



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 12:34 AM EST

PDB ID : 6EF1
EMDB ID : EMD-9043
Title : Yeast 26S proteasome bound to ubiquitinated substrate (5D 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 : 4.73 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

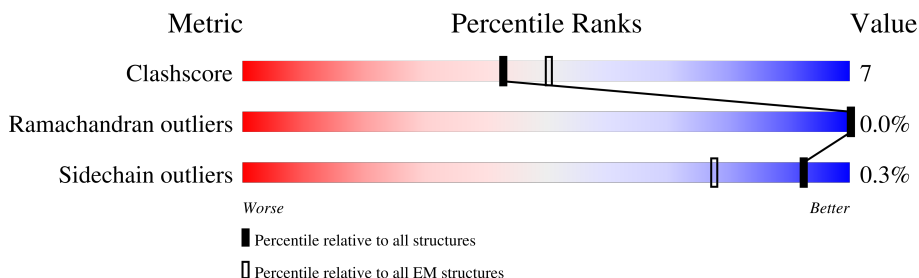
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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	239	
2	B	250	
3	C	238	
4	D	234	
5	E	242	
6	F	233	
7	G	243	
8	H	262	

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Mol	Chain	Length	Quality of chain
9	I	271	
10	J	273	
11	K	276	
12	L	271	
13	M	262	
14	s	15	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 23658 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	239	Total	C	N	O	S	0	0
			1818	1163	301	347	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
			1801	1149	299	350	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	238	Total	C	N	O	S	0	0
			1738	1110	286	340	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	234	Total	C	N	O	S	0	0
			1669	1052	287	326	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	242	Total	C	N	O	S	0	0
			1725	1086	297	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1736	1093	300	339	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	243	Total	C	N	O	S	0	0
			1822	1162	316	340	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	254	Total	C	N	O	S	0	0
			1764	1101	324	332	7		

- 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
			1918	1204	333	375	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	273	Total	C	N	O	S	0	0
			1923	1223	338	352	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	276	Total	C	N	O	S	0	0
			1856	1174	324	356	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	264	Total	C	N	O	S	0	0
			1867	1183	317	360	7		

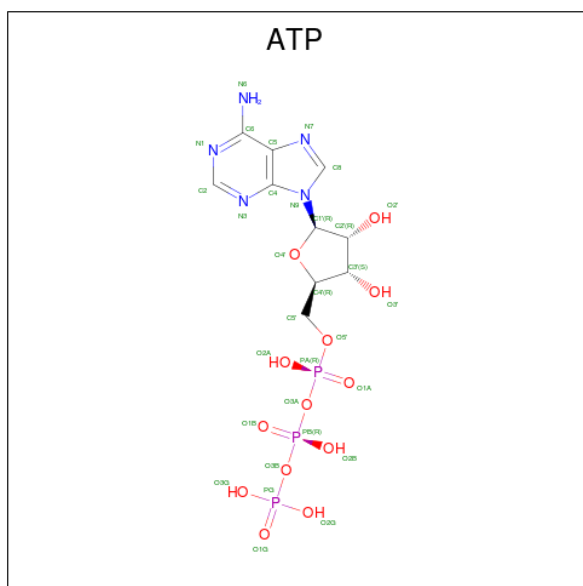
- Molecule 13 is a protein called 26S proteasome regulatory subunit 6A.

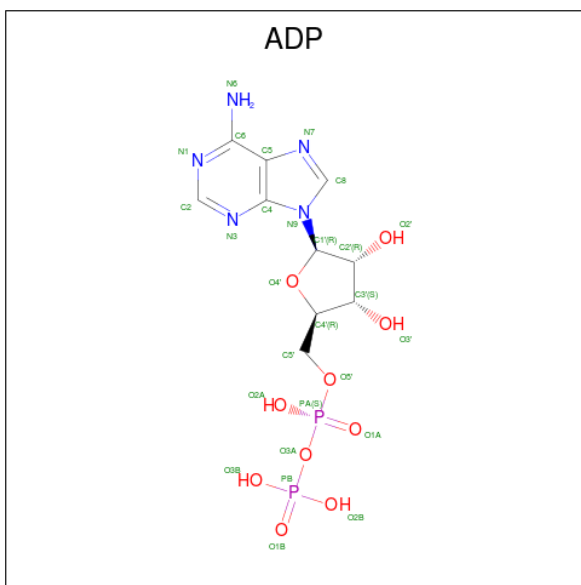
Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	262	Total	C	N	O	S	0	0
			1756	1088	312	352	4		

- Molecule 14 is a protein called model substrate polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	s	15	Total	C	N	O	0	0
			87	51	16	20		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



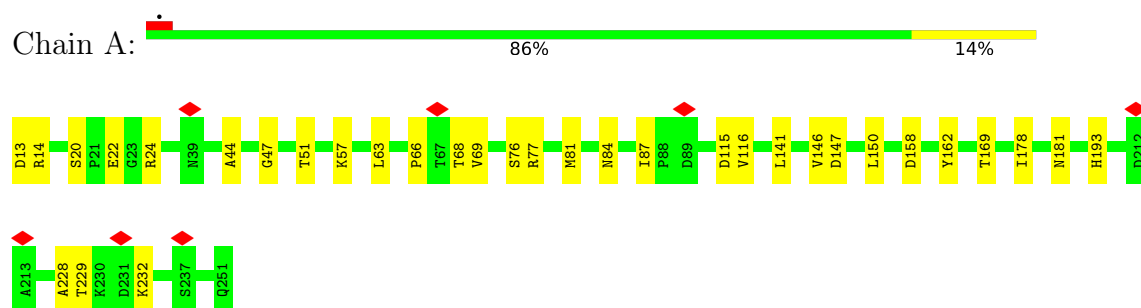


Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total 27	C 10	N 5	O 10	P 2	0
16	M	1	Total 27	C 10	N 5	O 10	P 2	0

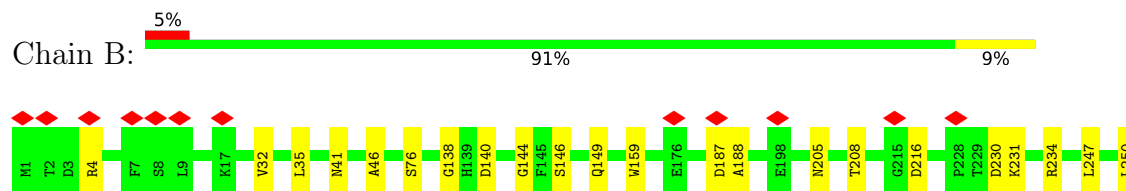
3 Residue-property plots

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.

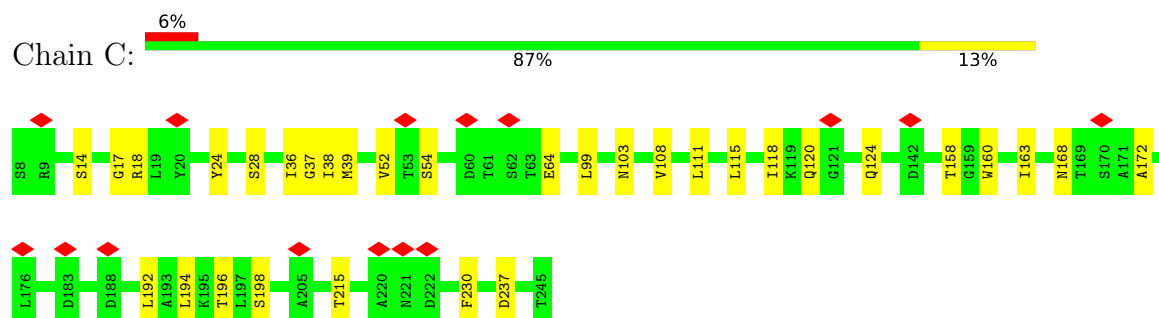
• Molecule 1: Proteasome subunit alpha type-1



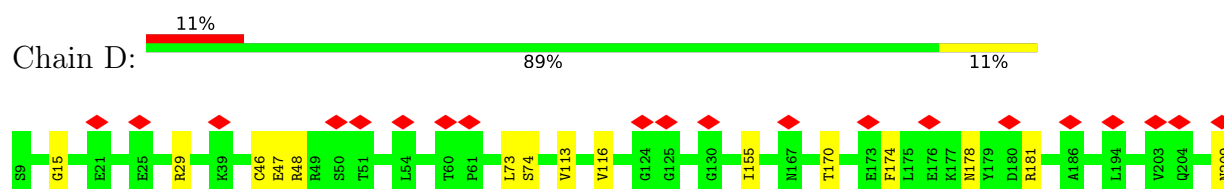
• Molecule 2: Proteasome subunit alpha type-2



• Molecule 3: Proteasome subunit alpha type-3

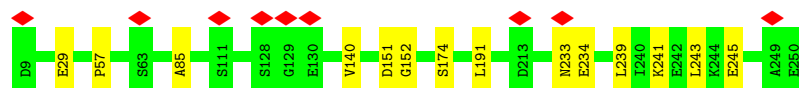


• Molecule 4: Proteasome subunit alpha type-4

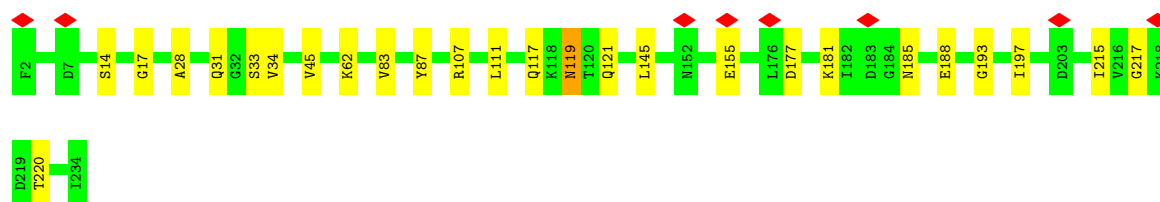




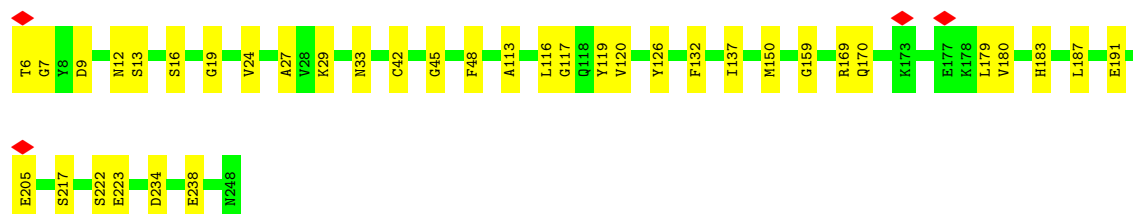
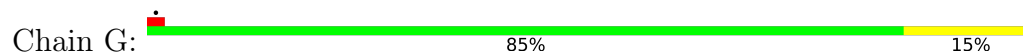
- Molecule 5: Proteasome subunit alpha type-5



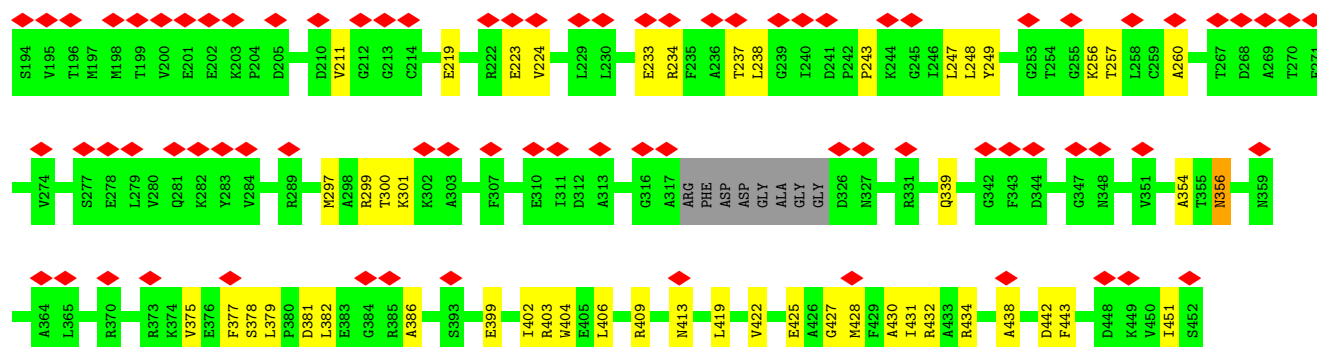
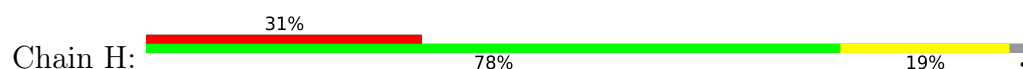
- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Probable proteasome subunit alpha type-7

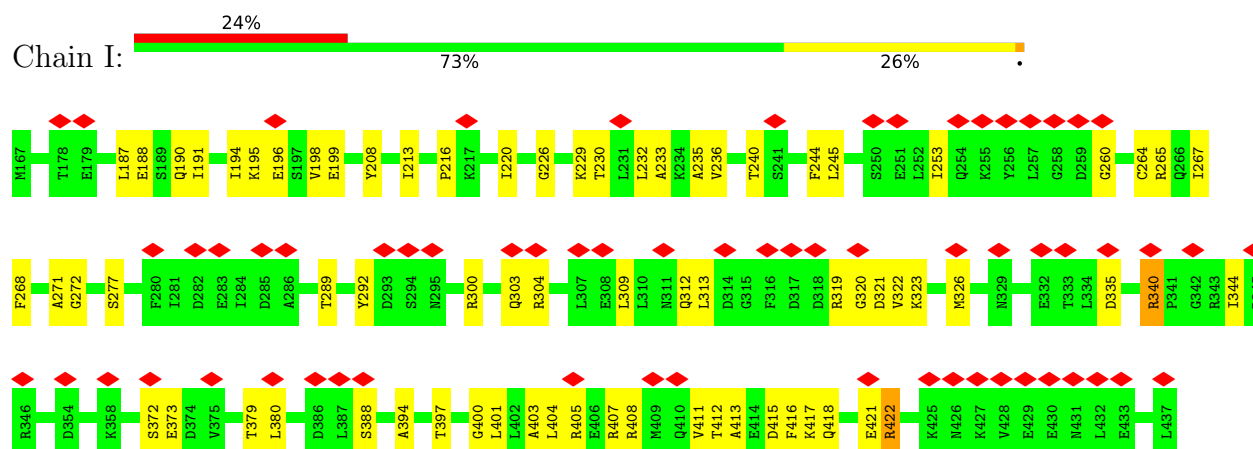


- Molecule 8: 26S proteasome regulatory subunit 7 homolog

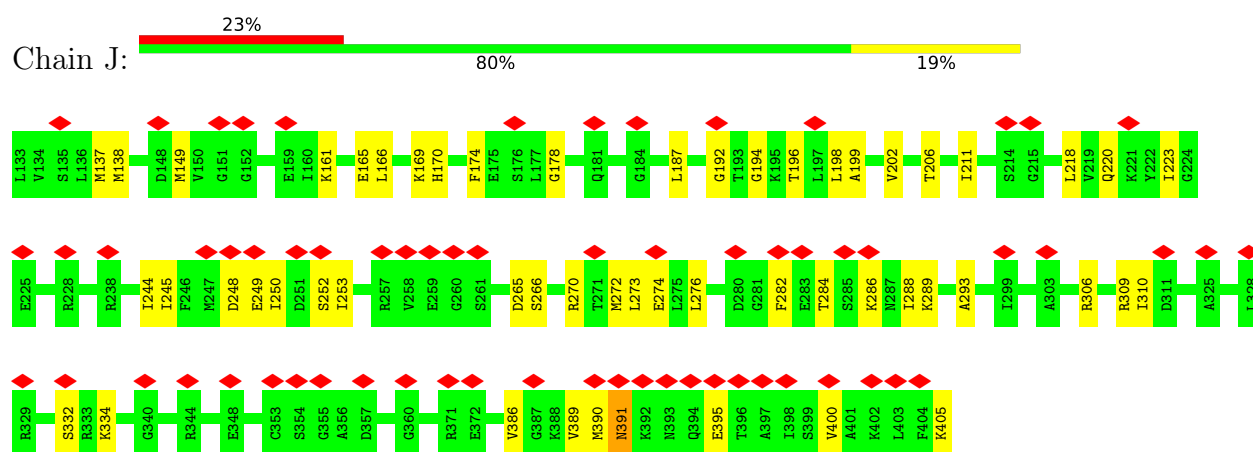




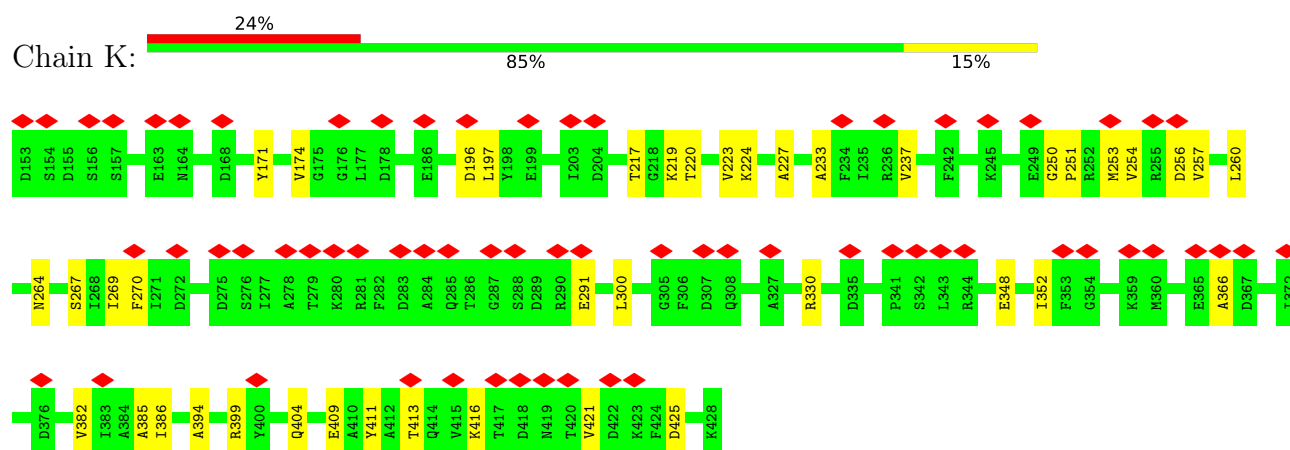
- Molecule 9: 26S proteasome regulatory subunit 4 homolog



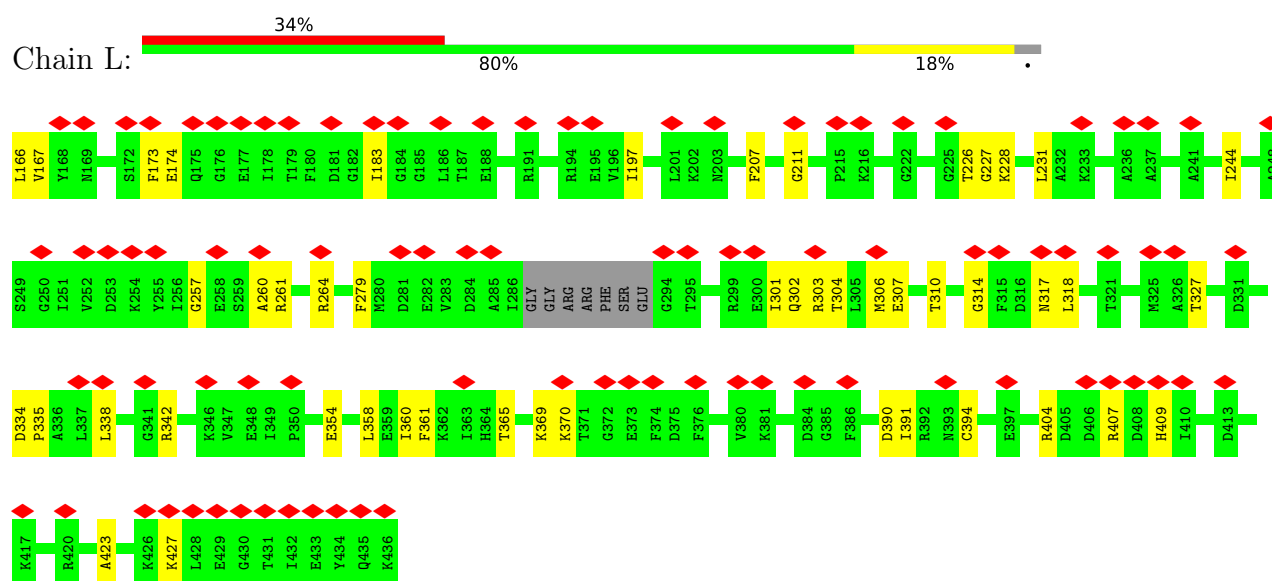
- Molecule 10: 26S proteasome regulatory subunit 8 homolog



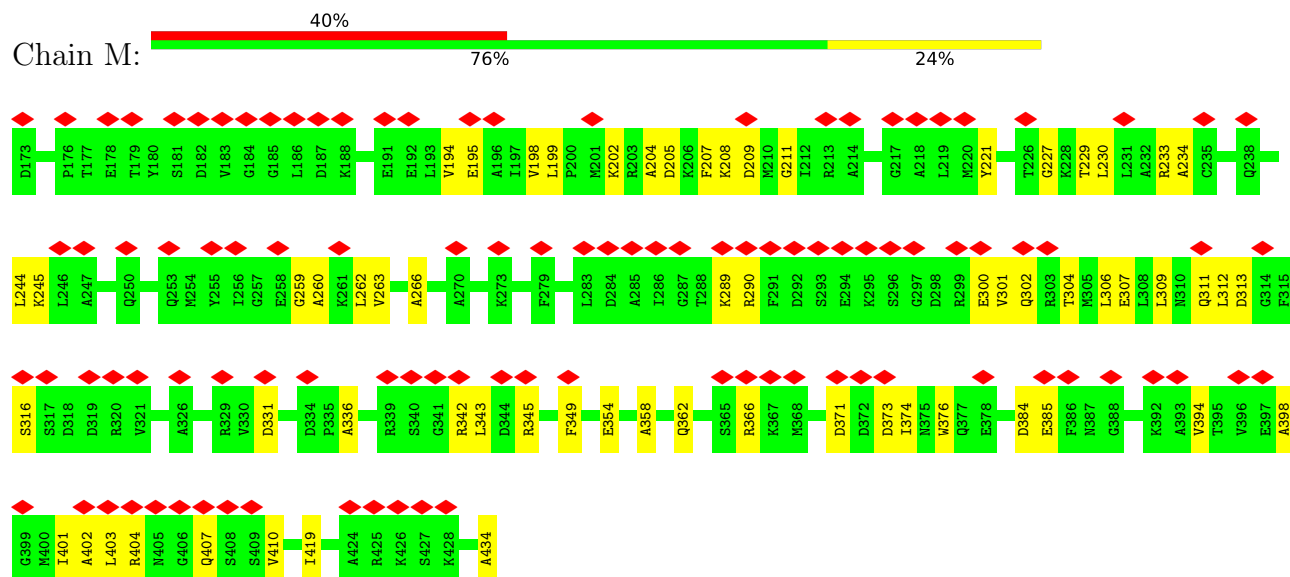
- Molecule 11: 26S proteasome regulatory subunit 6B homolog



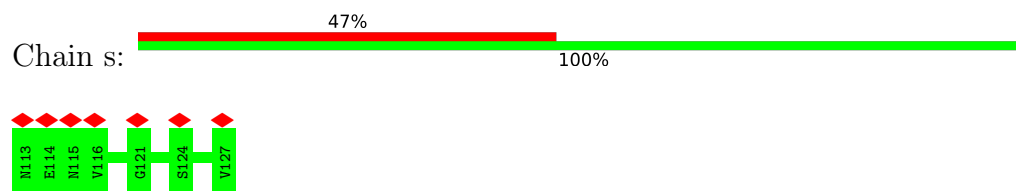
- Molecule 12: 26S proteasome subunit RPT4



• 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	31019	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	0.155	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	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	0.48	0/1854	0.58	0/2522
2	B	0.48	0/1837	0.61	0/2509
3	C	0.45	0/1767	0.64	1/2413 (0.0%)
4	D	0.45	0/1697	0.62	0/2325
5	E	0.44	0/1749	0.57	0/2377
6	F	0.47	0/1763	0.65	0/2392
7	G	0.50	0/1861	0.59	0/2526
8	H	0.34	0/1788	0.59	0/2437
9	I	0.34	0/1940	0.62	1/2638 (0.0%)
10	J	0.37	0/1952	0.60	0/2650
11	K	0.34	0/1882	0.57	0/2578
12	L	0.33	0/1898	0.56	0/2587
13	M	0.31	0/1777	0.58	0/2429
14	s	0.31	0/86	0.49	0/116
All	All	0.41	0/23851	0.60	2/32499 (0.0%)

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
10	J	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	237	ASP	CB-CG-OD1	7.01	124.61	118.30
9	I	340	ARG	NE-CZ-NH1	5.29	122.95	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	MET	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	1818	0	1762	21	0
2	B	1801	0	1724	11	0
3	C	1738	0	1657	21	0
4	D	1669	0	1544	16	0
5	E	1725	0	1631	9	0
6	F	1736	0	1689	15	0
7	G	1822	0	1757	21	0
8	H	1764	0	1624	37	0
9	I	1918	0	1817	50	0
10	J	1923	0	1845	34	0
11	K	1856	0	1639	27	0
12	L	1867	0	1717	31	0
13	M	1756	0	1522	42	0
14	s	87	0	70	0	0
15	H	31	0	12	5	0
15	I	31	0	12	2	0
15	J	31	0	12	2	0
15	K	31	0	12	3	0
16	L	27	0	12	4	0
16	M	27	0	12	1	0
All	All	23658	0	22070	323	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 7.

All (323) 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)
2:B:35:LEU:HD21	2:B:46:ALA:HB3	1.58	0.85
12:L:228:LYS:NZ	12:L:327:THR:O	2.18	0.77
10:J:284:THR:O	10:J:288:ILE:N	2.20	0.74
8:H:297:MET:O	8:H:300:THR:OG1	2.04	0.74
9:I:404:LEU:O	9:I:407:ARG:NH2	2.21	0.73
12:L:335:PRO:O	12:L:342:ARG:NH1	2.21	0.73
12:L:404:ARG:NH2	13:M:195:GLU:OE2	2.22	0.73
4:D:15:GLY:N	5:E:29:GLU:OE2	2.22	0.72
15:I:501:ATP:O3B	10:J:309:ARG:NH2	2.21	0.72
13:M:362:GLN:O	13:M:366:ARG:N	2.23	0.72
13:M:336:ALA:O	13:M:342:ARG:NH1	2.23	0.71
9:I:418:GLN:O	9:I:422:ARG:N	2.22	0.71
10:J:391:ASN:O	10:J:395:GLU:N	2.22	0.71
9:I:373:GLU:OE2	9:I:413:ALA:N	2.23	0.71
3:C:160:TRP:CD2	3:C:163:ILE:HD11	2.26	0.70
11:K:382:VAL:O	11:K:385:ALA:N	2.24	0.70
13:M:198:VAL:O	13:M:202:LYS:N	2.24	0.70
7:G:12:ASN:ND2	7:G:126:TYR:O	2.25	0.69
12:L:227:GLY:N	16:L:501:ADP:O3B	2.25	0.69
10:J:187:LEU:HD21	10:J:293:ALA:HB2	1.73	0.69
4:D:174:PHE:O	4:D:178:ASN:ND2	2.25	0.69
9:I:277:SER:OG	9:I:321:ASP:O	2.10	0.69
8:H:256:LYS:NZ	15:H:501:ATP:O1B	2.25	0.68
10:J:161:LYS:O	10:J:165:GLU:N	2.26	0.68
8:H:299:ARG:NH2	8:H:339:GLN:O	2.26	0.68
10:J:174:PHE:O	10:J:178:GLY:N	2.26	0.67
11:K:394:ALA:O	11:K:399:ARG:N	2.27	0.67
8:H:247:LEU:O	8:H:375:VAL:N	2.28	0.67
10:J:249:GLU:OE2	10:J:252:SER:N	2.28	0.67
3:C:158:THR:HG1	3:C:160:TRP:HE1	1.41	0.66
10:J:211:ILE:HD11	10:J:245:ILE:HG22	1.78	0.66
11:K:409:GLU:O	11:K:413:THR:N	2.29	0.66
12:L:334:ASP:O	12:L:338:LEU:N	2.29	0.66
9:I:236:VAL:O	9:I:240:THR:N	2.28	0.66
13:M:394:VAL:HB	13:M:419:ILE:HG21	1.76	0.66
7:G:169:ARG:NH1	7:G:170:GLN:OE1	2.29	0.65
8:H:432:ARG:NH2	9:I:196:GLU:OE1	2.29	0.65
8:H:211:VAL:HG23	15:H:501:ATP:N1	2.12	0.65
8:H:256:LYS:O	8:H:260:ALA:N	2.29	0.65
8:H:382:LEU:O	8:H:386:ALA:N	2.30	0.64
4:D:170:THR:O	4:D:174:PHE:N	2.31	0.64
9:I:417:LYS:NZ	9:I:421:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:GLU:O	10:J:405:LYS:NZ	2.30	0.64
12:L:303:ARG:O	12:L:307:GLU:N	2.31	0.64
13:M:300:GLU:O	13:M:304:THR:HG23	1.97	0.63
2:B:205:ASN:O	2:B:208:THR:OG1	2.14	0.63
9:I:415:ASP:HA	9:I:418:GLN:HE22	1.63	0.63
9:I:403:ALA:HB1	9:I:408:ARG:O	1.99	0.63
12:L:423:ALA:O	12:L:427:LYS:N	2.31	0.63
9:I:220:ILE:HD13	9:I:326:MET:HB2	1.81	0.63
15:J:501:ATP:O3A	11:K:330:ARG:NH1	2.32	0.63
12:L:226:THR:N	16:L:501:ADP:O3B	2.32	0.62
13:M:402:ALA:O	13:M:407:GLN:N	2.32	0.62
2:B:140:ASP:OD1	2:B:144:GLY:N	2.32	0.62
9:I:267:ILE:O	9:I:271:ALA:N	2.32	0.62
11:K:260:LEU:O	11:K:264:ASN:ND2	2.32	0.62
10:J:282:PHE:O	10:J:286:LYS:N	2.33	0.61
13:M:221:TYR:O	13:M:349:PHE:N	2.33	0.61
3:C:14:SER:N	3:C:18:ARG:O	2.33	0.61
9:I:194:ILE:O	9:I:198:VAL:N	2.33	0.61
13:M:259:GLY:O	13:M:263:VAL:N	2.34	0.61
8:H:248:LEU:HD22	8:H:354:ALA:CB	2.30	0.61
11:K:253:MET:O	11:K:257:VAL:N	2.34	0.61
13:M:300:GLU:O	13:M:304:THR:N	2.34	0.61
3:C:14:SER:OG	3:C:18:ARG:N	2.34	0.61
9:I:403:ALA:O	9:I:407:ARG:N	2.34	0.60
13:M:373:ASP:H	13:M:374:ILE:HD12	1.66	0.60
4:D:236:ILE:O	4:D:240:LYS:N	2.34	0.60
6:F:62:LYS:NZ	13:M:434:ALA:O	2.25	0.60
15:H:501:ATP:O3A	9:I:340:ARG:NH1	2.34	0.60
7:G:29:LYS:O	7:G:33:ASN:ND2	2.35	0.60
9:I:403:ALA:O	9:I:408:ARG:N	2.32	0.60
12:L:301:ILE:O	12:L:304:THR:OG1	2.09	0.60
9:I:292:TYR:O	9:I:303:GLN:NE2	2.28	0.60
12:L:390:ASP:O	12:L:394:CYS:N	2.36	0.59
8:H:234:ARG:HD3	13:M:403:LEU:HD11	1.84	0.59
3:C:192:LEU:O	3:C:196:THR:N	2.34	0.59
1:A:147:ASP:OD2	1:A:150:LEU:N	2.35	0.58
9:I:401:LEU:O	9:I:405:ARG:N	2.36	0.58
13:M:358:ALA:HB1	13:M:376:TRP:HE1	1.67	0.58
9:I:226:GLY:O	9:I:388:SER:OG	2.21	0.58
5:E:241:LYS:O	5:E:245:GLU:N	2.36	0.58
12:L:174:GLU:OE1	12:L:174:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:69:VAL:HG12	1.86	0.58
12:L:244:ILE:HD11	12:L:279:PHE:O	2.04	0.58
8:H:219:GLU:OE1	13:M:404:ARG:NE	2.37	0.57
8:H:442:ASP:OD1	8:H:443:PHE:N	2.37	0.57
11:K:421:VAL:O	11:K:425:ASP:N	2.38	0.57
9:I:373:GLU:OE1	9:I:373:GLU:N	2.37	0.57
7:G:16:SER:OG	7:G:19:GLY:N	2.38	0.57
8:H:219:GLU:O	8:H:223:GLU:N	2.38	0.57
12:L:354:GLU:O	12:L:358:LEU:HD23	2.05	0.57
12:L:369:LYS:NZ	12:L:407:ARG:O	2.35	0.57
13:M:198:VAL:HG13	13:M:199:LEU:HD22	1.87	0.56
13:M:207:PHE:O	13:M:211:GLY:N	2.37	0.56
13:M:307:GLU:O	13:M:311:GLN:N	2.35	0.56
10:J:306:ARG:O	10:J:309:ARG:N	2.37	0.56
8:H:248:LEU:HD22	8:H:354:ALA:HB1	1.87	0.56
12:L:173:PHE:N	12:L:174:GLU:OE1	2.38	0.55
12:L:260:ALA:O	12:L:264:ARG:NH1	2.38	0.55
3:C:194:LEU:O	3:C:198:SER:N	2.38	0.55
13:M:302:GLN:O	13:M:306:LEU:N	2.39	0.55
9:I:229:LYS:NZ	15:I:501:ATP:O3A	2.33	0.55
6:F:107:ARG:O	6:F:111:LEU:N	2.39	0.55
11:K:171:TYR:O	11:K:174:VAL:HG12	2.07	0.55
7:G:234:ASP:O	7:G:238:GLU:N	2.40	0.54
4:D:46:CYS:SG	4:D:47:GLU:N	2.81	0.54
10:J:137:MET:SD	10:J:138:MET:N	2.81	0.54
7:G:42:CYS:SG	7:G:45:GLY:N	2.80	0.54
4:D:234:THR:O	4:D:238:GLN:N	2.40	0.54
7:G:48:PHE:N	7:G:217:SER:O	2.41	0.53
11:K:220:THR:O	11:K:223:VAL:HG12	2.07	0.53
13:M:194:VAL:O	13:M:198:VAL:HG12	2.09	0.53
2:B:35:LEU:CD2	2:B:46:ALA:HB3	2.35	0.53
13:M:354:GLU:O	13:M:358:ALA:N	2.41	0.53
5:E:174:SER:OG	8:H:409:ARG:NH1	2.41	0.52
8:H:257:THR:OG1	15:H:501:ATP:O1A	2.27	0.52
3:C:215:THR:HG21	3:C:230:PHE:CZ	2.45	0.52
8:H:419:LEU:HA	8:H:422:VAL:HG12	1.91	0.52
9:I:415:ASP:O	9:I:418:GLN:NE2	2.41	0.52
7:G:205:GLU:N	7:G:205:GLU:OE1	2.42	0.52
1:A:44:ALA:N	1:A:169:THR:O	2.41	0.52
8:H:428:MET:SD	8:H:432:ARG:NH2	2.82	0.52
3:C:120:GLN:O	3:C:124:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:372:SER:N	9:I:411:VAL:O	2.40	0.51
1:A:76:SER:OG	1:A:77:ARG:N	2.43	0.51
8:H:238:LEU:HD13	8:H:238:LEU:O	2.11	0.51
13:M:289:LYS:NZ	13:M:331:ASP:O	2.26	0.51
10:J:272:MET:SD	10:J:273:LEU:N	2.84	0.51
13:M:309:LEU:O	13:M:313:ASP:N	2.40	0.51
4:D:181:ARG:NH2	5:E:57:PRO:O	2.44	0.51
13:M:371:ASP:OD1	13:M:410:VAL:N	2.43	0.51
1:A:51:THR:HG22	1:A:228:ALA:HB3	1.92	0.51
8:H:399:GLU:N	8:H:438:ALA:O	2.44	0.51
9:I:400:GLY:O	9:I:403:ALA:HB3	2.10	0.51
2:B:32:VAL:O	2:B:76:SER:OG	2.17	0.50
4:D:212:ILE:HD11	4:D:224:LEU:HB2	1.94	0.50
11:K:233:ALA:HB3	11:K:267:SER:CB	2.41	0.50
11:K:382:VAL:O	11:K:386:ILE:HD12	2.11	0.50
10:J:253:ILE:O	10:J:253:ILE:HG22	2.11	0.50
8:H:377:PHE:O	8:H:378:SER:OG	2.27	0.50
1:A:87:ILE:H	1:A:87:ILE:HD12	1.77	0.50
3:C:168:ASN:O	3:C:172:ALA:N	2.41	0.50
8:H:451:ILE:O	8:H:455:LYS:N	2.43	0.50
10:J:244:ILE:HG22	10:J:289:LYS:O	2.11	0.50
8:H:402:ILE:HD11	8:H:404:TRP:CD2	2.47	0.50
11:K:411:TYR:O	11:K:416:LYS:NZ	2.45	0.50
10:J:250:ILE:HG22	10:J:250:ILE:O	2.12	0.50
6:F:33:SER:OG	6:F:34:VAL:N	2.44	0.50
2:B:247:LEU:HA	2:B:250:LEU:HD23	1.94	0.49
8:H:356:ASN:O	8:H:356:ASN:ND2	2.43	0.49
13:M:205:ASP:O	13:M:209:ASP:N	2.41	0.49
9:I:380:LEU:HD22	9:I:416:PHE:CD2	2.47	0.49
1:A:63:LEU:HD23	1:A:63:LEU:H	1.76	0.49
9:I:232:LEU:O	9:I:235:ALA:HB3	2.12	0.49
7:G:6:THR:OG1	7:G:7:GLY:N	2.46	0.49
8:H:379:LEU:HD21	8:H:413:ASN:HD22	1.77	0.49
2:B:138:GLY:N	2:B:146:SER:O	2.45	0.49
5:E:191:LEU:HD23	5:E:191:LEU:H	1.78	0.48
12:L:390:ASP:OD1	12:L:391:ILE:N	2.46	0.48
13:M:230:LEU:O	13:M:234:ALA:N	2.46	0.48
6:F:14:SER:OG	6:F:17:GLY:N	2.45	0.48
13:M:204:ALA:O	13:M:208:LYS:N	2.40	0.48
7:G:120:VAL:HG12	7:G:132:PHE:CD2	2.48	0.48
9:I:319:ARG:O	9:I:321:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LEU:O	3:C:118:ILE:HG22	2.13	0.48
11:K:224:LYS:O	11:K:227:ALA:HB3	2.13	0.48
9:I:220:ILE:HG22	9:I:344:ILE:HG21	1.94	0.48
1:A:47:GLY:O	1:A:193:HIS:ND1	2.47	0.48
13:M:384:ASP:OD1	13:M:385:GLU:N	2.46	0.48
8:H:248:LEU:HD23	8:H:249:TYR:N	2.28	0.47
11:K:348:GLU:O	11:K:352:ILE:HG22	2.13	0.47
9:I:380:LEU:HD22	9:I:416:PHE:HD2	1.79	0.47
13:M:312:LEU:O	13:M:316:SER:N	2.41	0.47
6:F:177:ASP:O	6:F:181:LYS:NZ	2.48	0.47
8:H:427:GLY:O	8:H:431:ILE:N	2.43	0.47
10:J:248:ASP:OD1	10:J:249:GLU:N	2.48	0.47
8:H:402:ILE:HD11	8:H:404:TRP:CE2	2.49	0.47
13:M:262:LEU:O	13:M:266:ALA:N	2.43	0.47
13:M:312:LEU:HD21	13:M:342:ARG:HA	1.97	0.47
4:D:73:LEU:HD23	4:D:74:SER:N	2.30	0.47
12:L:227:GLY:O	12:L:231:LEU:N	2.41	0.47
2:B:230:ASP:OD1	2:B:231:LYS:N	2.49	0.46
9:I:319:ARG:O	9:I:322:VAL:HG22	2.16	0.46
13:M:301:VAL:O	13:M:304:THR:OG1	2.21	0.46
1:A:158:ASP:OD1	1:A:162:TYR:N	2.48	0.46
9:I:268:PHE:O	9:I:272:GLY:N	2.44	0.46
10:J:265:ASP:OD1	10:J:266:SER:N	2.47	0.46
7:G:183:HIS:HB3	7:G:187:LEU:HD21	1.98	0.46
9:I:232:LEU:O	9:I:236:VAL:N	2.43	0.46
11:K:220:THR:O	11:K:224:LYS:NZ	2.46	0.46
7:G:12:ASN:OD1	7:G:13:SER:N	2.49	0.46
9:I:309:LEU:O	9:I:313:LEU:N	2.47	0.46
10:J:400:VAL:HG13	10:J:400:VAL:O	2.15	0.46
9:I:412:THR:OG1	9:I:415:ASP:OD1	2.34	0.46
10:J:187:LEU:HD23	10:J:187:LEU:H	1.81	0.46
10:J:270:ARG:O	10:J:274:GLU:N	2.42	0.46
12:L:257:GLY:O	12:L:261:ARG:N	2.48	0.46
3:C:24:TYR:O	3:C:28:SER:N	2.46	0.46
6:F:217:GLY:N	6:F:220:THR:OG1	2.49	0.46
8:H:211:VAL:HG23	15:H:501:ATP:C2	2.52	0.46
8:H:430:ALA:O	8:H:434:ARG:N	2.48	0.46
7:G:113:ALA:O	7:G:117:GLY:N	2.45	0.45
9:I:195:LYS:O	9:I:199:GLU:N	2.48	0.45
5:E:85:ALA:HB2	5:E:140:VAL:HG11	1.99	0.45
11:K:220:THR:HG22	15:K:501:ATP:O2B	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:302:GLN:O	12:L:306:MET:N	2.45	0.45
12:L:317:ASN:OD1	12:L:318:LEU:N	2.49	0.45
7:G:116:LEU:O	7:G:119:TYR:N	2.44	0.45
1:A:178:ILE:O	1:A:181:ASN:N	2.49	0.45
10:J:386:VAL:O	10:J:390:MET:N	2.49	0.45
11:K:237:VAL:HG12	11:K:270:PHE:O	2.17	0.45
1:A:115:ASP:OD1	1:A:116:VAL:N	2.50	0.45
9:I:260:GLY:O	9:I:264:CYS:N	2.46	0.45
10:J:332:SER:O	10:J:334:LYS:N	2.48	0.45
1:A:229:THR:N	1:A:232:LYS:O	2.50	0.45
6:F:33:SER:HB3	6:F:62:LYS:HZ3	1.82	0.45
6:F:145:LEU:HD21	6:F:155:GLU:OE2	2.17	0.45
8:H:224:VAL:HG23	8:H:243:PRO:HG2	1.99	0.45
9:I:322:VAL:HG23	9:I:322:VAL:O	2.17	0.45
3:C:14:SER:OG	3:C:17:GLY:N	2.50	0.45
11:K:217:THR:N	15:K:501:ATP:O3A	2.49	0.45
13:M:398:ALA:HB3	13:M:419:ILE:HD11	1.98	0.45
6:F:28:ALA:O	6:F:31:GLN:N	2.50	0.45
11:K:300:LEU:HD21	11:K:330:ARG:NH2	2.32	0.45
11:K:196:ASP:OD1	11:K:197:LEU:N	2.50	0.44
13:M:244:LEU:HD23	13:M:245:LYS:N	2.32	0.44
13:M:401:ILE:HD12	13:M:404:ARG:HD3	2.00	0.44
6:F:83:VAL:O	6:F:87:TYR:N	2.46	0.44
8:H:381:ASP:OD1	8:H:382:LEU:N	2.48	0.44
9:I:300:ARG:O	9:I:304:ARG:N	2.47	0.44
10:J:386:VAL:O	10:J:389:VAL:N	2.51	0.44
2:B:187:ASP:OD1	2:B:188:ALA:N	2.49	0.44
8:H:403:ARG:HB3	8:H:406:LEU:HD23	2.00	0.44
3:C:108:VAL:O	3:C:111:LEU:N	2.50	0.44
5:E:233:ASN:OD1	5:E:234:GLU:N	2.50	0.44
9:I:253:ILE:HD12	10:J:223:ILE:CG2	2.48	0.44
1:A:84:ASN:OD1	1:A:84:ASN:N	2.51	0.44
8:H:431:ILE:O	8:H:434:ARG:NE	2.49	0.44
4:D:48:ARG:N	4:D:209:ASN:O	2.43	0.43
9:I:397:THR:HG22	9:I:401:LEU:HD23	2.00	0.43
10:J:194:GLY:O	10:J:198:LEU:N	2.45	0.43
12:L:197:ILE:O	12:L:197:ILE:HG22	2.18	0.43
13:M:227:GLY:N	16:M:501:ADP:O4'	2.51	0.43
3:C:36:ILE:HD12	3:C:37:GLY:N	2.33	0.43
12:L:310:THR:O	12:L:314:GLY:N	2.51	0.43
13:M:259:GLY:O	13:M:262:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASP:OD1	1:A:14:ARG:N	2.51	0.43
3:C:38:ILE:HD12	3:C:39:MET:N	2.34	0.43
6:F:45:VAL:HA	6:F:215:ILE:HG22	2.00	0.43
10:J:192:GLY:N	15:J:501:ATP:O2A	2.42	0.43
1:A:68:THR:HG21	7:G:159:GLY:H	1.82	0.43
11:K:250:GLY:O	11:K:253:MET:N	2.48	0.43
2:B:216:ASP:OD1	2:B:234:ARG:NH1	2.52	0.43
3:C:52:VAL:HG12	3:C:54:SER:H	1.84	0.43
11:K:291:GLU:OE1	11:K:291:GLU:N	2.48	0.43
13:M:229:THR:O	13:M:233:ARG:N	2.45	0.43
5:E:151:ASP:OD1	5:E:152:GLY:N	2.52	0.43
6:F:119:ASN:O	6:F:119:ASN:ND2	2.45	0.43
12:L:361:PHE:O	12:L:365:THR:N	2.48	0.43
3:C:99:LEU:O	3:C:103:ASN:N	2.49	0.42
11:K:251:PRO:HA	11:K:254:VAL:HG22	2.01	0.42
12:L:167:VAL:HG12	12:L:167:VAL:O	2.19	0.42
1:A:81:MET:CE	1:A:141:LEU:HD22	2.49	0.42
11:K:253:MET:O	11:K:256:ASP:N	2.52	0.42
12:L:361:PHE:O	12:L:365:THR:HG22	2.19	0.42
3:C:158:THR:OG1	3:C:160:TRP:NE1	2.39	0.42
9:I:394:ALA:O	9:I:397:THR:N	2.51	0.42
12:L:207:PHE:O	12:L:211:GLY:N	2.50	0.42
3:C:160:TRP:CG	3:C:163:ILE:HD11	2.54	0.42
4:D:229:ILE:O	4:D:233:VAL:HG12	2.19	0.42
9:I:244:PHE:C	9:I:245:LEU:HD22	2.40	0.42
5:E:239:LEU:O	5:E:243:LEU:N	2.52	0.42
9:I:289:THR:O	9:I:335:ASP:N	2.51	0.42
1:A:20:SER:OG	1:A:24:ARG:O	2.34	0.42
7:G:222:SER:OG	7:G:223:GLU:N	2.53	0.42
10:J:309:ARG:O	10:J:310:ILE:HD13	2.20	0.42
7:G:24:VAL:O	7:G:27:ALA:HB3	2.19	0.42
9:I:265:ARG:NH1	9:I:312:GLN:OE1	2.53	0.42
11:K:219:LYS:NZ	15:K:501:ATP:O1B	2.51	0.42
7:G:191:GLU:OE1	7:G:191:GLU:N	2.49	0.42
9:I:230:THR:O	9:I:233:ALA:N	2.49	0.42
10:J:202:VAL:O	10:J:206:THR:HG22	2.19	0.42
12:L:166:LEU:HD13	12:L:166:LEU:O	2.19	0.42
9:I:190:GLN:HB3	9:I:191:ILE:HD12	2.02	0.42
9:I:379:THR:HG22	9:I:379:THR:O	2.19	0.42
13:M:309:LEU:CD2	13:M:342:ARG:HE	2.32	0.42
13:M:373:ASP:N	13:M:374:ILE:HD12	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:GLN:OE1	6:F:121:GLN:NE2	2.53	0.42
8:H:297:MET:SD	8:H:301:LYS:NZ	2.76	0.42
10:J:166:LEU:O	10:J:170:HIS:N	2.50	0.41
1:A:51:THR:CG2	1:A:228:ALA:HB3	2.50	0.41
3:C:17:GLY:O	4:D:29:ARG:NH1	2.53	0.41
10:J:165:GLU:O	10:J:169:LYS:N	2.50	0.41
12:L:370:LYS:O	12:L:409:HIS:ND1	2.53	0.41
12:L:183:ILE:HG23	16:L:501:ADP:C6	2.55	0.41
13:M:343:LEU:HD23	13:M:345:ARG:H	1.85	0.41
1:A:57:LYS:HD3	1:A:69:VAL:HG11	2.02	0.41
1:A:146:VAL:HG12	1:A:147:ASP:N	2.35	0.41
8:H:233:GLU:O	8:H:237:THR:N	2.53	0.41
9:I:187:LEU:HD23	9:I:188:GLU:N	2.34	0.41
11:K:269:ILE:HD12	11:K:270:PHE:N	2.35	0.41
6:F:185:ASN:ND2	6:F:188:GLU:OE2	2.54	0.41
4:D:155:ILE:HG23	4:D:155:ILE:O	2.21	0.41
7:G:179:LEU:HD23	7:G:180:VAL:HA	2.02	0.41
7:G:6:THR:N	7:G:9:ASP:OD2	2.54	0.41
9:I:216:PRO:O	9:I:323:LYS:NZ	2.53	0.41
4:D:113:VAL:HA	4:D:116:VAL:HG12	2.02	0.41
4:D:230:ASN:HA	4:D:233:VAL:HG12	2.03	0.41
9:I:220:ILE:HD13	9:I:326:MET:CB	2.51	0.41
10:J:218:LEU:O	10:J:220:GLN:NE2	2.54	0.41
10:J:272:MET:O	10:J:276:LEU:N	2.54	0.41
1:A:22:GLU:OE2	1:A:24:ARG:N	2.54	0.41
7:G:137:ILE:HD13	7:G:150:MET:HG3	2.03	0.40
10:J:196:THR:O	10:J:199:ALA:N	2.54	0.40
11:K:366:ALA:O	11:K:404:GLN:NE2	2.53	0.40
12:L:360:ILE:HG23	16:L:501:ADP:C2	2.56	0.40
2:B:149:GLN:OE1	2:B:159:TRP:NE1	2.54	0.40
8:H:425:GLU:OE1	8:H:425:GLU:N	2.49	0.40
9:I:208:TYR:O	9:I:213:ILE:N	2.48	0.40
13:M:260:ALA:HB2	13:M:304:THR:HG22	2.03	0.40
4:D:231:GLN:O	4:D:234:THR:OG1	2.39	0.40
6:F:193:GLY:O	6:F:197:ILE:N	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	237/239 (99%)	205 (86%)	32 (14%)	0	100	100
2	B	248/250 (99%)	217 (88%)	31 (12%)	0	100	100
3	C	236/238 (99%)	198 (84%)	38 (16%)	0	100	100
4	D	232/234 (99%)	208 (90%)	24 (10%)	0	100	100
5	E	240/242 (99%)	210 (88%)	30 (12%)	0	100	100
6	F	231/233 (99%)	203 (88%)	28 (12%)	0	100	100
7	G	241/243 (99%)	216 (90%)	25 (10%)	0	100	100
8	H	250/262 (95%)	212 (85%)	38 (15%)	0	100	100
9	I	269/271 (99%)	216 (80%)	52 (19%)	1 (0%)	34	72
10	J	271/273 (99%)	224 (83%)	47 (17%)	0	100	100
11	K	274/276 (99%)	225 (82%)	49 (18%)	0	100	100
12	L	260/271 (96%)	223 (86%)	37 (14%)	0	100	100
13	M	260/262 (99%)	223 (86%)	37 (14%)	0	100	100
14	s	13/15 (87%)	9 (69%)	4 (31%)	0	100	100
All	All	3262/3309 (99%)	2789 (86%)	472 (14%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	320	GLY

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	186/205 (91%)	186 (100%)	0	100	100
2	B	180/209 (86%)	178 (99%)	2 (1%)	73	85
3	C	168/198 (85%)	168 (100%)	0	100	100
4	D	165/208 (79%)	165 (100%)	0	100	100
5	E	164/198 (83%)	164 (100%)	0	100	100
6	F	177/192 (92%)	176 (99%)	1 (1%)	86	92
7	G	183/201 (91%)	183 (100%)	0	100	100
8	H	156/219 (71%)	155 (99%)	1 (1%)	86	92
9	I	183/234 (78%)	182 (100%)	1 (0%)	88	93
10	J	179/231 (78%)	178 (99%)	1 (1%)	86	92
11	K	150/235 (64%)	150 (100%)	0	100	100
12	L	170/224 (76%)	170 (100%)	0	100	100
13	M	141/217 (65%)	140 (99%)	1 (1%)	84	90
14	s	6/10 (60%)	6 (100%)	0	100	100
All	All	2208/2781 (79%)	2201 (100%)	7 (0%)	92	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4	ARG
2	B	41	ASN
6	F	119	ASN
8	H	356	ASN
9	I	422	ARG
10	J	391	ASN
13	M	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	178	ASN
6	F	117	GLN
6	F	121	GLN
7	G	33	ASN
8	H	413	ASN

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Mol	Chain	Res	Type
9	I	204	HIS
9	I	365	HIS
9	I	418	GLN
10	J	156	GLN
10	J	391	ASN
12	L	189	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	ATP	H	501	-	26,33,33	0.84	1 (3%)	31,52,52	1.82	6 (19%)
16	ADP	L	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
15	ATP	K	501	-	26,33,33	0.85	1 (3%)	31,52,52	1.76	5 (16%)
15	ATP	J	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.50	7 (22%)
16	ADP	M	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.58	5 (17%)
15	ATP	I	501	-	26,33,33	0.89	1 (3%)	31,52,52	1.49	5 (16%)

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	ATP	H	501	-	-	3/18/38/38	0/3/3/3
16	ADP	L	501	-	-	2/12/32/32	0/3/3/3
15	ATP	K	501	-	-	6/18/38/38	0/3/3/3
15	ATP	J	501	-	-	5/18/38/38	0/3/3/3
16	ADP	M	501	-	-	2/12/32/32	0/3/3/3
15	ATP	I	501	-	-	5/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	501	ADP	C5-C4	2.48	1.47	1.40
16	L	501	ADP	C5-C4	2.39	1.47	1.40
15	J	501	ATP	C5-C4	2.27	1.46	1.40
15	K	501	ATP	C5-C4	2.07	1.46	1.40
15	I	501	ATP	C5-C4	2.05	1.46	1.40
15	H	501	ATP	C5-C4	2.02	1.46	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	501	ATP	PA-O3A-PB	-5.76	113.06	132.83
15	K	501	ATP	PA-O3A-PB	-5.04	115.52	132.83
16	M	501	ADP	PA-O3A-PB	-4.18	118.50	132.83
15	H	501	ATP	N3-C2-N1	-4.14	122.21	128.68
15	K	501	ATP	PB-O3B-PG	-3.93	119.34	132.83
15	I	501	ATP	N3-C2-N1	-3.75	122.81	128.68
15	J	501	ATP	N3-C2-N1	-3.71	122.88	128.68
16	M	501	ADP	N3-C2-N1	-3.69	122.91	128.68
15	K	501	ATP	N3-C2-N1	-3.58	123.08	128.68
15	H	501	ATP	PB-O3B-PG	-3.49	120.85	132.83
15	I	501	ATP	C3'-C2'-C1'	3.43	106.14	100.98
16	L	501	ADP	N3-C2-N1	-3.40	123.37	128.68
15	J	501	ATP	PA-O3A-PB	-3.14	122.04	132.83
15	K	501	ATP	C3'-C2'-C1'	3.09	105.63	100.98
16	L	501	ADP	C3'-C2'-C1'	3.06	105.59	100.98
16	L	501	ADP	PA-O3A-PB	-3.02	122.47	132.83
15	I	501	ATP	PA-O3A-PB	-2.81	123.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	501	ATP	PB-O3B-PG	-2.71	123.53	132.83
15	J	501	ATP	C3'-C2'-C1'	2.65	104.97	100.98
15	H	501	ATP	C2-N1-C6	2.63	123.26	118.75
16	L	501	ADP	C4-C5-N7	-2.50	106.79	109.40
15	K	501	ATP	C4-C5-N7	-2.47	106.83	109.40
15	J	501	ATP	PB-O3B-PG	-2.46	124.38	132.83
16	M	501	ADP	C4-C5-N7	-2.45	106.84	109.40
15	J	501	ATP	C4-C5-N7	-2.44	106.86	109.40
15	J	501	ATP	O4'-C1'-C2'	-2.23	103.67	106.93
16	M	501	ADP	C1'-N9-C4	2.22	130.54	126.64
16	M	501	ADP	C3'-C2'-C1'	2.20	104.29	100.98
15	H	501	ATP	C3'-C2'-C1'	2.19	104.27	100.98
15	I	501	ATP	C4-C5-N7	-2.18	107.13	109.40
15	J	501	ATP	O3G-PG-O2G	2.05	115.47	107.64
15	H	501	ATP	O2B-PB-O1B	2.03	122.26	112.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	501	ATP	C5'-O5'-PA-O2A
15	I	501	ATP	C5'-O5'-PA-O1A
15	I	501	ATP	C5'-O5'-PA-O2A
15	I	501	ATP	C5'-O5'-PA-O3A
15	I	501	ATP	O4'-C4'-C5'-O5'
15	J	501	ATP	C5'-O5'-PA-O3A
15	J	501	ATP	O4'-C4'-C5'-O5'
15	J	501	ATP	C3'-C4'-C5'-O5'
15	K	501	ATP	C5'-O5'-PA-O1A
16	M	501	ADP	C3'-C4'-C5'-O5'
15	I	501	ATP	C3'-C4'-C5'-O5'
16	M	501	ADP	O4'-C4'-C5'-O5'
15	H	501	ATP	C5'-O5'-PA-O3A
15	K	501	ATP	C5'-O5'-PA-O3A
16	L	501	ADP	PB-O3A-PA-O2A
15	H	501	ATP	C5'-O5'-PA-O1A
15	J	501	ATP	C5'-O5'-PA-O1A
15	J	501	ATP	C5'-O5'-PA-O2A
15	K	501	ATP	C5'-O5'-PA-O2A
16	L	501	ADP	O4'-C4'-C5'-O5'
15	K	501	ATP	PA-O3A-PB-O1B
15	K	501	ATP	PA-O3A-PB-O2B

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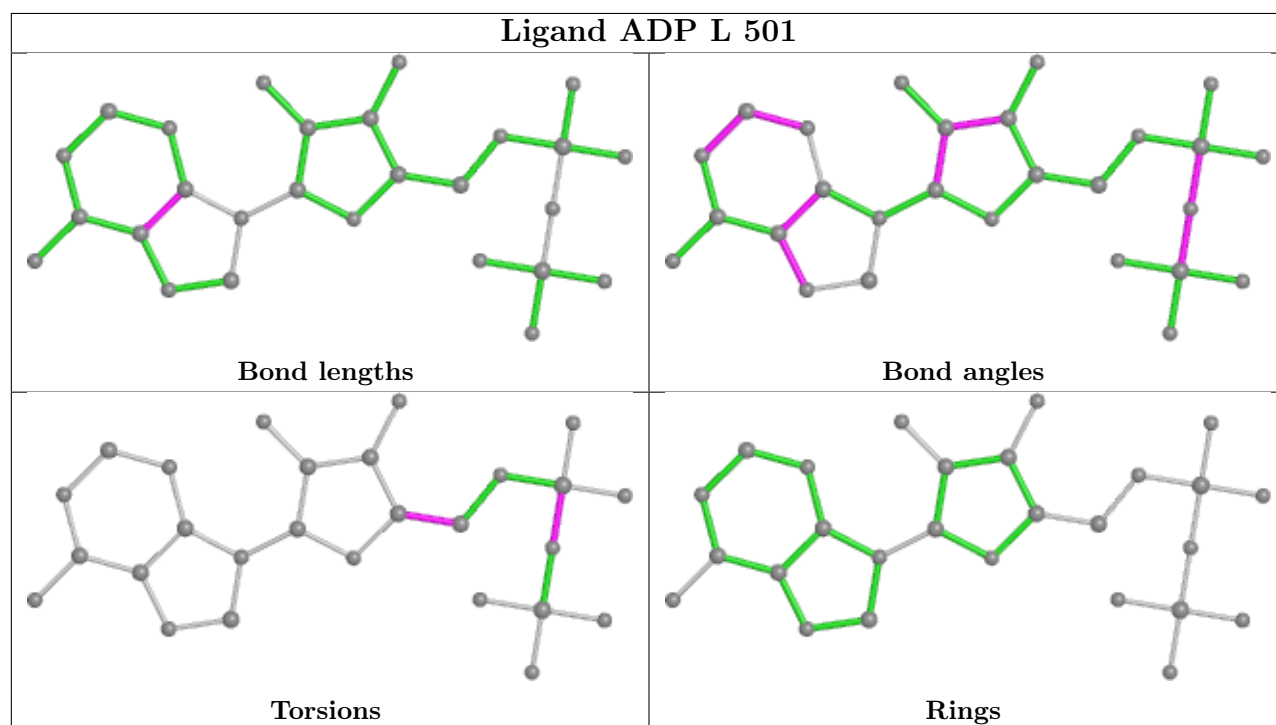
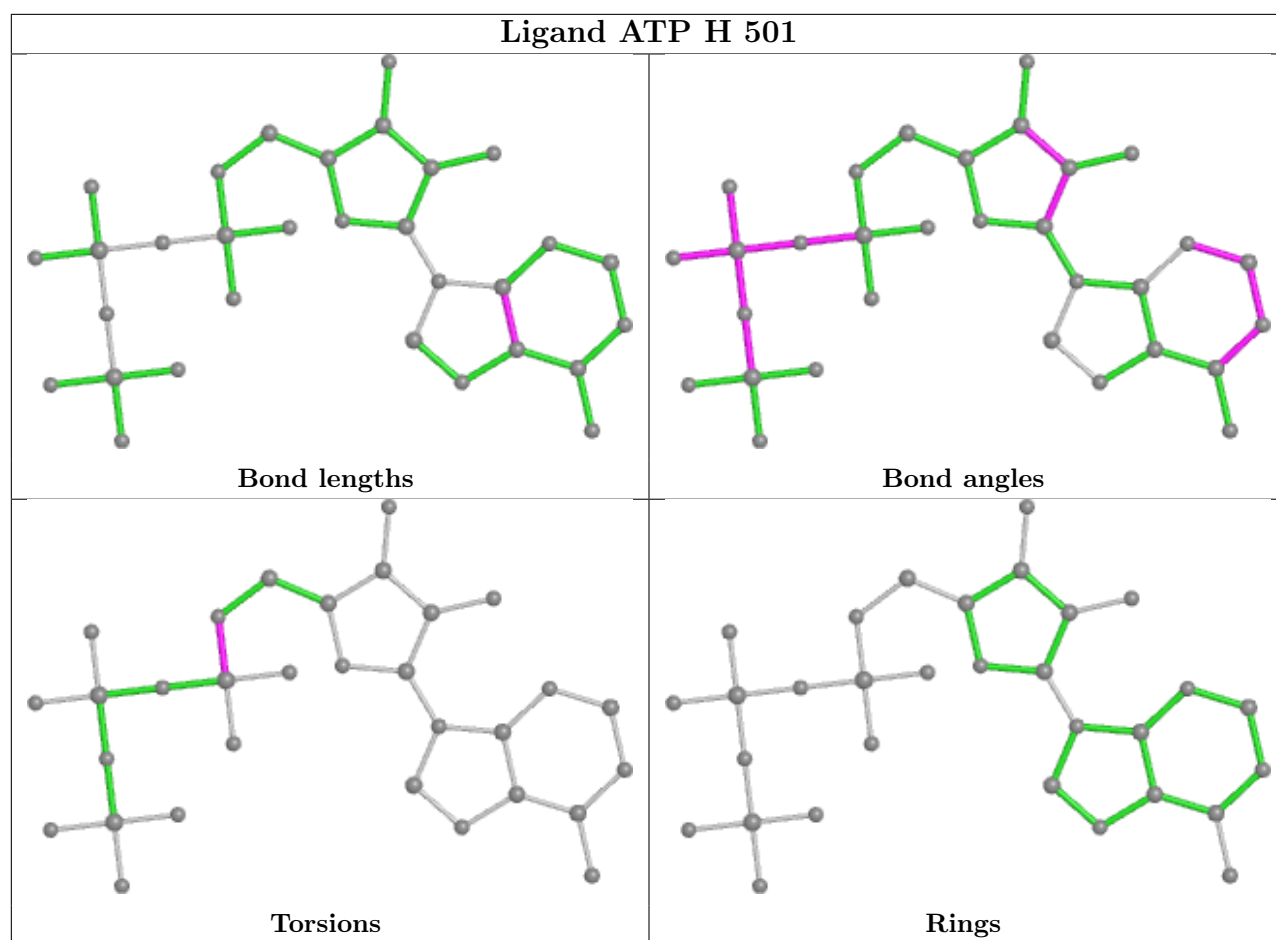
Mol	Chain	Res	Type	Atoms
15	K	501	ATP	C4'-C5'-O5'-PA

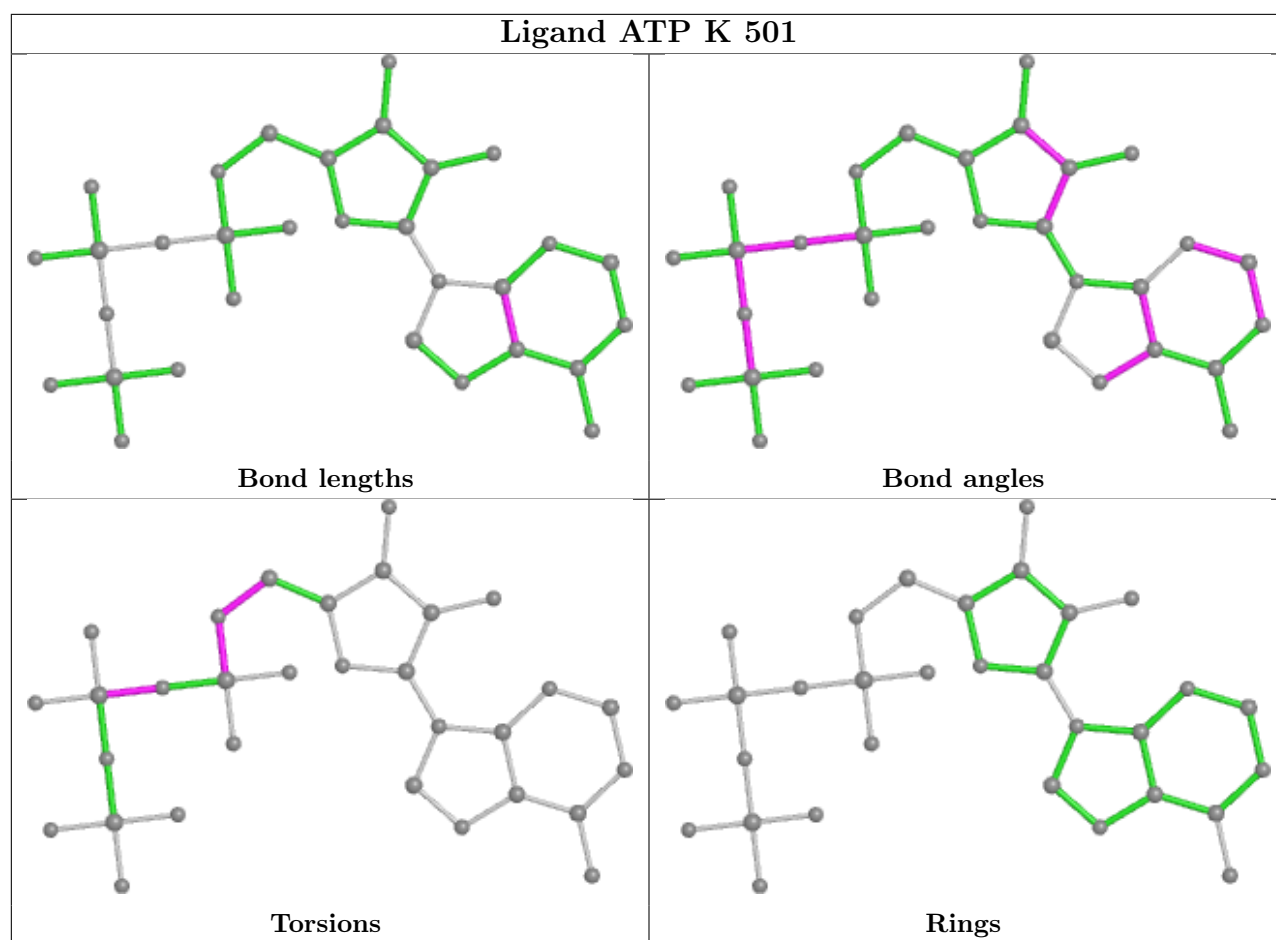
There are no ring outliers.

6 monomers are involved in 17 short contacts:

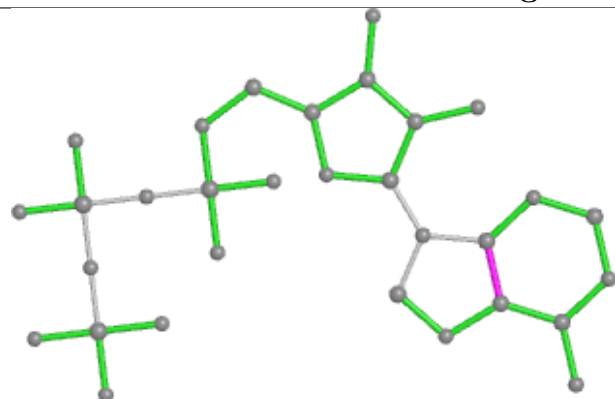
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	501	ATP	5	0
16	L	501	ADP	4	0
15	K	501	ATP	3	0
15	J	501	ATP	2	0
16	M	501	ADP	1	0
15	I	501	ATP	2	0

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.

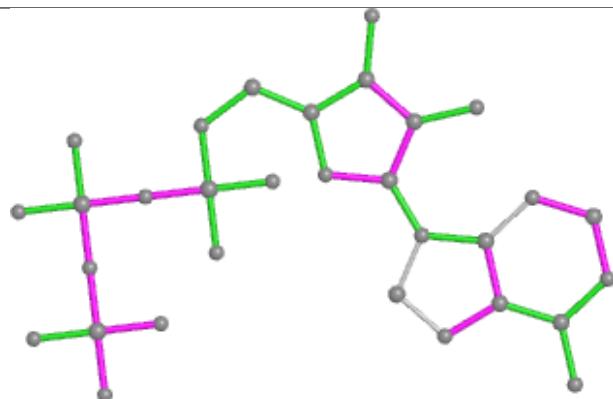




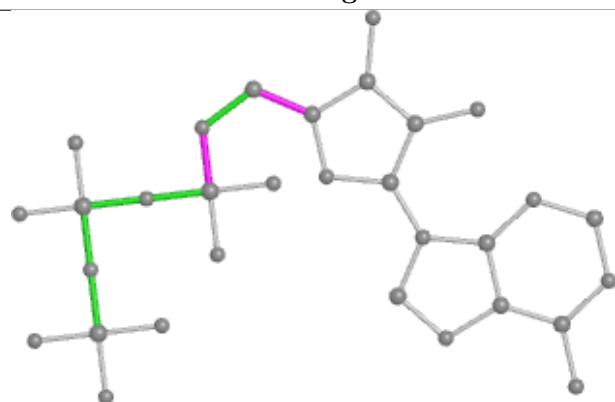
Ligand ATP J 501



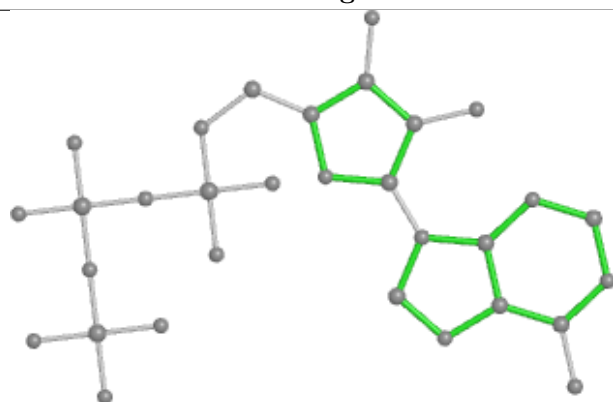
Bond lengths



Bond angles

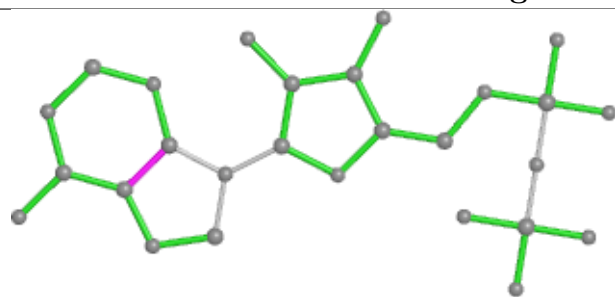


Torsions

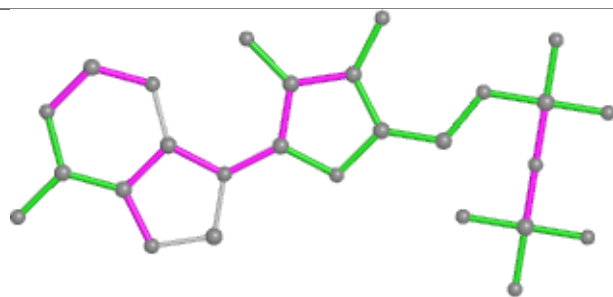


Rings

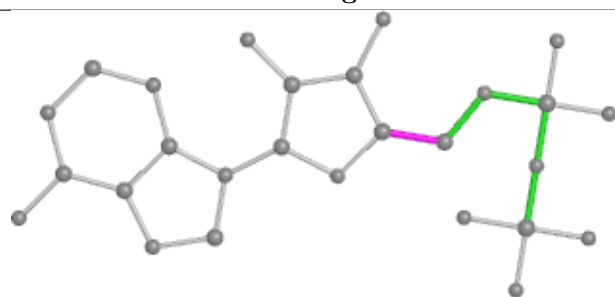
Ligand ADP M 501



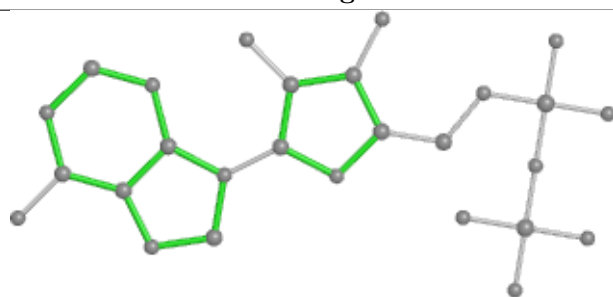
Bond lengths



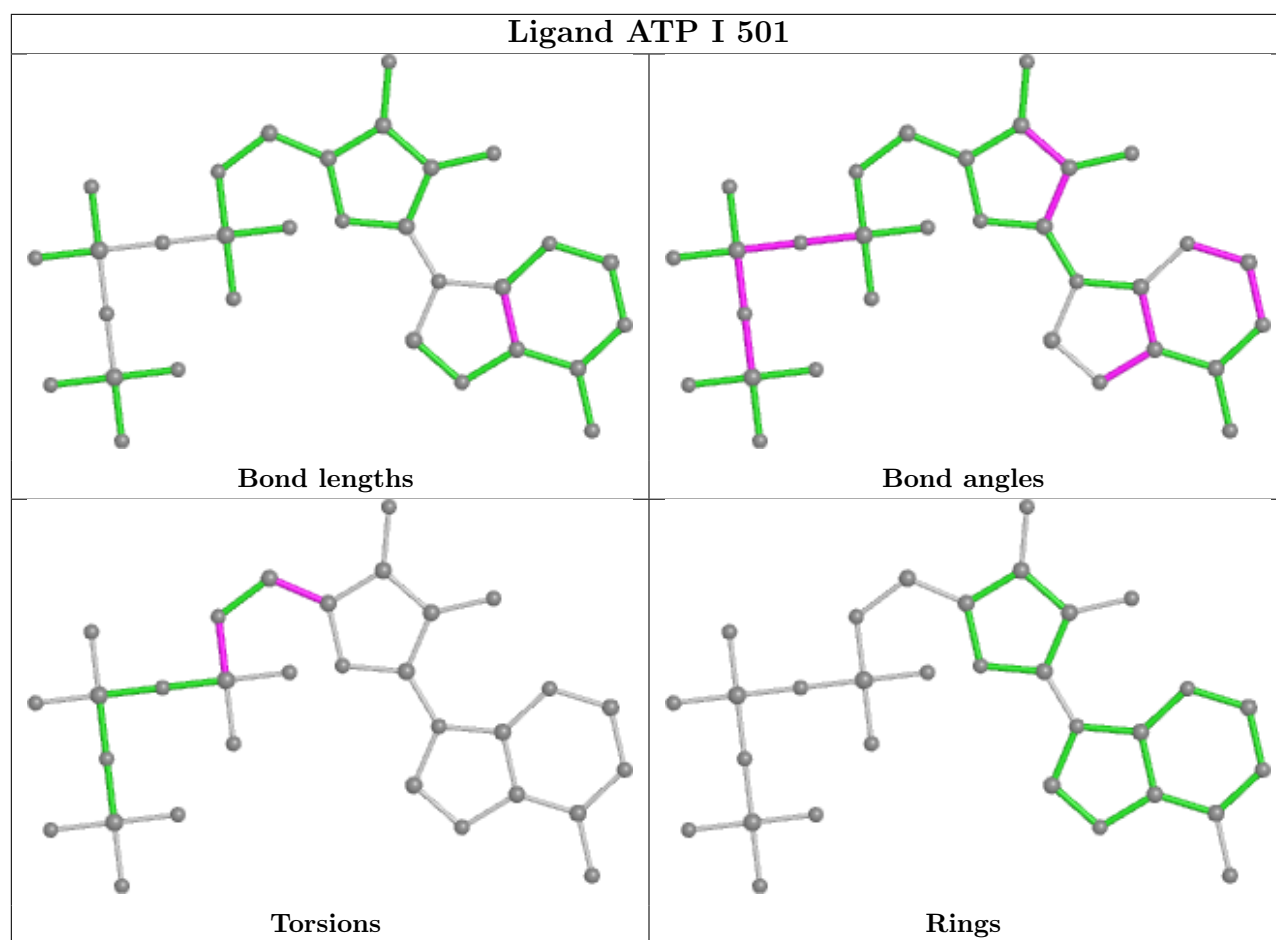
Bond angles



Torsions



Rings



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.

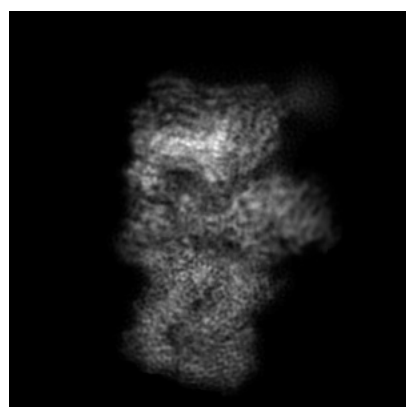
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9043. These allow visual inspection of the internal detail of the map and identification of artifacts.

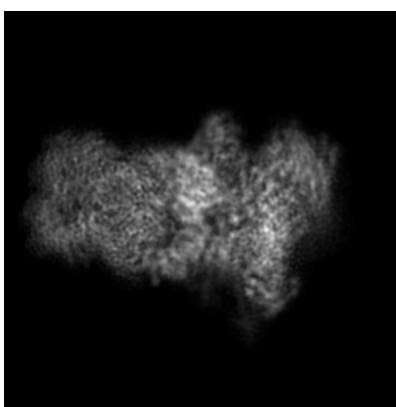
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

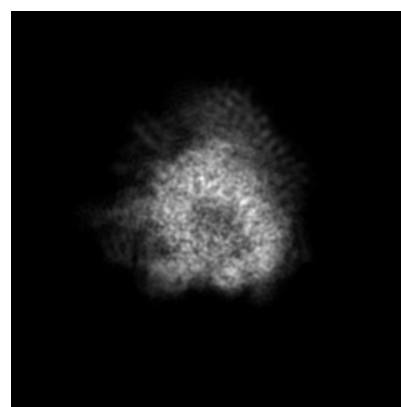
6.1.1 Primary map



X



Y

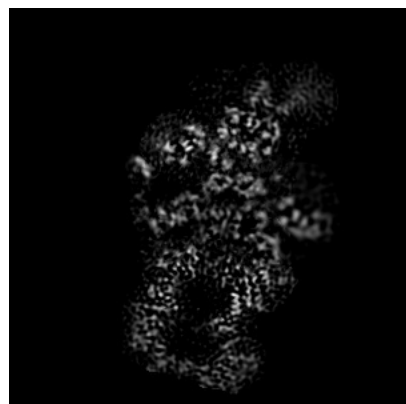


Z

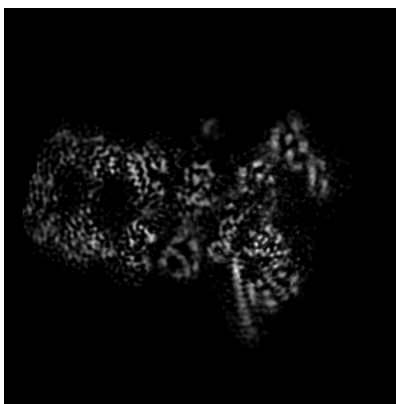
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 170



Y Index: 170

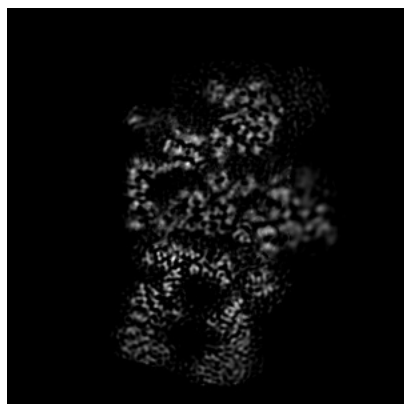


Z Index: 170

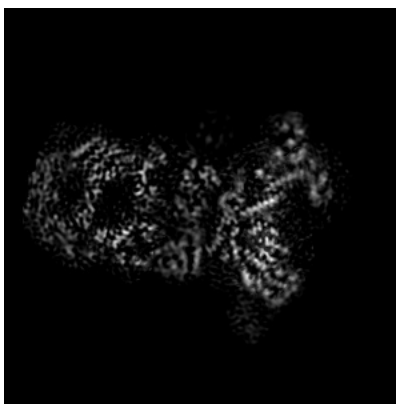
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

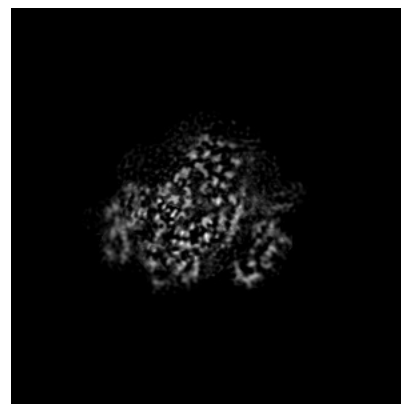
6.3.1 Primary map



X Index: 179



Y Index: 175

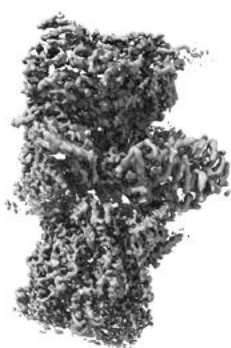


Z Index: 227

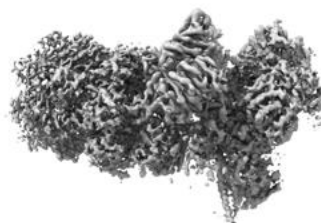
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

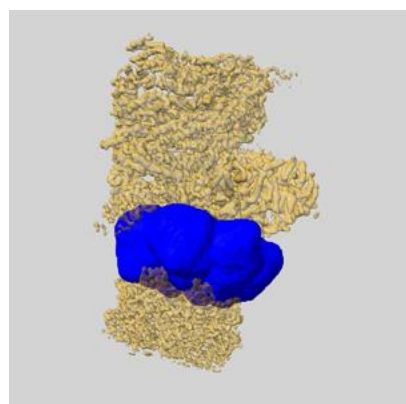
6.5 Mask visualisation [i](#)

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

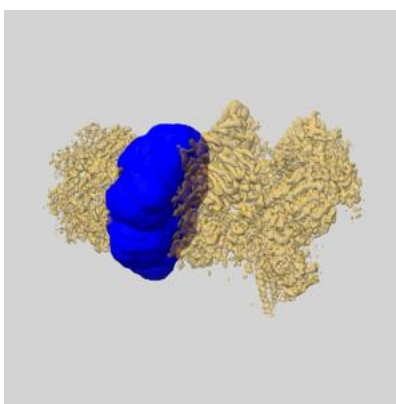
A mask typically either:

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

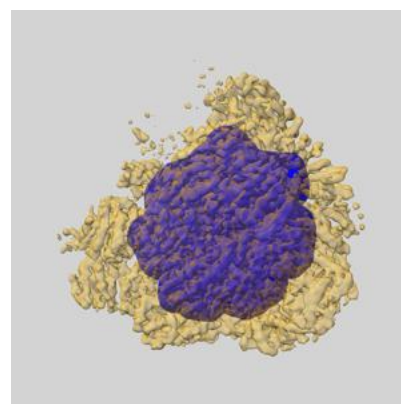
6.5.1 emd_9043_msk_2.map [i](#)



X

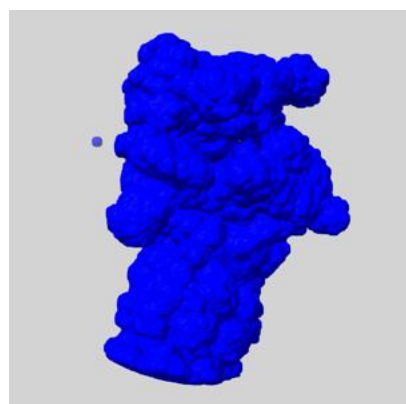


Y

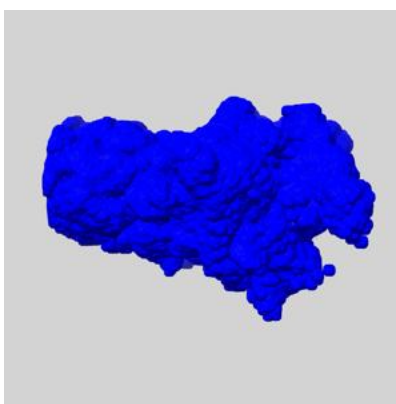


Z

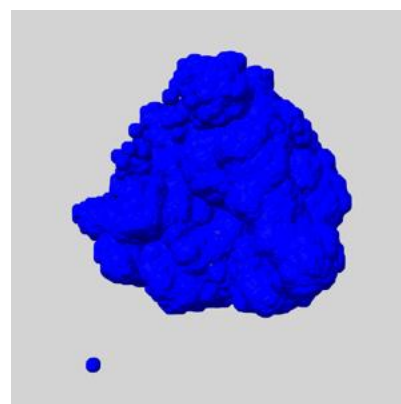
6.5.2 emd_9043_msk_3.map [i](#)



X

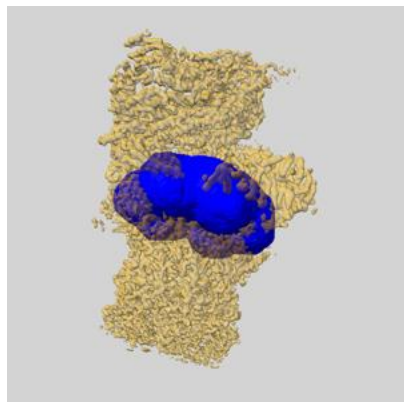


Y

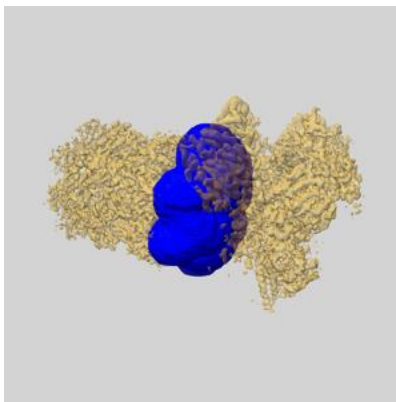


Z

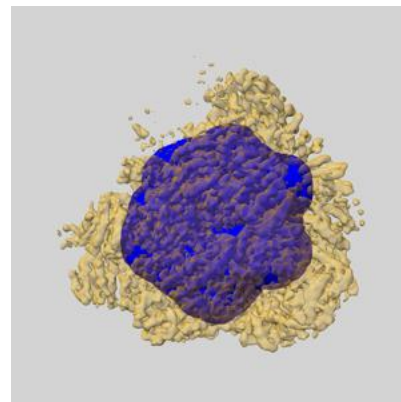
6.5.3 emd_9043_msk_1.map [i](#)



X



Y

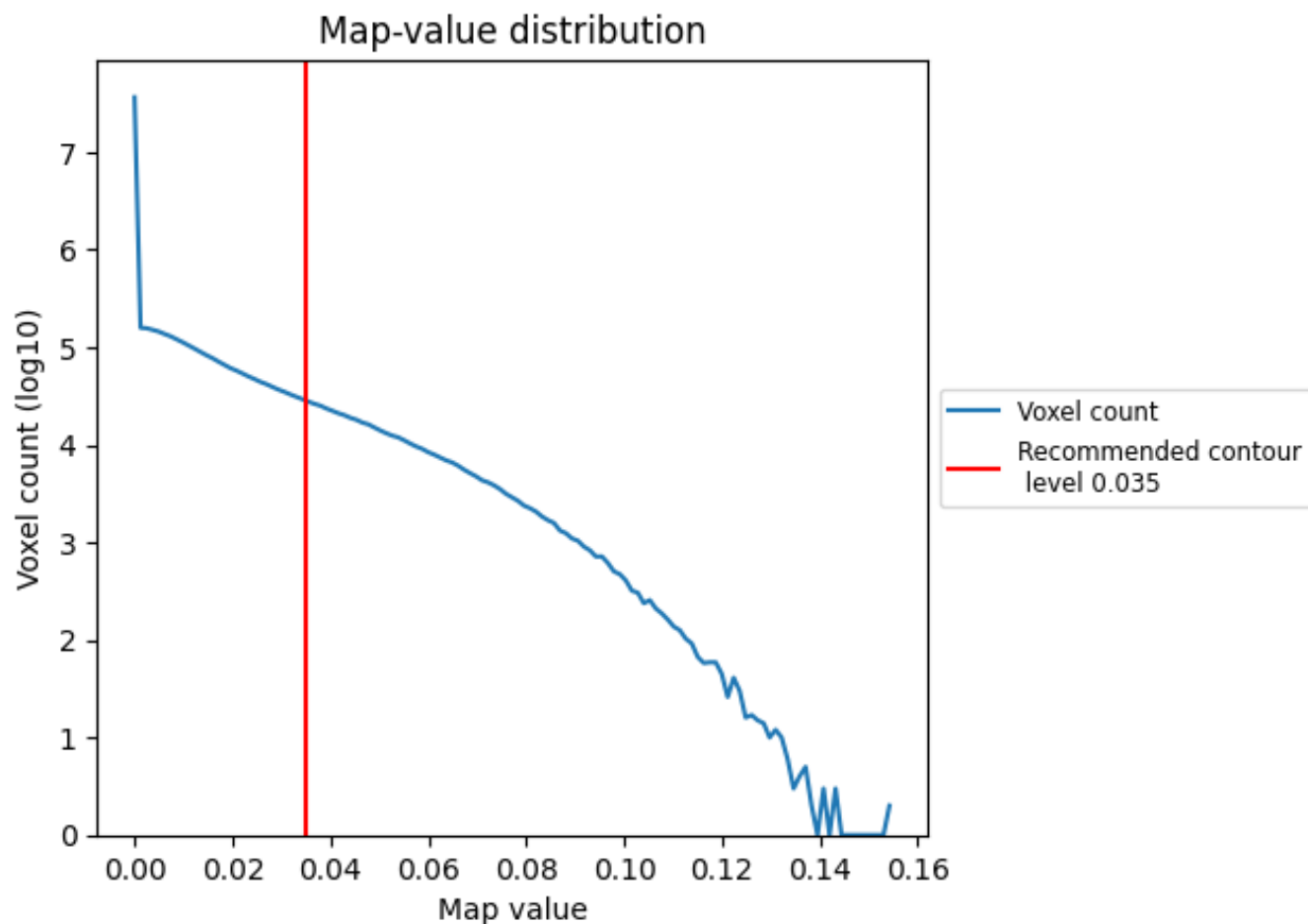


Z

7 Map analysis [i](#)

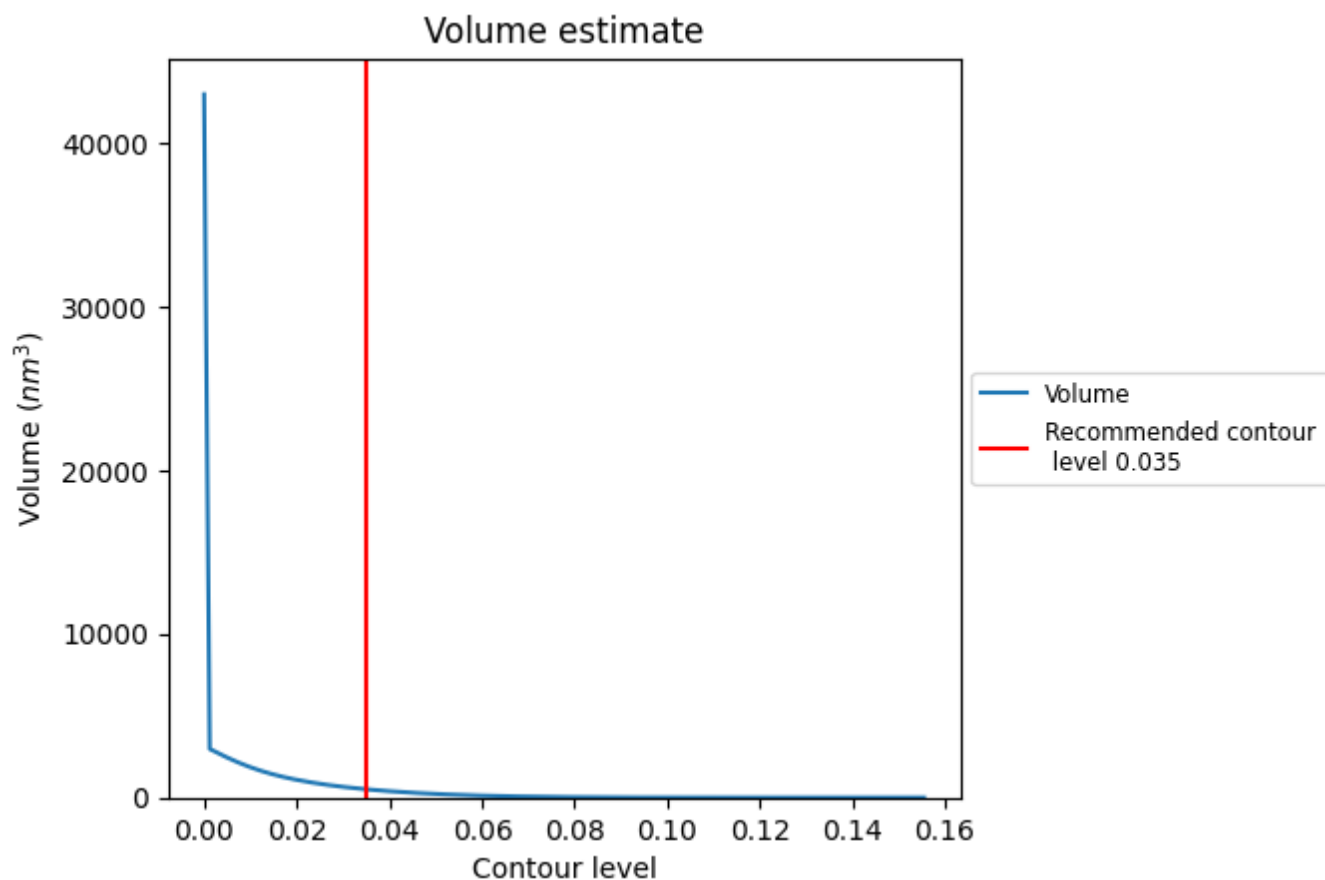
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

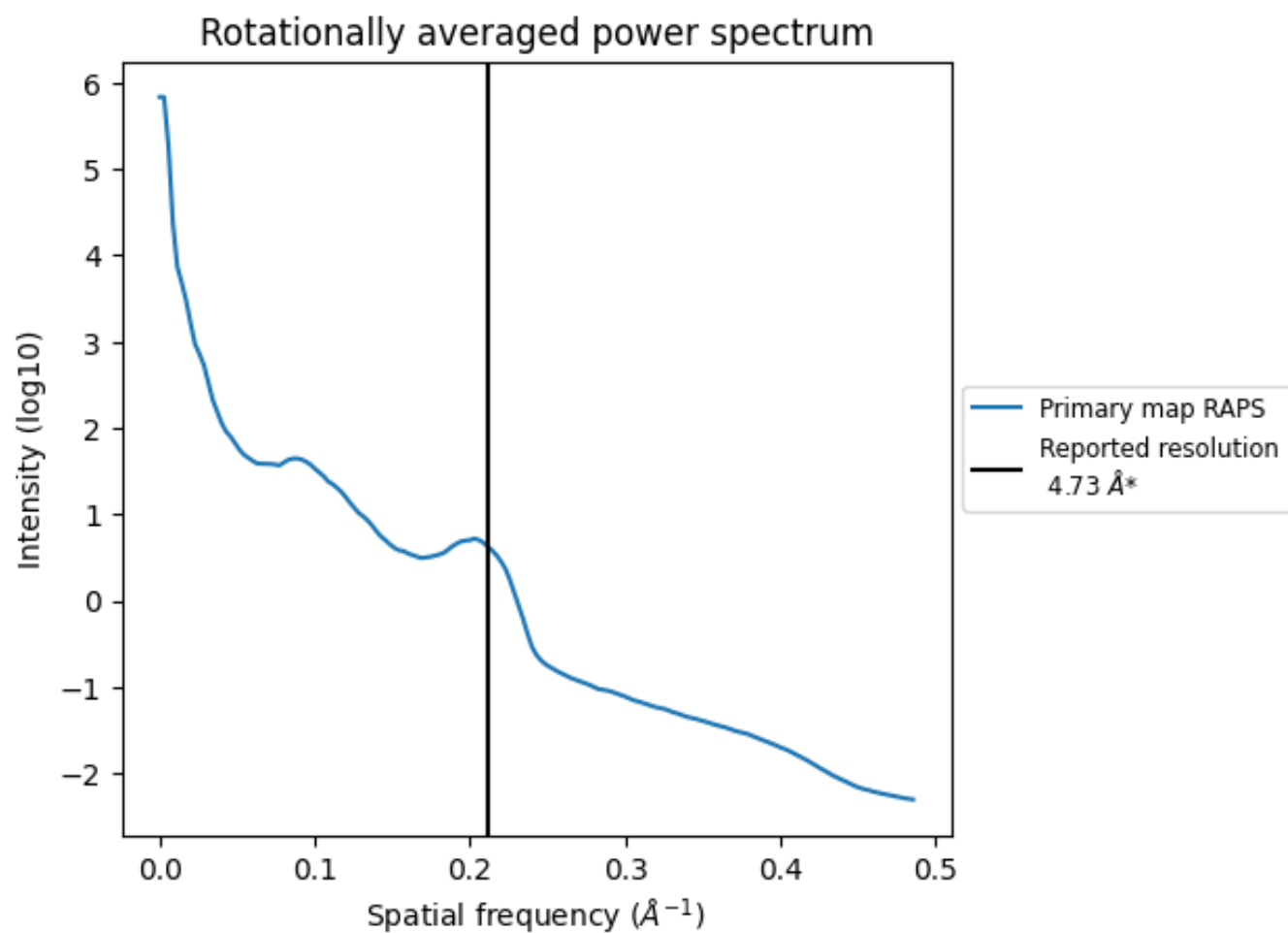
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 506 nm³; this corresponds to an approximate mass of 457 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 0.211 Å⁻¹

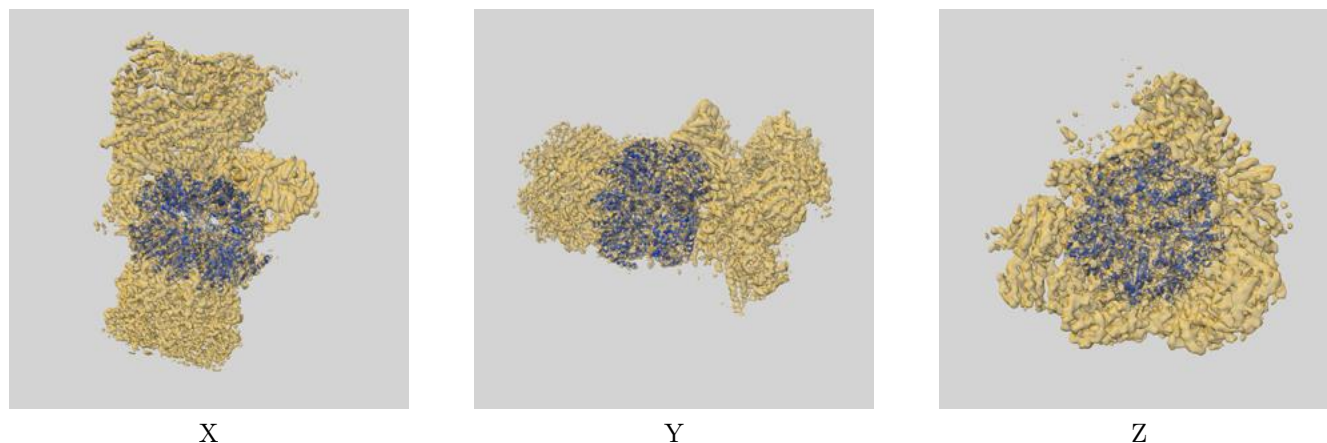
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

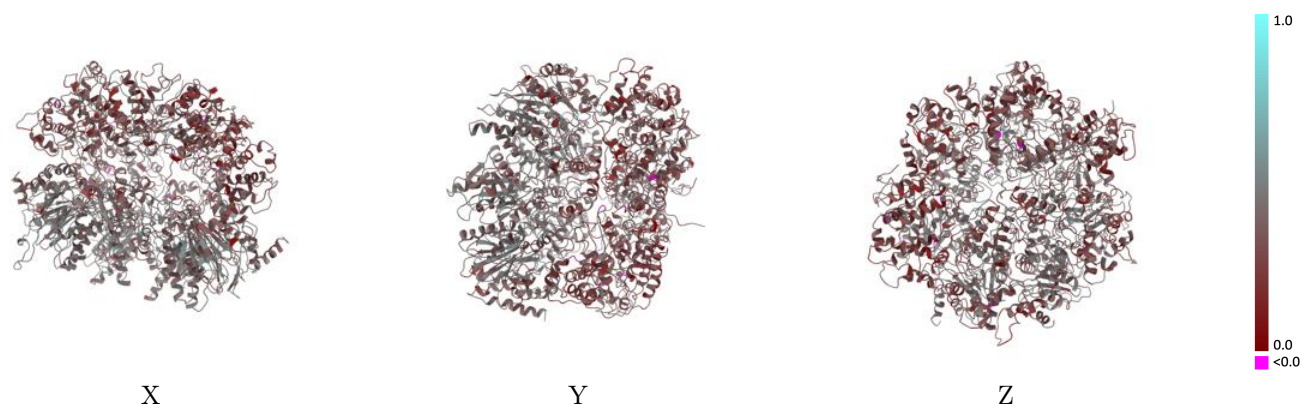
This section contains information regarding the fit between EMDB map EMD-9043 and PDB model 6EF1. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



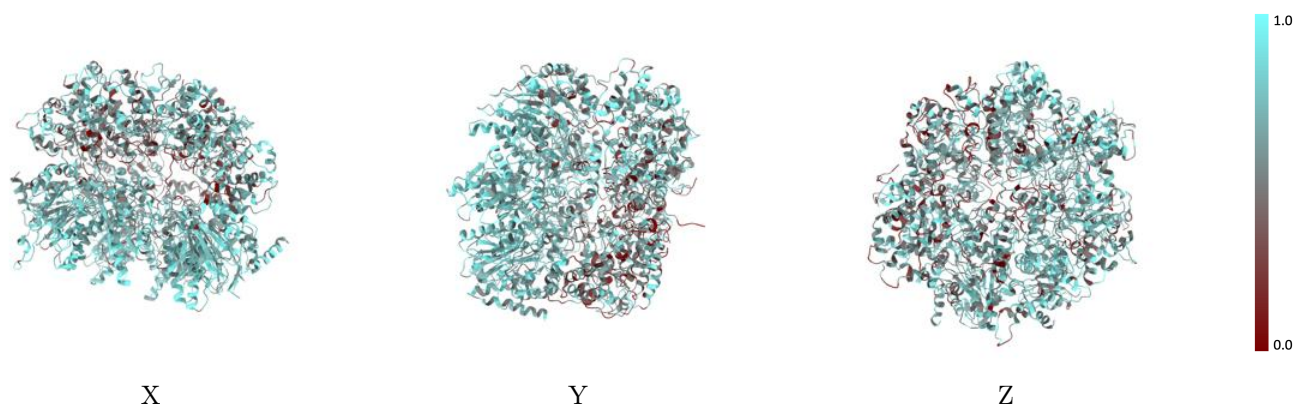
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



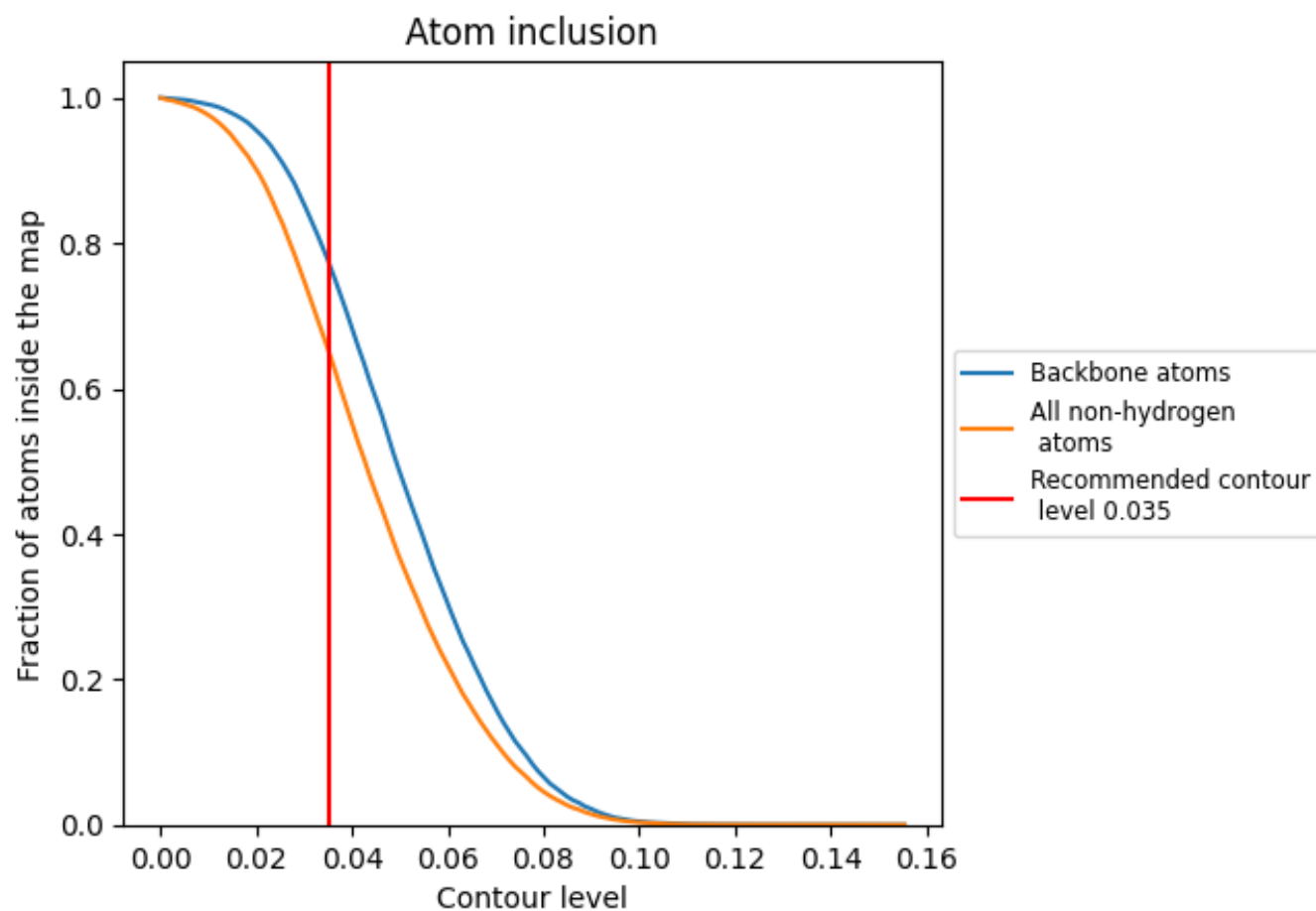
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 65% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6546	<div></div> 0.3710
A	<div></div> 0.7306	<div></div> 0.4120
B	<div></div> 0.7428	<div></div> 0.4310
C	<div></div> 0.7082	<div></div> 0.4050
D	<div></div> 0.7091	<div></div> 0.3990
E	<div></div> 0.7428	<div></div> 0.4250
F	<div></div> 0.7438	<div></div> 0.4100
G	<div></div> 0.7414	<div></div> 0.4200
H	<div></div> 0.5518	<div></div> 0.3210
I	<div></div> 0.6003	<div></div> 0.3180
J	<div></div> 0.6197	<div></div> 0.3400
K	<div></div> 0.6198	<div></div> 0.3470
L	<div></div> 0.5302	<div></div> 0.3110
M	<div></div> 0.5062	<div></div> 0.3040
s	<div></div> 0.4253	<div></div> 0.4480

