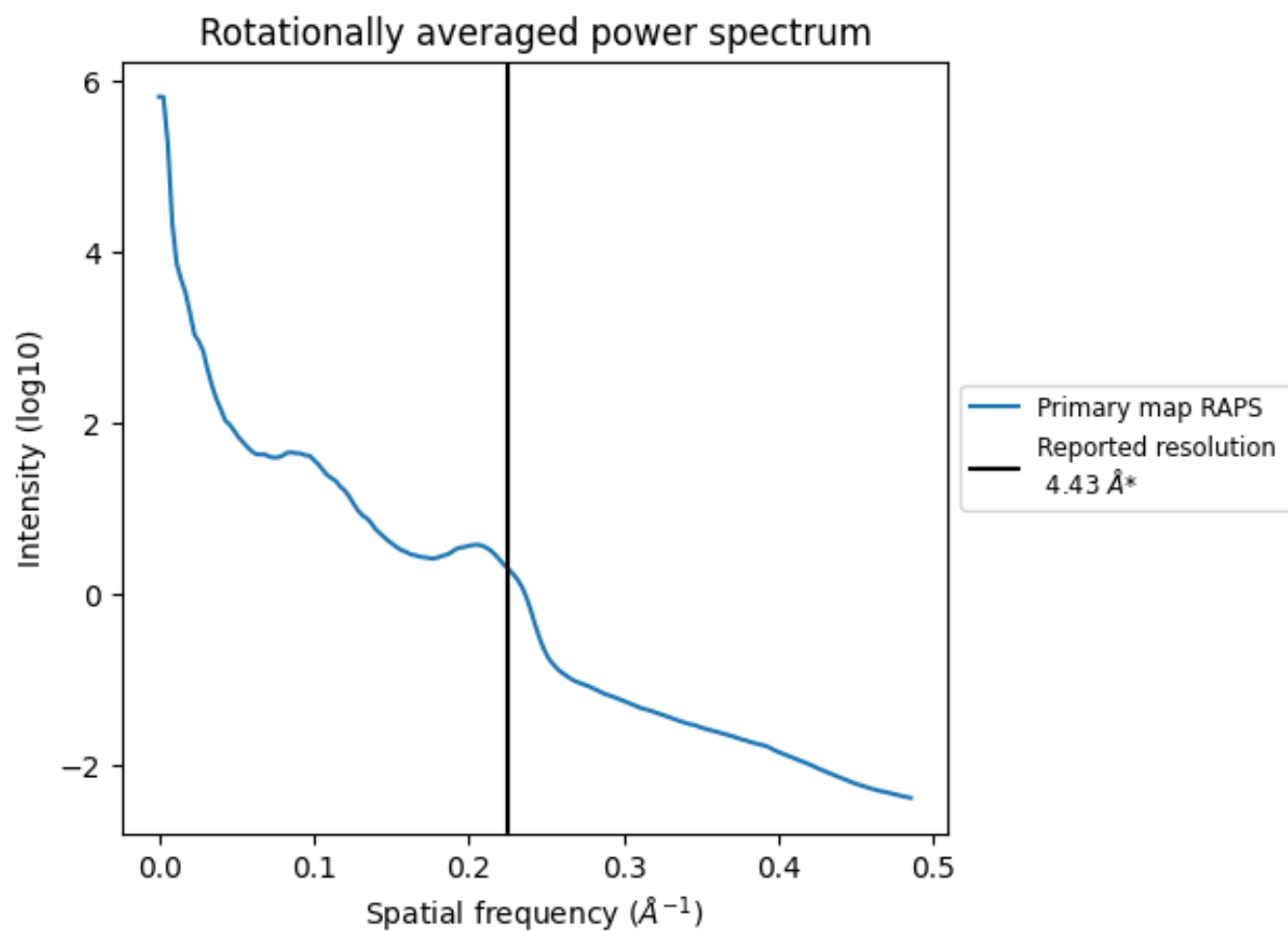
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 589 nm³; this corresponds to an approximate mass of 532 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 0.226 Å⁻¹

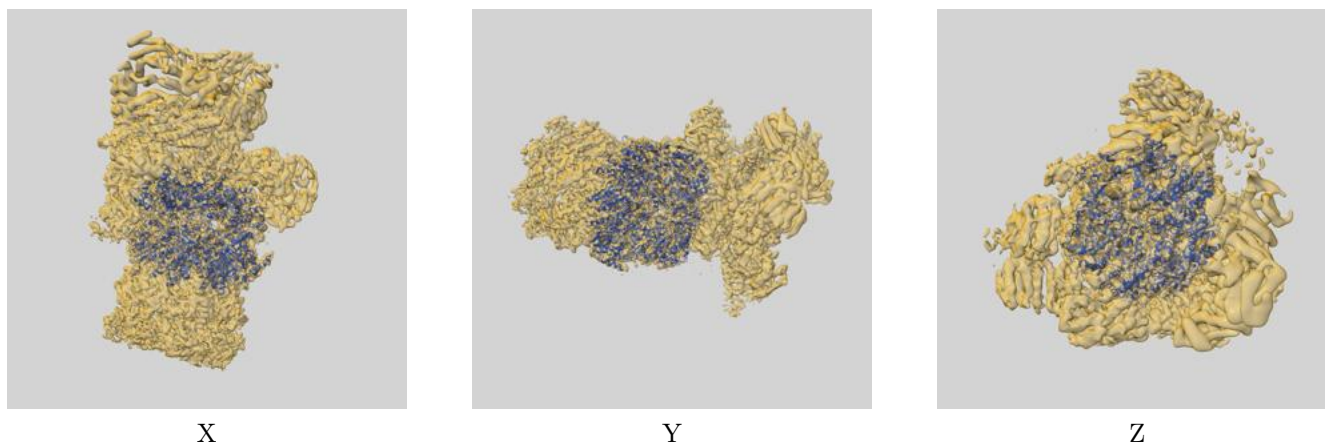
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

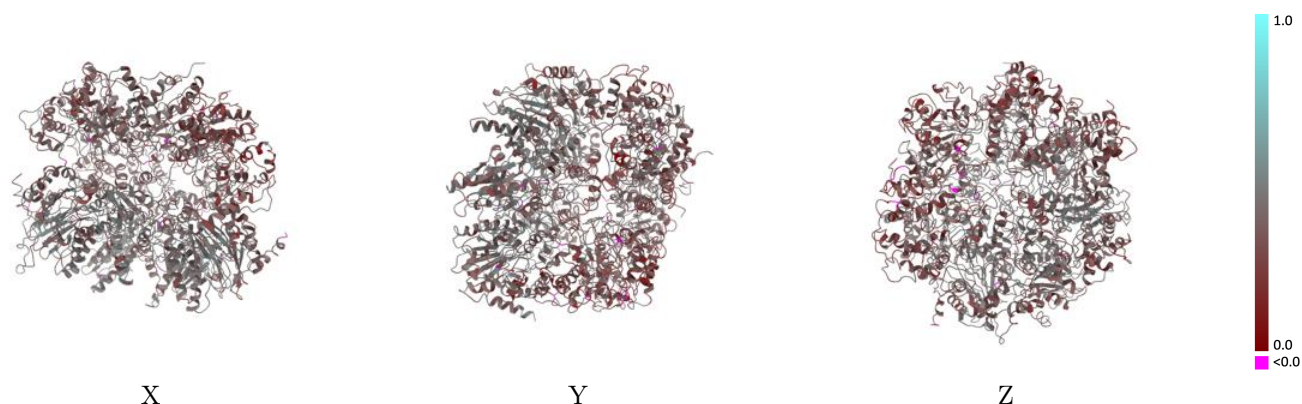
This section contains information regarding the fit between EMDB map EMD-9042 and PDB model 6EF0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



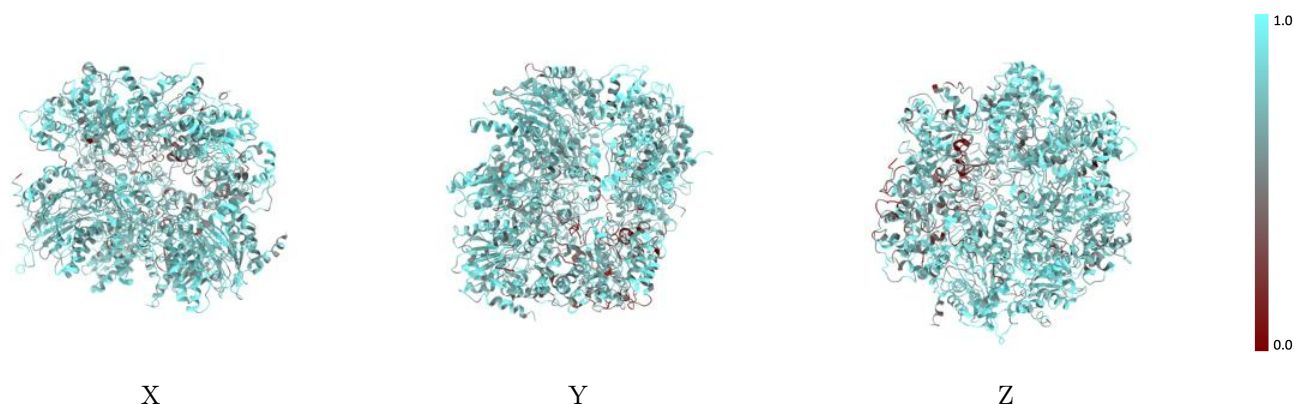
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



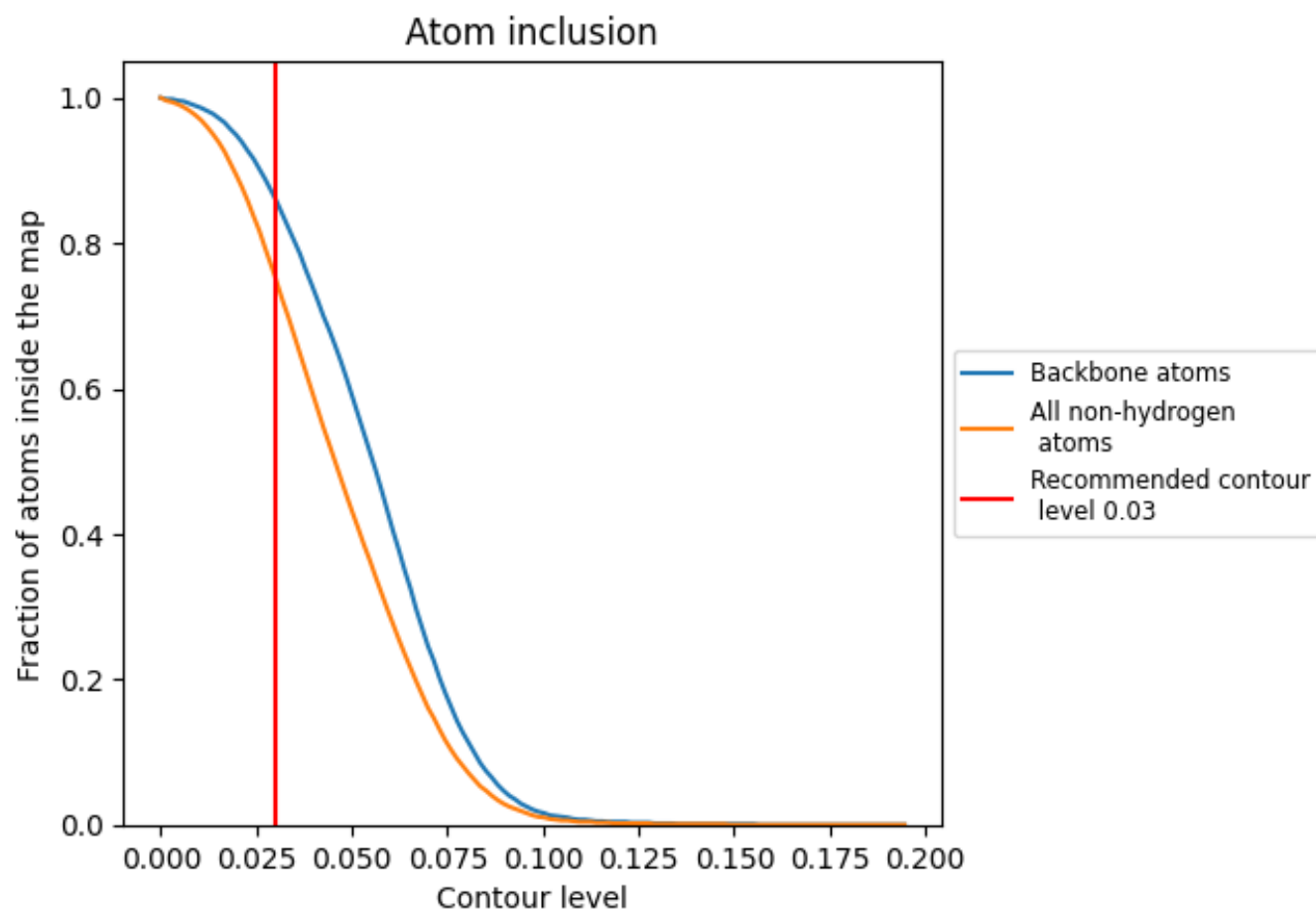
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.3830
A	0.7820	0.4100
B	0.7940	0.4290
C	0.7630	0.4230
D	0.7800	0.4090
E	0.7530	0.4120
F	0.7640	0.4020
G	0.7740	0.4230
H	0.6780	0.3250
I	0.7830	0.3310
J	0.7610	0.3710
K	0.7990	0.3810
L	0.7350	0.3640
M	0.6070	0.3040
s	0.7270	0.4720

1.0

0.0

<0.0