



## Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 01:37 PM EST

PDB ID : 6EF2  
EMDB ID : EMD-9044  
Title : Yeast 26S proteasome bound to ubiquitinated substrate (5T 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 : 4.27 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

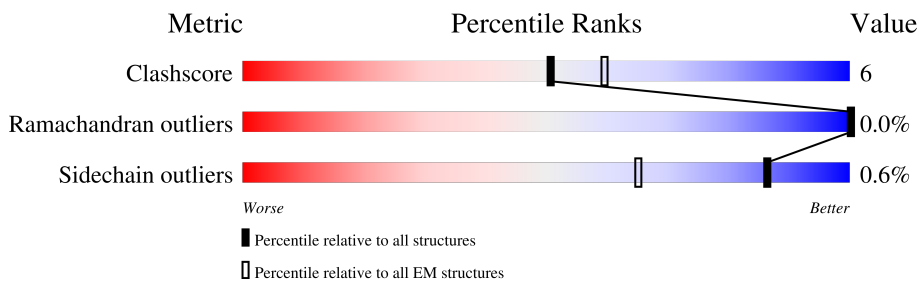
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.27 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.






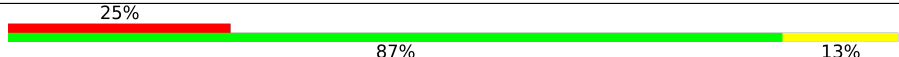
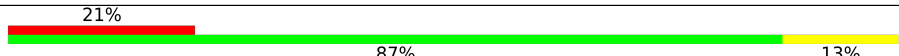
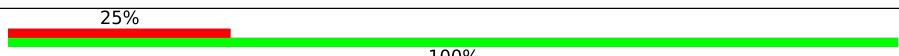
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	249	
3	C	241	
4	D	241	
5	E	247	
6	F	232	
7	G	246	
8	H	273	

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Mol	Chain	Length	Quality of chain
9	I	260	 7% 80% 20%
10	J	262	 7% 77% 22%
11	K	259	 7% 84% 15%
12	L	264	 25% 87% 13%
13	M	270	 21% 87% 13%
14	s	16	 25% 100%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 24659 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
			Total	C	N	O	S		
1	A	238	1835	1169	309	349	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	249	1816	1164	308	341	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	241	1795	1140	301	352	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	241	1782	1121	309	348	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	247	1869	1173	319	370	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	232	1739	1097	307	331	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	246	1778	1135	313	326	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	265	1986	1246	358	369	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	260	1958	1230	337	382	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	262	1976	1242	358	363	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	259	1956	1231	351	367	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	264	1860	1189	315	348	8	0	0

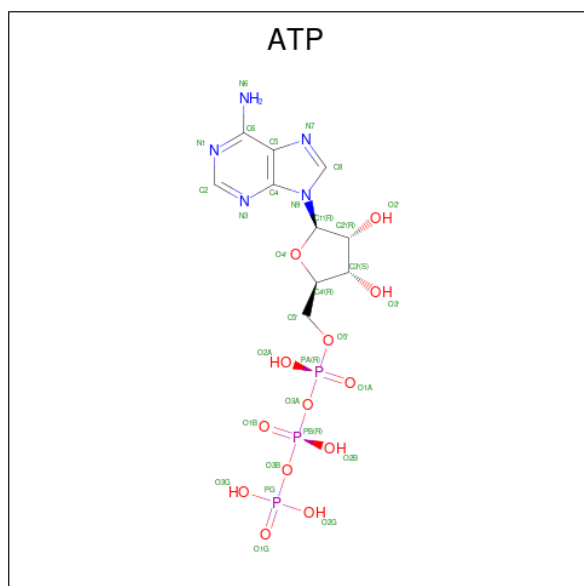
- Molecule 13 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	270	2035	1272	356	400	7	0	0

- Molecule 14 is a protein called model substrate polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	s	16	96	58	18	20	0	0

- 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
			Total	C	N	O	P	
15	H	1	31	10	5	13	3	0
15	I	1	31	10	5	13	3	0
15	J	1	31	10	5	13	3	0
15	M	1	31	10	5	13	3	0

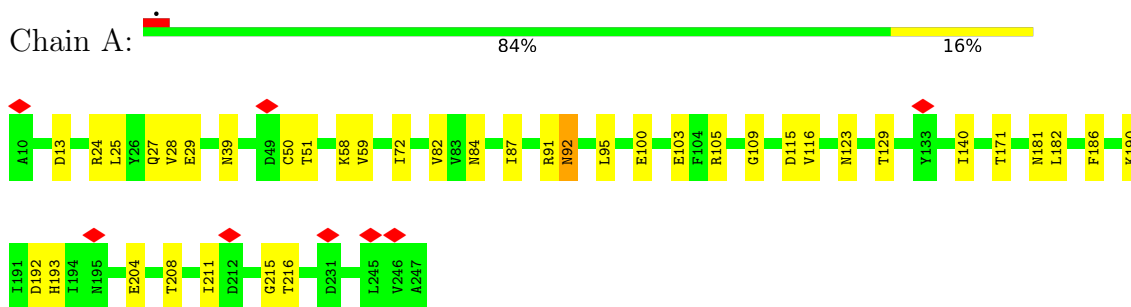
- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



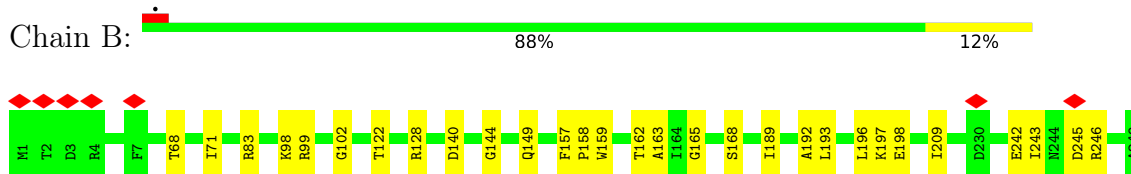
### 3 Residue-property plots [i](#)

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

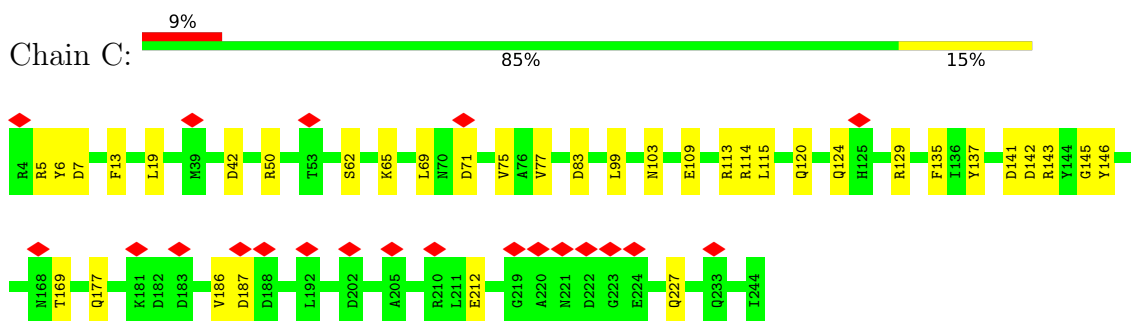
- Molecule 1: Proteasome subunit alpha type-1



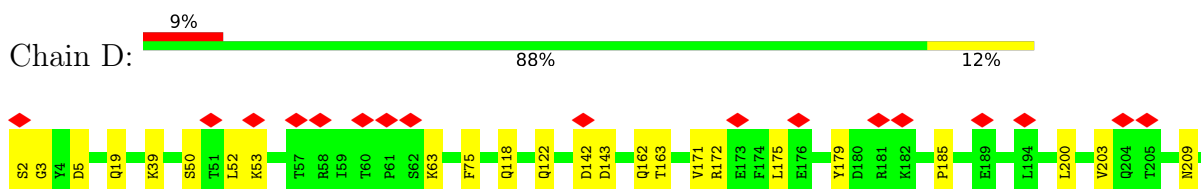
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 3: Proteasome subunit alpha type-3



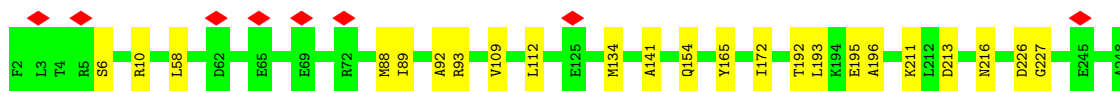
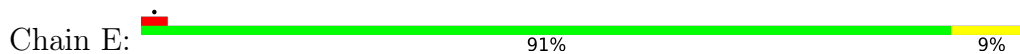
- Molecule 4: Proteasome subunit alpha type-4



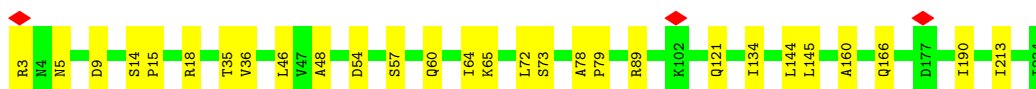
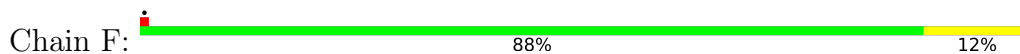




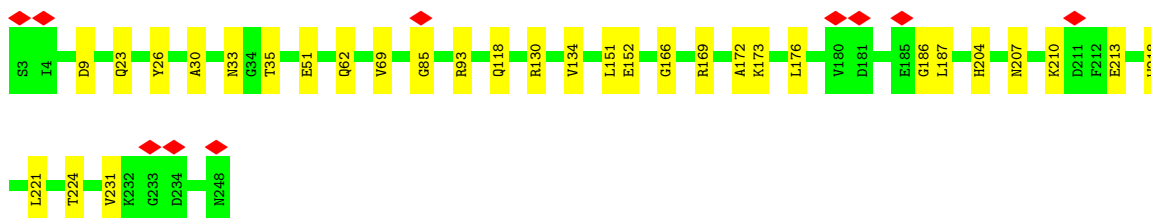
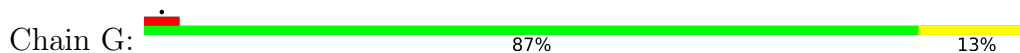
- Molecule 5: Proteasome subunit alpha type-5



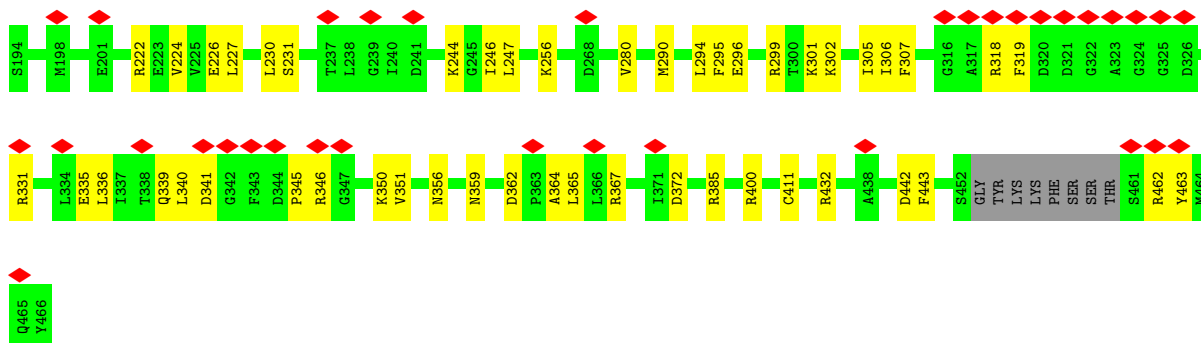
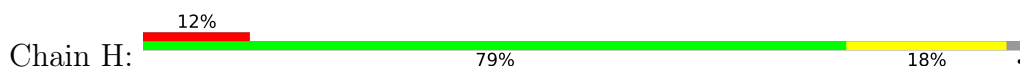
- Molecule 6: Proteasome subunit alpha type-6



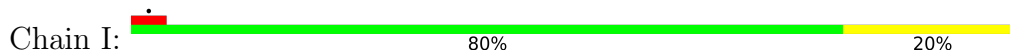
- Molecule 7: Probable proteasome subunit alpha type-7

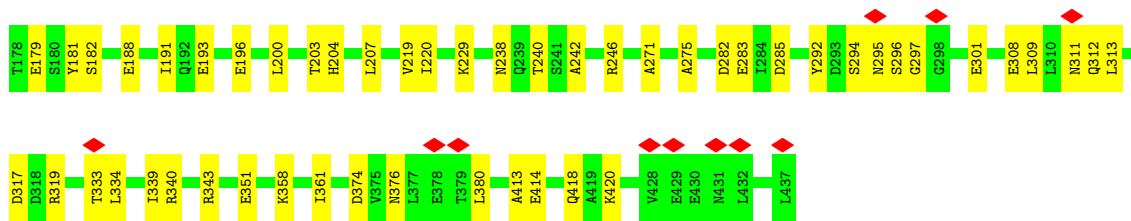


- Molecule 8: 26S proteasome regulatory subunit 7 homolog

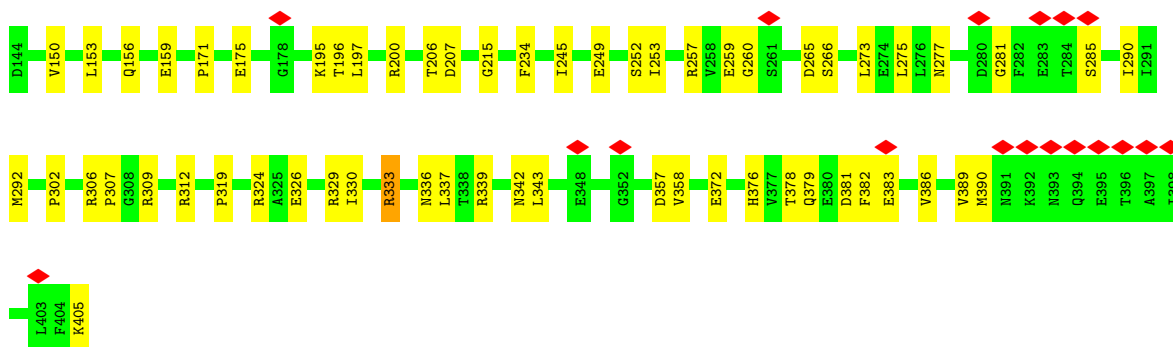
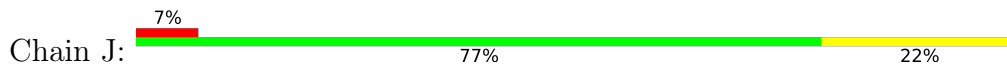


- Molecule 9: 26S proteasome regulatory subunit 4 homolog

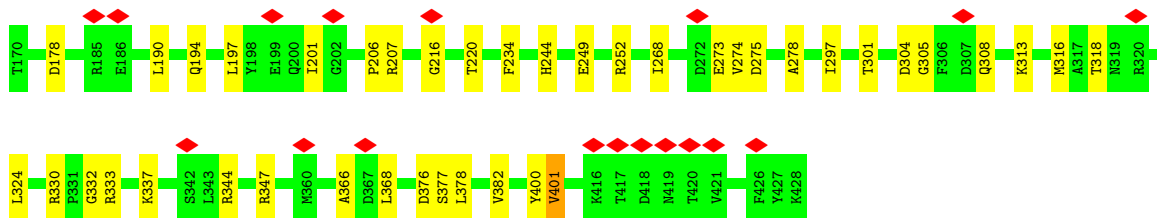
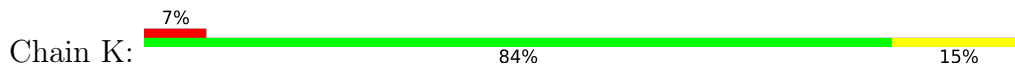




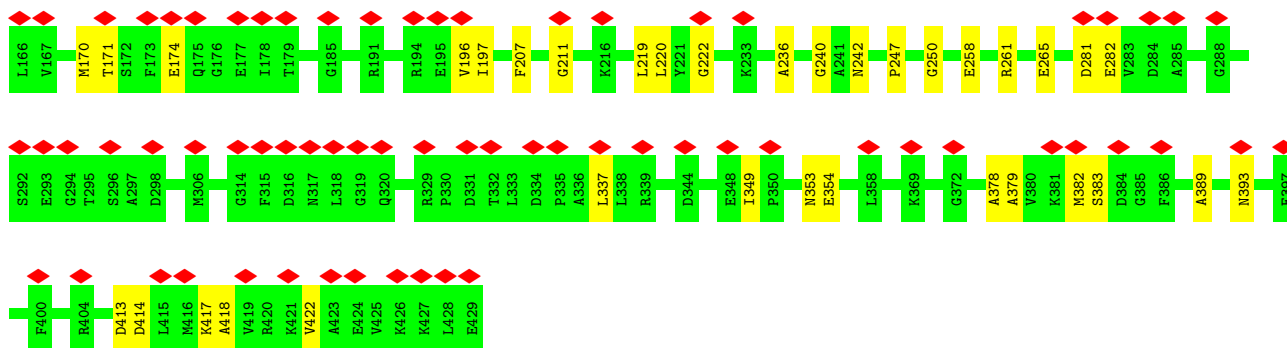
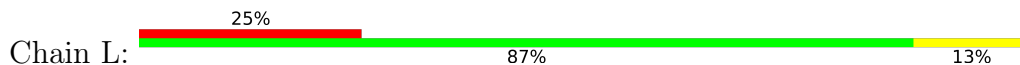
- Molecule 10: 26S proteasome regulatory subunit 8 homolog



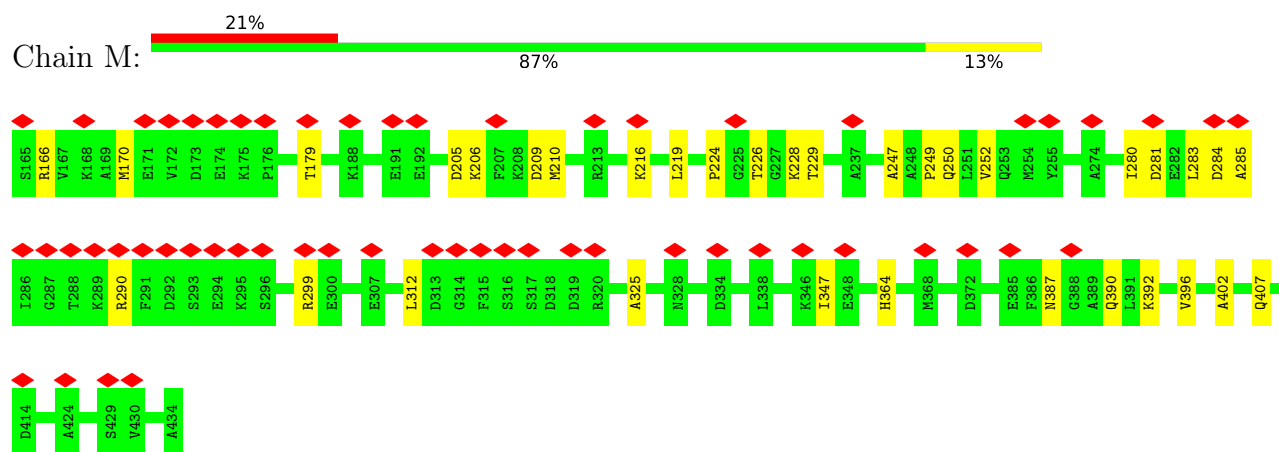
- Molecule 11: 26S proteasome regulatory subunit 6B homolog



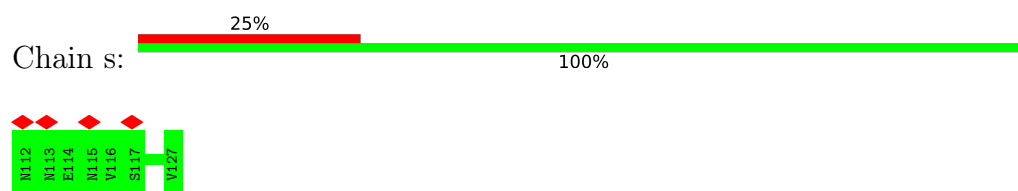
- Molecule 12: 26S proteasome subunit RPT4



- 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	47349	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	0.192	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.54	0/1873	0.62	0/2544
2	B	0.55	0/1852	0.61	0/2519
3	C	0.50	0/1825	0.60	0/2488
4	D	0.50	0/1811	0.62	0/2472
5	E	0.53	0/1896	0.61	0/2561
6	F	0.54	0/1766	0.63	0/2393
7	G	0.52	0/1816	0.60	0/2474
8	H	0.47	0/2016	0.66	0/2724
9	I	0.52	0/1981	0.66	0/2673
10	J	0.54	0/2003	0.67	0/2696
11	K	0.51	0/1982	0.64	0/2681
12	L	0.37	0/1891	0.58	0/2578
13	M	0.39	0/2062	0.61	0/2785
14	s	0.35	0/95	0.70	0/129
All	All	0.50	0/24869	0.62	0/33717

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
2	B	0	1
11	K	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	157	PHE	Peptide
11	K	401	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1835	0	1781	26	0
2	B	1816	0	1796	16	0
3	C	1795	0	1720	23	0
4	D	1782	0	1706	17	0
5	E	1869	0	1818	15	0
6	F	1739	0	1722	16	0
7	G	1778	0	1672	19	0
8	H	1986	0	1958	28	0
9	I	1958	0	1960	35	0
10	J	1976	0	2018	36	0
11	K	1956	0	1948	27	0
12	L	1860	0	1747	20	0
13	M	2035	0	1998	29	0
14	s	96	0	88	0	0
15	H	31	0	12	3	0
15	I	31	0	12	3	0
15	J	31	0	12	2	0
15	M	31	0	12	6	0
16	K	27	0	12	2	0
16	L	27	0	12	0	0
All	All	24659	0	24004	287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (287) 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)
11:K:304:ASP:OD2	11:K:330:ARG:NH2	2.14	0.81
8:H:385:ARG:NH1	8:H:411:CYS:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:330:ILE:O	10:J:333:ARG:NH1	2.15	0.78
11:K:206:PRO:O	11:K:313:LYS:NZ	2.18	0.77
9:I:414:GLU:O	9:I:418:GLN:NE2	2.18	0.77
12:L:261:ARG:NH2	12:L:265:GLU:OE2	2.19	0.75
8:H:318:ARG:NH1	8:H:362:ASP:OD1	2.19	0.75
4:D:63:LYS:NZ	4:D:75:PHE:O	2.21	0.74
2:B:198:GLU:O	11:K:344:ARG:NH2	2.21	0.74
1:A:105:ARG:NH1	1:A:109:GLY:O	2.21	0.73
12:L:258:GLU:OE1	12:L:261:ARG:NE	2.21	0.72
10:J:195:LYS:NZ	15:J:501:ATP:O1B	2.22	0.72
10:J:200:ARG:NH2	11:K:305:GLY:O	2.22	0.72
13:M:280:ILE:HD11	13:M:325:ALA:HB1	1.72	0.71
10:J:245:ILE:HD11	10:J:290:ILE:HG23	1.71	0.71
9:I:380:LEU:O	9:I:420:LYS:NZ	2.25	0.70
11:K:244:HIS:ND1	11:K:249:GLU:OE2	2.25	0.69
1:A:24:ARG:NH2	1:A:29:GLU:OE1	2.26	0.69
3:C:120:GLN:OE1	3:C:124:GLN:NE2	2.26	0.68
6:F:190:ILE:HD11	6:F:213:ILE:HG21	1.75	0.68
2:B:242:GLU:O	2:B:246:ARG:NH1	2.27	0.68
7:G:62:GLN:NE2	7:G:213:GLU:OE2	2.27	0.67
11:K:178:ASP:OD2	11:K:347:ARG:NH2	2.26	0.67
10:J:273:LEU:HD22	10:J:309:ARG:NH2	2.09	0.67
8:H:345:PRO:O	8:H:346:ARG:NE	2.25	0.66
9:I:317:ASP:O	9:I:319:ARG:NH1	2.28	0.66
13:M:216:LYS:HG3	13:M:312:LEU:HD22	1.77	0.65
11:K:304:ASP:OD1	11:K:333:ARG:NH1	2.29	0.65
13:M:228:LYS:NZ	15:M:501:ATP:O3B	2.29	0.65
10:J:281:GLY:O	10:J:285:SER:N	2.29	0.64
1:A:84:ASN:ND2	1:A:171:THR:OG1	2.30	0.64
2:B:149:GLN:OE1	2:B:159:TRP:NE1	2.31	0.64
6:F:65:LYS:O	6:F:89:ARG:NH2	2.31	0.63
3:C:65:LYS:NZ	10:J:405:LYS:O	2.26	0.63
10:J:171:PRO:O	10:J:175:GLU:N	2.32	0.63
4:D:52:LEU:HD13	4:D:53:LYS:N	2.14	0.62
13:M:224:PRO:O	13:M:226:THR:OG1	2.17	0.62
8:H:244:LYS:N	8:H:372:ASP:OD2	2.32	0.62
12:L:196:VAL:HG23	12:L:197:ILE:HD12	1.83	0.61
13:M:228:LYS:N	15:M:501:ATP:O1A	2.33	0.60
5:E:211:LYS:O	5:E:216:ASN:ND2	2.34	0.60
4:D:5:ASP:O	4:D:19:GLN:NE2	2.31	0.60
9:I:229:LYS:NZ	15:I:501:ATP:O1A	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:181:TYR:HE1	9:I:191:ILE:HD11	1.67	0.60
8:H:226:GLU:O	8:H:230:LEU:N	2.34	0.59
11:K:308:GLN:N	11:K:308:GLN:OE1	2.35	0.59
11:K:216:GLY:N	16:K:501:ADP:O1A	2.35	0.59
5:E:213:ASP:N	5:E:216:ASN:OD1	2.34	0.59
6:F:121:GLN:OE1	7:G:130:ARG:NH2	2.35	0.59
10:J:302:PRO:O	10:J:306:ARG:N	2.35	0.59
4:D:234:THR:O	4:D:238:GLN:N	2.34	0.59
1:A:39:ASN:O	1:A:58:LYS:NZ	2.36	0.58
1:A:95:LEU:HD22	7:G:118:GLN:HE22	1.68	0.58
12:L:389:ALA:O	12:L:393:ASN:ND2	2.36	0.58
8:H:335:GLU:O	8:H:339:GLN:N	2.36	0.58
12:L:170:MET:O	12:L:171:THR:OG1	2.20	0.58
10:J:252:SER:OG	10:J:253:ILE:HD12	2.03	0.58
13:M:290:ARG:O	13:M:299:ARG:NH2	2.38	0.57
8:H:341:ASP:OD2	8:H:367:ARG:NH2	2.37	0.57
3:C:177:GLN:OE1	4:D:52:LEU:HD11	2.05	0.57
7:G:169:ARG:O	7:G:173:LYS:N	2.38	0.56
8:H:256:LYS:NZ	15:H:501:ATP:O1B	2.37	0.56
8:H:290:MET:O	8:H:294:LEU:N	2.38	0.56
3:C:164:SER:HG	3:C:169:THR:HG1	1.48	0.56
9:I:229:LYS:N	15:I:501:ATP:O2A	2.36	0.56
10:J:306:ARG:NH2	10:J:307:PRO:O	2.39	0.56
2:B:165:GLY:O	2:B:168:SER:OG	2.19	0.55
4:D:39:LYS:N	4:D:185:PRO:O	2.40	0.55
9:I:181:TYR:O	9:I:182:SER:OG	2.20	0.55
8:H:331:ARG:NH1	13:M:252:VAL:O	2.38	0.55
9:I:193:GLU:OE1	9:I:193:GLU:N	2.39	0.55
5:E:192:THR:OG1	5:E:195:GLU:N	2.40	0.55
12:L:418:ALA:O	12:L:422:VAL:HG22	2.06	0.55
7:G:35:THR:OG1	7:G:51:GLU:O	2.24	0.55
12:L:379:ALA:O	12:L:383:SER:N	2.40	0.55
5:E:165:TYR:OH	6:F:60:GLN:NE2	2.41	0.54
8:H:442:ASP:OD1	8:H:443:PHE:N	2.40	0.54
1:A:115:ASP:OD1	1:A:116:VAL:N	2.40	0.54
1:A:123:ASN:OD1	2:B:83:ARG:NH1	2.40	0.54
7:G:172:ALA:HB1	7:G:176:LEU:HD23	1.90	0.54
5:E:6:SER:O	5:E:10:ARG:NH1	2.38	0.53
7:G:166:GLY:O	7:G:169:ARG:NH1	2.41	0.53
7:G:69:VAL:O	7:G:93:ARG:NH1	2.42	0.53
8:H:296:GLU:OE1	8:H:299:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:229:THR:OG1	15:M:501:ATP:O2B	2.16	0.53
9:I:179:GLU:O	9:I:238:ASN:ND2	2.41	0.53
6:F:54:ASP:OD1	6:F:57:SER:N	2.41	0.53
6:F:64:ILE:HD11	6:F:72:LEU:HD11	1.91	0.53
9:I:294:SER:OG	9:I:295:ASN:N	2.42	0.53
9:I:339:ILE:HD12	9:I:339:ILE:O	2.07	0.53
13:M:206:LYS:O	13:M:210:MET:N	2.42	0.53
2:B:245:ASP:OD1	2:B:246:ARG:N	2.42	0.53
13:M:364:HIS:CE1	15:M:501:ATP:HO2'	2.27	0.53
4:D:200:LEU:HA	4:D:203:VAL:HG12	1.91	0.52
7:G:204:HIS:NE2	7:G:210:LYS:O	2.42	0.52
1:A:84:ASN:HD21	1:A:171:THR:CG2	2.23	0.52
12:L:219:LEU:C	12:L:220:LEU:HD12	2.30	0.52
4:D:175:LEU:O	4:D:179:TYR:N	2.42	0.52
1:A:25:LEU:HD11	1:A:28:VAL:HG22	1.91	0.52
8:H:227:LEU:O	8:H:231:SER:N	2.43	0.52
3:C:5:ARG:NH2	3:C:7:ASP:OD2	2.44	0.51
13:M:205:ASP:O	13:M:209:ASP:N	2.43	0.51
8:H:306:ILE:HD11	8:H:351:VAL:HG13	1.92	0.51
10:J:234:PHE:CD2	10:J:275:LEU:HD13	2.45	0.51
3:C:42:ASP:O	3:C:146:TYR:OH	2.15	0.51
9:I:240:THR:HG23	9:I:242:ALA:H	1.75	0.51
2:B:98:LYS:O	2:B:102:GLY:N	2.44	0.51
4:D:50:SER:N	4:D:209:ASN:OD1	2.43	0.51
1:A:192:ASP:OD1	1:A:193:HIS:N	2.43	0.51
9:I:285:ASP:OD2	10:J:257:ARG:NH1	2.43	0.51
9:I:374:ASP:HB3	9:I:413:ALA:HB2	1.92	0.50
12:L:207:PHE:O	12:L:211:GLY:N	2.42	0.50
11:K:278:ALA:HB1	11:K:324:LEU:HB2	1.93	0.50
10:J:319:PRO:O	10:J:324:ARG:NH1	2.45	0.50
5:E:109:VAL:O	5:E:112:LEU:N	2.45	0.50
10:J:159:GLU:OE2	10:J:312:ARG:NH1	2.44	0.50
4:D:142:ASP:OD1	4:D:143:ASP:N	2.42	0.49
9:I:188:GLU:HA	9:I:191:ILE:HG22	1.94	0.49
11:K:376:ASP:OD1	11:K:377:SER:N	2.45	0.49
10:J:150:VAL:HG23	10:J:197:LEU:HD12	1.94	0.49
12:L:247:PRO:O	12:L:250:GLY:N	2.42	0.49
12:L:414:ASP:O	12:L:418:ALA:N	2.40	0.49
6:F:9:ASP:OD1	6:F:9:ASP:N	2.44	0.49
1:A:186:PHE:O	1:A:190:LYS:N	2.44	0.49
7:G:9:ASP:O	7:G:23:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:265:ASP:OD1	10:J:266:SER:N	2.46	0.49
11:K:220:THR:HG22	16:K:501:ADP:O2A	2.11	0.49
3:C:142:ASP:OD1	3:C:143:ARG:N	2.46	0.49
8:H:224:VAL:HG11	8:H:246:ILE:HG21	1.95	0.49
12:L:281:ASP:OD1	12:L:282:GLU:N	2.45	0.49
3:C:115:LEU:HD23	3:C:137:TYR:OH	2.12	0.48
8:H:336:LEU:O	8:H:340:LEU:N	2.44	0.48
13:M:166:ARG:O	13:M:170:MET:N	2.43	0.48
13:M:364:HIS:NE2	15:M:501:ATP:O2'	2.46	0.48
5:E:88:MET:O	5:E:92:ALA:N	2.47	0.48
1:A:13:ASP:O	1:A:27:GLN:NE2	2.46	0.48
2:B:68:THR:OG1	2:B:71:ILE:N	2.46	0.48
13:M:249:PRO:O	13:M:252:VAL:N	2.45	0.48
9:I:351:GLU:N	9:I:351:GLU:OE1	2.47	0.48
15:H:501:ATP:O3B	9:I:340:ARG:NH2	2.47	0.47
13:M:280:ILE:HD13	13:M:283:LEU:HD21	1.95	0.47
13:M:402:ALA:O	13:M:407:GLN:N	2.44	0.47
3:C:69:LEU:HD13	3:C:75:VAL:HG13	1.96	0.47
9:I:308:GLU:O	9:I:312:GLN:N	2.47	0.47
3:C:109:GLU:OE2	3:C:113:ARG:NH1	2.47	0.47
10:J:196:THR:OG1	15:J:501:ATP:O2A	2.32	0.47
3:C:6:TYR:OH	4:D:5:ASP:OD2	2.31	0.47
4:D:2:SER:OG	4:D:3:GLY:N	2.47	0.47
1:A:92:ASN:O	1:A:92:ASN:ND2	2.46	0.47
2:B:140:ASP:OD1	2:B:144:GLY:N	2.46	0.47
4:D:229:ILE:O	4:D:233:VAL:N	2.48	0.47
5:E:226:ASP:OD1	5:E:227:GLY:N	2.48	0.47
6:F:36:VAL:HG23	6:F:160:ALA:HB2	1.97	0.47
8:H:301:LYS:NZ	8:H:302:LYS:O	2.44	0.47
13:M:280:ILE:HD11	13:M:325:ALA:CB	2.43	0.47
9:I:301:GLU:OE1	9:I:301:GLU:N	2.46	0.47
12:L:174:GLU:OE2	12:L:242:ASN:ND2	2.47	0.47
9:I:282:ASP:OD1	9:I:283:GLU:N	2.47	0.47
9:I:292:TYR:OH	10:J:260:GLY:O	2.20	0.47
11:K:190:LEU:O	11:K:194:GLN:N	2.45	0.47
3:C:13:PHE:CE1	3:C:19:LEU:HD11	2.50	0.46
2:B:122:THR:O	3:C:129:ARG:NH2	2.46	0.46
10:J:342:ASN:OD1	10:J:343:LEU:N	2.48	0.46
8:H:305:ILE:HG22	8:H:350:LYS:CB	2.46	0.46
3:C:99:LEU:O	3:C:103:ASN:N	2.45	0.46
6:F:14:SER:N	6:F:18:ARG:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ASP:OD2	3:C:129:ARG:NH1	2.42	0.46
7:G:204:HIS:NE2	7:G:207:ASN:O	2.48	0.46
15:H:501:ATP:O2G	9:I:343:ARG:NH1	2.47	0.46
7:G:30:ALA:O	7:G:33:ASN:N	2.47	0.46
11:K:207:ARG:NH2	11:K:332:GLY:O	2.49	0.46
1:A:181:ASN:OD1	1:A:182:LEU:N	2.49	0.45
12:L:378:ALA:O	12:L:382:MET:N	2.43	0.45
3:C:71:ASP:O	3:C:227:GLN:NE2	2.48	0.45
7:G:186:GLY:C	7:G:187:LEU:HD22	2.36	0.45
6:F:144:LEU:C	6:F:145:LEU:HD12	2.37	0.45
8:H:432:ARG:NH2	9:I:196:GLU:OE1	2.50	0.45
10:J:249:GLU:OE1	11:K:297:ILE:HG23	2.16	0.45
5:E:141:ALA:HB3	5:E:172:ILE:HD13	1.98	0.45
10:J:372:GLU:OE1	10:J:372:GLU:N	2.49	0.45
12:L:337:LEU:O	12:L:337:LEU:HD23	2.17	0.45
11:K:330:ARG:NH1	11:K:333:ARG:HE	2.14	0.45
11:K:400:TYR:CD2	11:K:401:VAL:HG23	2.52	0.45
12:L:413:ASP:O	12:L:417:LYS:N	2.50	0.45
1:A:72:ILE:HD12	1:A:82:VAL:HG12	1.99	0.45
9:I:200:LEU:O	9:I:203:THR:N	2.44	0.45
10:J:337:LEU:O	10:J:339:ARG:NH1	2.40	0.45
10:J:357:ASP:OD1	10:J:358:VAL:N	2.50	0.45
10:J:378:THR:HG22	10:J:379:GLN:N	2.32	0.45
13:M:387:ASN:O	13:M:390:GLN:N	2.50	0.45
5:E:89:ILE:HA	5:E:92:ALA:HB3	1.99	0.45
5:E:154:GLN:N	5:E:154:GLN:OE1	2.50	0.45
8:H:462:ARG:NH1	8:H:463:TYR:O	2.50	0.44
5:E:89:ILE:HD12	5:E:93:ARG:HH12	1.81	0.44
6:F:134:ILE:N	6:F:145:LEU:O	2.47	0.44
9:I:271:ALA:O	9:I:275:ALA:N	2.51	0.44
10:J:215:GLY:HA3	11:K:301:THR:HG21	2.00	0.44
2:B:209:ILE:HD11	2:B:243:ILE:HD13	1.99	0.44
9:I:229:LYS:NZ	15:I:501:ATP:O3B	2.50	0.44
11:K:234:PHE:HD1	11:K:268:ILE:HD11	1.83	0.44
1:A:25:LEU:CD1	1:A:28:VAL:HG22	2.48	0.44
1:A:72:ILE:CD1	1:A:82:VAL:HG12	2.48	0.43
1:A:129:THR:O	2:B:128:ARG:NE	2.51	0.43
3:C:141:ASP:O	3:C:145:GLY:N	2.51	0.43
6:F:35:THR:OG1	6:F:48:ALA:HB2	2.18	0.43
10:J:389:VAL:HG13	10:J:390:MET:SD	2.58	0.43
9:I:296:SER:OG	9:I:297:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:O	1:A:51:THR:OG1	2.31	0.43
7:G:151:LEU:HD13	7:G:152:GLU:N	2.33	0.43
8:H:280:VAL:HG12	8:H:280:VAL:O	2.18	0.43
10:J:150:VAL:HG22	10:J:150:VAL:O	2.18	0.43
3:C:13:PHE:CD1	3:C:19:LEU:HD11	2.54	0.43
5:E:58:LEU:HD23	5:E:58:LEU:H	1.84	0.43
1:A:204:GLU:O	1:A:208:THR:HG22	2.18	0.43
3:C:77:VAL:HG23	3:C:135:PHE:HE1	1.83	0.43
10:J:326:GLU:O	10:J:329:ARG:N	2.52	0.43
13:M:219:LEU:O	13:M:347:ILE:N	2.44	0.43
1:A:211:ILE:HG23	1:A:216:THR:O	2.18	0.43
8:H:295:PHE:O	8:H:299:ARG:N	2.42	0.43
13:M:219:LEU:HD23	13:M:325:ALA:HB3	2.00	0.43
2:B:162:THR:HG22	2:B:163:ALA:N	2.34	0.43
3:C:50:ARG:NH2	3:C:62:SER:O	2.48	0.43
7:G:85:GLY:N	7:G:134:VAL:HG11	2.34	0.43
11:K:201:ILE:HD12	11:K:201:ILE:H	1.83	0.43
13:M:284:ASP:OD1	13:M:285:ALA:N	2.52	0.43
4:D:122:GLN:NE2	5:E:134:MET:SD	2.92	0.43
8:H:364:ALA:C	8:H:365:LEU:HD22	2.39	0.43
10:J:259:GLU:N	10:J:259:GLU:OE1	2.52	0.43
11:K:194:GLN:HB3	11:K:197:LEU:HD22	2.01	0.43
12:L:196:VAL:CG2	12:L:197:ILE:HD12	2.47	0.43
9:I:204:HIS:HB3	9:I:207:LEU:HD23	2.00	0.42
11:K:366:ALA:O	11:K:368:LEU:N	2.51	0.42
13:M:166:ARG:NE	13:M:250:GLN:OE1	2.50	0.42
10:J:153:LEU:HD13	10:J:156:GLN:HB2	2.00	0.42
12:L:353:ASN:OD1	12:L:354:GLU:N	2.50	0.42
13:M:247:ALA:HB3	13:M:250:GLN:HG2	2.00	0.42
2:B:192:ALA:O	2:B:196:LEU:N	2.48	0.42
4:D:163:THR:HG21	4:D:171:VAL:HG11	2.00	0.42
8:H:318:ARG:HE	8:H:319:PHE:N	2.17	0.42
13:M:364:HIS:HE2	15:M:501:ATP:HO2'	1.60	0.42
4:D:229:ILE:O	4:D:232:TYR:N	2.53	0.42
13:M:280:ILE:HD12	13:M:281:ASP:O	2.18	0.42
8:H:246:ILE:HD12	8:H:247:LEU:N	2.34	0.42
10:J:383:GLU:HA	10:J:386:VAL:HG12	2.01	0.42
2:B:193:LEU:O	2:B:197:LYS:N	2.49	0.42
7:G:224:THR:HG22	7:G:224:THR:O	2.19	0.42
9:I:333:THR:C	9:I:334:LEU:HD22	2.40	0.42
1:A:211:ILE:O	1:A:215:GLY:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:306:ILE:HD12	8:H:307:PHE:N	2.35	0.42
11:K:275:ASP:OD2	11:K:318:THR:OG1	2.38	0.42
12:L:236:ALA:O	12:L:240:GLY:N	2.49	0.42
6:F:78:ALA:HB3	6:F:79:PRO:HD3	2.02	0.42
9:I:193:GLU:O	9:I:196:GLU:N	2.53	0.42
7:G:221:LEU:HD23	7:G:221:LEU:H	1.85	0.41
11:K:378:LEU:HD22	11:K:382:VAL:HG21	2.02	0.41
13:M:205:ASP:OD1	13:M:206:LYS:N	2.53	0.41
1:A:87:ILE:HD11	1:A:91:ARG:NH2	2.36	0.41
3:C:212:GLU:N	3:C:212:GLU:OE1	2.54	0.41
10:J:336:ASN:HD22	10:J:376:HIS:HA	1.85	0.41
11:K:273:GLU:OE2	11:K:275:ASP:N	2.53	0.41
2:B:189:ILE:HD12	2:B:189:ILE:H	1.86	0.41
9:I:181:TYR:CE1	9:I:191:ILE:HD11	2.53	0.41
9:I:219:VAL:HG12	9:I:220:ILE:N	2.35	0.41
6:F:3:ARG:HE	6:F:5:ASN:HB2	1.86	0.41
7:G:218:TRP:HE1	7:G:231:VAL:HG12	1.85	0.41
12:L:222:GLY:HA3	12:L:349:ILE:HG21	2.03	0.41
13:M:219:LEU:HD22	13:M:325:ALA:O	2.20	0.41
13:M:392:LYS:O	13:M:396:VAL:N	2.54	0.41
1:A:59:VAL:HG13	1:A:59:VAL:O	2.21	0.41
8:H:362:ASP:OD2	8:H:364:ALA:N	2.54	0.41
8:H:222:ARG:NH2	8:H:226:GLU:OE1	2.53	0.41
9:I:309:LEU:O	9:I:313:LEU:N	2.49	0.41
11:K:274:VAL:HG11	11:K:316:MET:CE	2.51	0.41
3:C:186:VAL:HG23	3:C:187:ASP:N	2.36	0.41
9:I:358:LYS:HA	9:I:361:ILE:HG22	2.02	0.41
10:J:215:GLY:CA	11:K:301:THR:HG21	2.51	0.41
10:J:381:ASP:OD1	10:J:382:PHE:N	2.54	0.41
1:A:100:GLU:O	1:A:103:GLU:N	2.54	0.40
1:A:140:ILE:HG23	1:A:140:ILE:O	2.21	0.40
3:C:77:VAL:HG23	3:C:135:PHE:CE1	2.56	0.40
4:D:162:GLN:OE1	4:D:172:ARG:NH2	2.48	0.40
5:E:193:LEU:O	5:E:196:ALA:HB3	2.21	0.40
6:F:15:PRO:HA	7:G:26:TYR:CD1	2.56	0.40
9:I:203:THR:OG1	9:I:204:HIS:N	2.54	0.40
13:M:179:THR:O	13:M:179:THR:HG22	2.21	0.40
10:J:206:THR:HG23	10:J:207:ASP:N	2.36	0.40
6:F:46:LEU:HD13	6:F:73:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	205 (87%)	31 (13%)	0	100	100
2	B	247/249 (99%)	216 (87%)	30 (12%)	1 (0%)	34	72
3	C	239/241 (99%)	207 (87%)	32 (13%)	0	100	100
4	D	239/241 (99%)	211 (88%)	28 (12%)	0	100	100
5	E	245/247 (99%)	217 (89%)	28 (11%)	0	100	100
6	F	230/232 (99%)	206 (90%)	24 (10%)	0	100	100
7	G	244/246 (99%)	219 (90%)	25 (10%)	0	100	100
8	H	261/273 (96%)	226 (87%)	35 (13%)	0	100	100
9	I	258/260 (99%)	211 (82%)	47 (18%)	0	100	100
10	J	260/262 (99%)	222 (85%)	38 (15%)	0	100	100
11	K	257/259 (99%)	226 (88%)	31 (12%)	0	100	100
12	L	262/264 (99%)	218 (83%)	44 (17%)	0	100	100
13	M	268/270 (99%)	226 (84%)	42 (16%)	0	100	100
14	s	14/16 (88%)	11 (79%)	3 (21%)	0	100	100
All	All	3260/3298 (99%)	2821 (86%)	438 (13%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	PRO

### 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	190/203 (94%)	189 (100%)	1 (0%)	88	93
2	B	184/208 (88%)	183 (100%)	1 (0%)	88	93
3	C	177/201 (88%)	176 (99%)	1 (1%)	86	92
4	D	185/213 (87%)	184 (100%)	1 (0%)	88	93
5	E	192/204 (94%)	192 (100%)	0	100	100
6	F	178/191 (93%)	177 (99%)	1 (1%)	86	92
7	G	168/203 (83%)	168 (100%)	0	100	100
8	H	202/230 (88%)	199 (98%)	3 (2%)	65	80
9	I	205/223 (92%)	202 (98%)	3 (2%)	65	80
10	J	207/220 (94%)	204 (99%)	3 (1%)	67	80
11	K	197/219 (90%)	195 (99%)	2 (1%)	76	86
12	L	169/218 (78%)	169 (100%)	0	100	100
13	M	207/224 (92%)	207 (100%)	0	100	100
14	s	8/11 (73%)	8 (100%)	0	100	100
All	All	2469/2768 (89%)	2453 (99%)	16 (1%)	86	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
2	B	99	ARG
3	C	114	ARG
4	D	118	GLN
6	F	166	GLN
8	H	356	ASN
8	H	359	ASN
8	H	400	ARG
9	I	246	ARG
9	I	311	ASN
9	I	376	ASN
10	J	277	ASN
10	J	292	MET
10	J	333	ARG
11	K	252	ARG
11	K	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
3	C	120	GLN
3	C	124	GLN
3	C	147	GLN
4	D	118	GLN
7	G	118	GLN
9	I	376	ASN
10	J	277	ASN
13	M	362	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	J	501	-	26,33,33	0.89	0	31,52,52	1.67	4 (12%)
15	ATP	I	501	-	26,33,33	0.90	0	31,52,52	1.76	6 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	ATP	H	501	-	26,33,33	0.94	1 (3%)	31,52,52	1.85	6 (19%)
15	ATP	M	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.81	4 (12%)
16	ADP	K	501	-	24,29,29	0.98	2 (8%)	29,45,45	1.53	7 (24%)
16	ADP	L	501	-	24,29,29	0.89	1 (4%)	29,45,45	1.66	5 (17%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	501	ADP	C5-C4	2.14	1.46	1.40
16	K	501	ADP	C5-C4	2.12	1.46	1.40
15	M	501	ATP	C5-C4	2.11	1.46	1.40
15	H	501	ATP	C5-C4	2.06	1.46	1.40
16	K	501	ADP	O4'-C1'	2.01	1.43	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	501	ATP	PA-O3A-PB	-5.53	113.84	132.83
15	H	501	ATP	PB-O3B-PG	-5.21	114.96	132.83
15	J	501	ATP	PA-O3A-PB	-5.03	115.58	132.83
15	H	501	ATP	PA-O3A-PB	-4.84	116.22	132.83
15	M	501	ATP	PB-O3B-PG	-4.82	116.27	132.83
16	L	501	ADP	PA-O3A-PB	-4.68	116.75	132.83
15	I	501	ATP	PA-O3A-PB	-4.25	118.26	132.83
15	J	501	ATP	PB-O3B-PG	-4.15	118.59	132.83
15	I	501	ATP	PB-O3B-PG	-4.04	118.96	132.83
15	I	501	ATP	N3-C2-N1	-3.65	122.97	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	501	ATP	C3'-C2'-C1'	3.58	106.37	100.98
16	L	501	ADP	N3-C2-N1	-3.51	123.19	128.68
15	H	501	ATP	C3'-C2'-C1'	3.48	106.22	100.98
16	K	501	ADP	N3-C2-N1	-3.47	123.25	128.68
16	K	501	ADP	PA-O3A-PB	-3.40	121.15	132.83
15	M	501	ATP	N3-C2-N1	-3.36	123.43	128.68
16	L	501	ADP	C3'-C2'-C1'	3.32	105.97	100.98
15	J	501	ATP	N3-C2-N1	-3.30	123.52	128.68
15	H	501	ATP	N3-C2-N1	-3.22	123.65	128.68
16	K	501	ADP	C3'-C2'-C1'	3.07	105.60	100.98
16	K	501	ADP	C2'-C3'-C4'	2.39	107.28	102.64
16	L	501	ADP	C4-C5-N7	-2.33	106.97	109.40
15	J	501	ATP	N6-C6-N1	2.28	123.31	118.57
15	M	501	ATP	C3'-C2'-C1'	2.26	104.38	100.98
16	K	501	ADP	C4-C5-N7	-2.21	107.09	109.40
16	K	501	ADP	O3B-PB-O2B	2.16	115.89	107.64
15	H	501	ATP	C4-C5-N7	-2.15	107.16	109.40
15	I	501	ATP	O3G-PG-O2G	2.10	115.65	107.64
15	I	501	ATP	C4-C5-N7	-2.09	107.22	109.40
16	L	501	ADP	C2-N1-C6	2.05	122.26	118.75
15	H	501	ATP	O3G-PG-O2G	2.04	115.42	107.64
16	K	501	ADP	N6-C6-N1	2.02	122.76	118.57

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	501	ATP	C5'-O5'-PA-O1A
15	J	501	ATP	PB-O3B-PG-O2G
15	J	501	ATP	C5'-O5'-PA-O3A
15	M	501	ATP	C5'-O5'-PA-O1A
16	K	501	ADP	C5'-O5'-PA-O1A
16	K	501	ADP	C5'-O5'-PA-O2A
16	L	501	ADP	C5'-O5'-PA-O1A
16	L	501	ADP	C5'-O5'-PA-O3A
15	J	501	ATP	C5'-O5'-PA-O1A
15	J	501	ATP	PB-O3A-PA-O2A
15	J	501	ATP	PB-O3B-PG-O1G
15	H	501	ATP	C5'-O5'-PA-O3A
15	M	501	ATP	C5'-O5'-PA-O3A
16	K	501	ADP	C5'-O5'-PA-O3A
15	H	501	ATP	PA-O3A-PB-O2B

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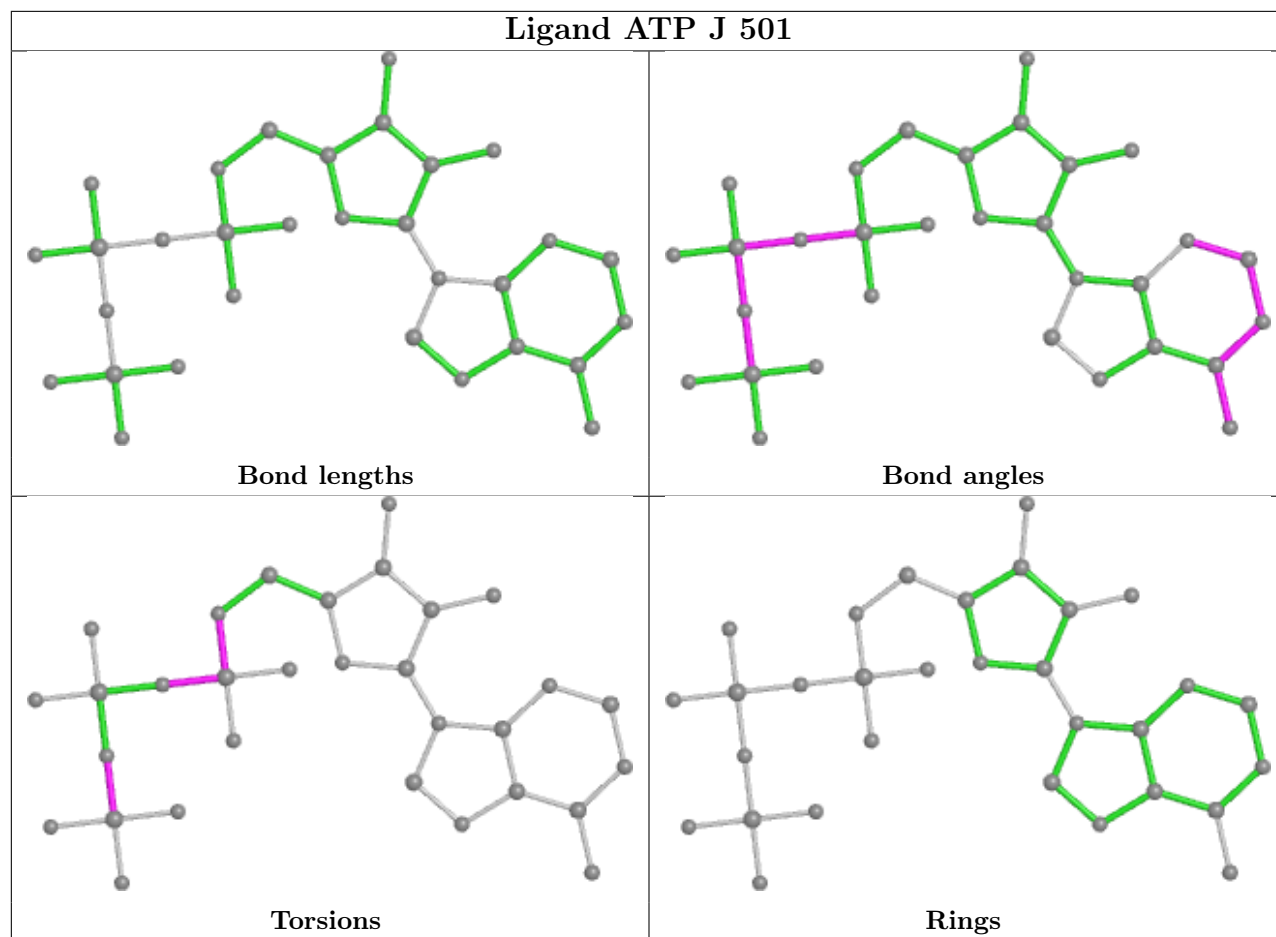
Mol	Chain	Res	Type	Atoms
15	M	501	ATP	PB-O3A-PA-O2A

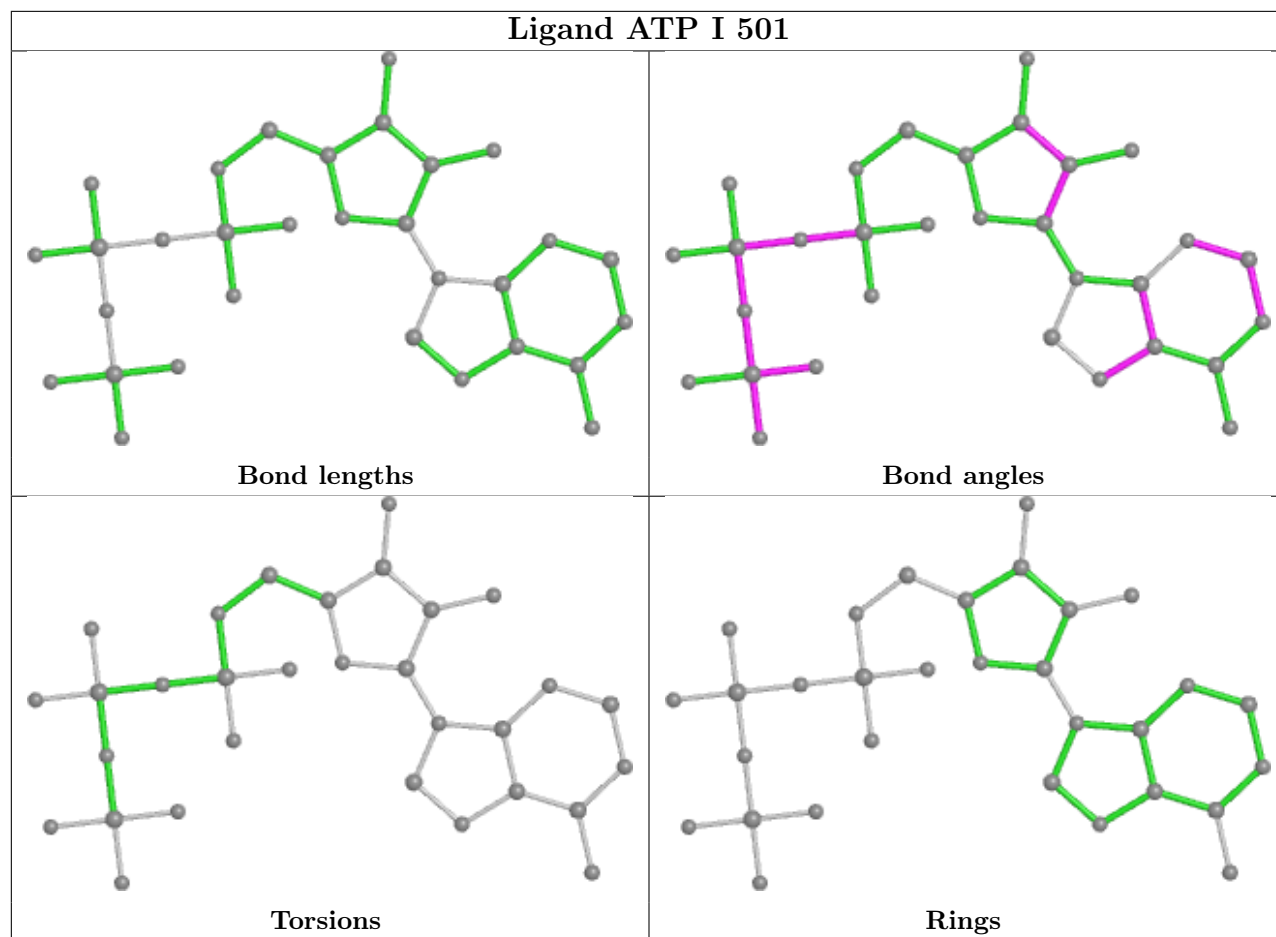
There are no ring outliers.

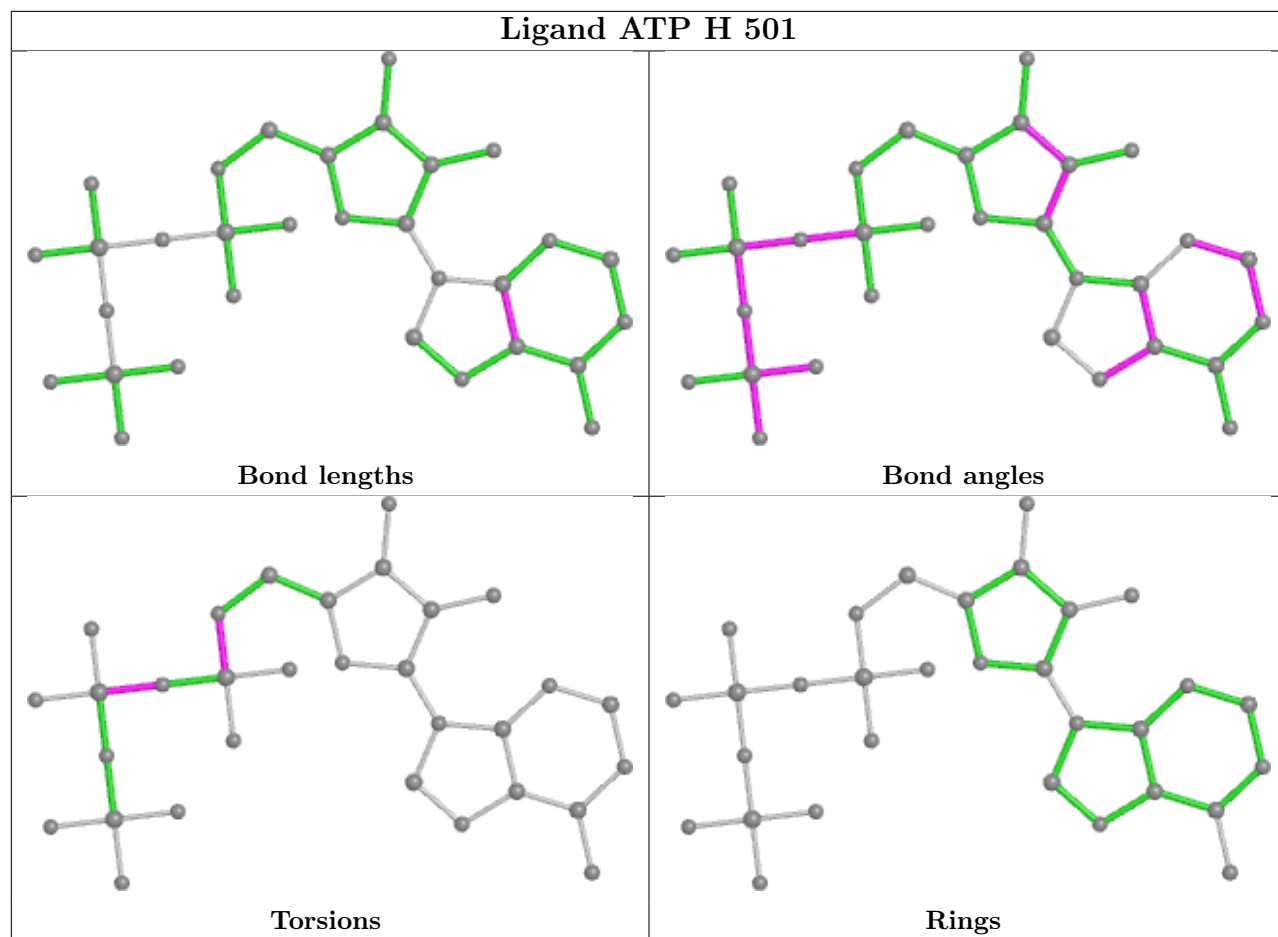
5 monomers are involved in 16 short contacts:

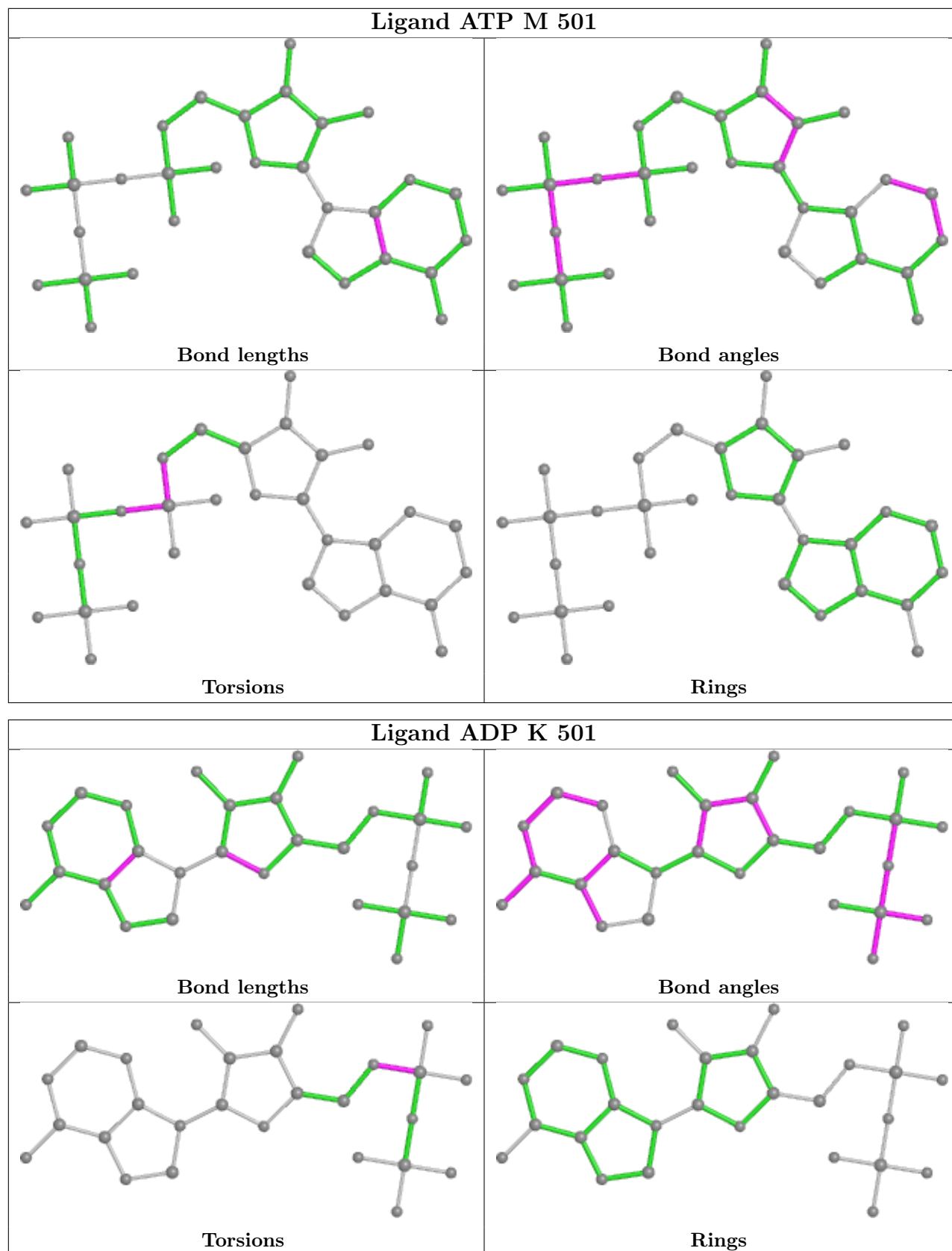
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	J	501	ATP	2	0
15	I	501	ATP	3	0
15	H	501	ATP	3	0
15	M	501	ATP	6	0
16	K	501	ADP	2	0

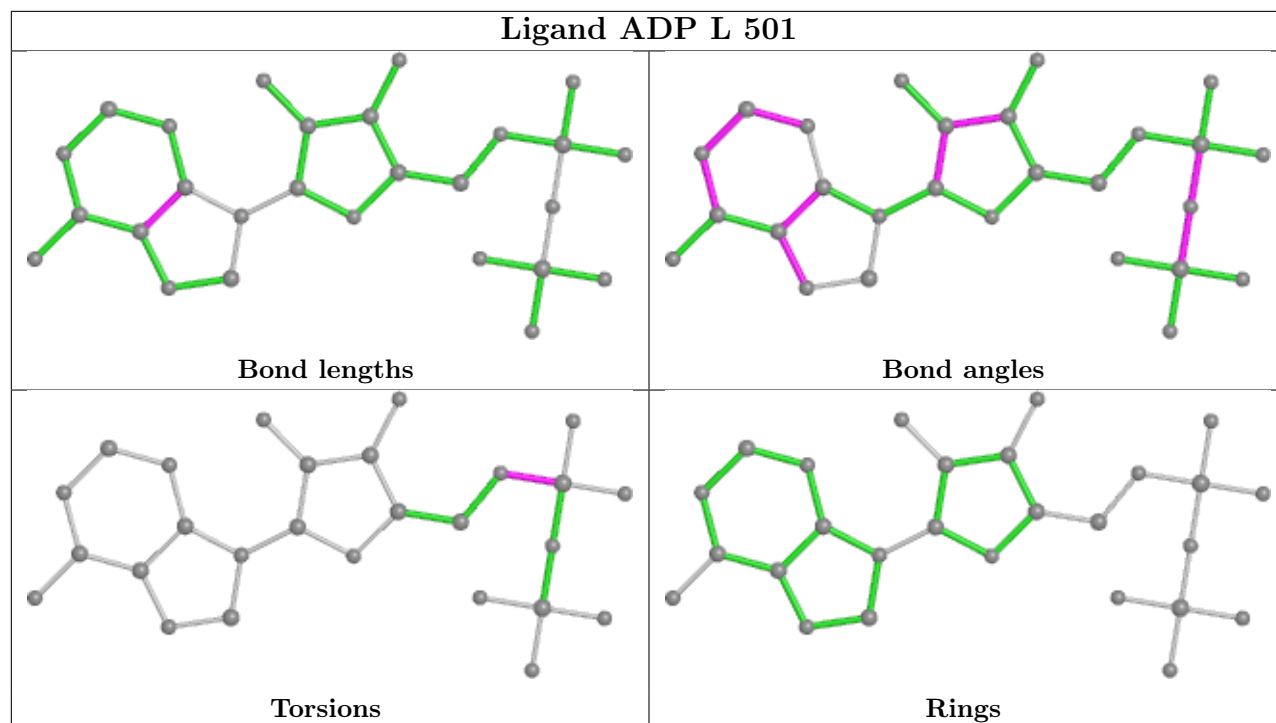
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



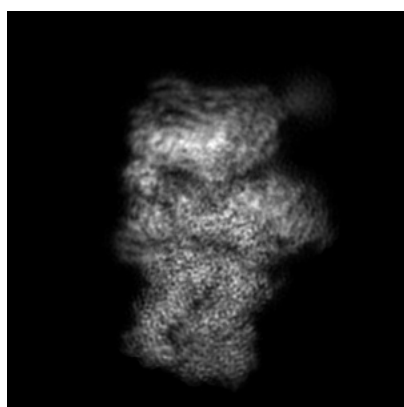
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9044. These allow visual inspection of the internal detail of the map and identification of artifacts.

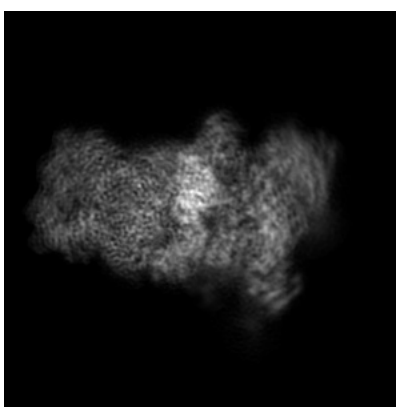
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

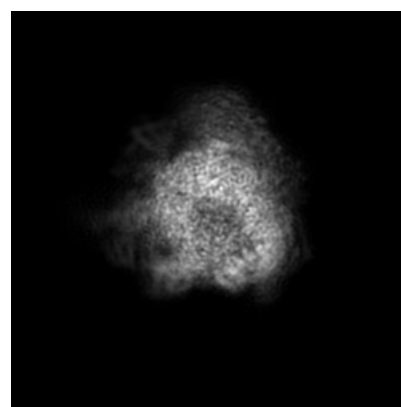
#### 6.1.1 Primary map



X



Y

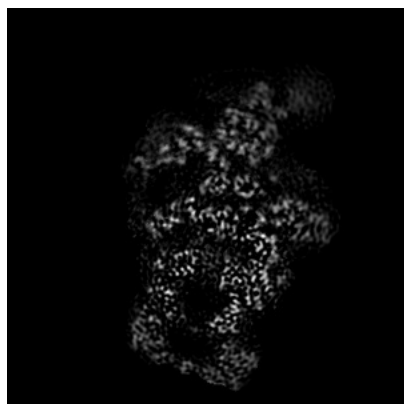


Z

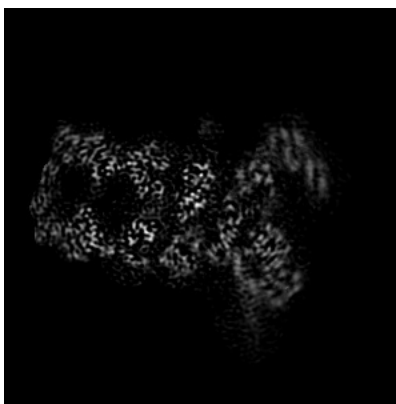
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

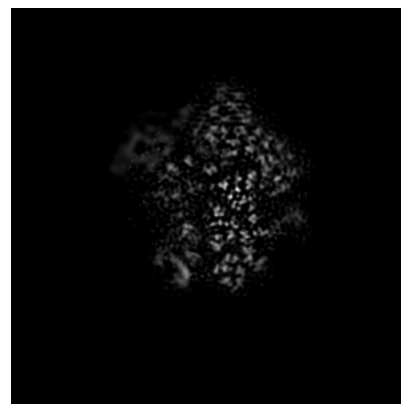
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

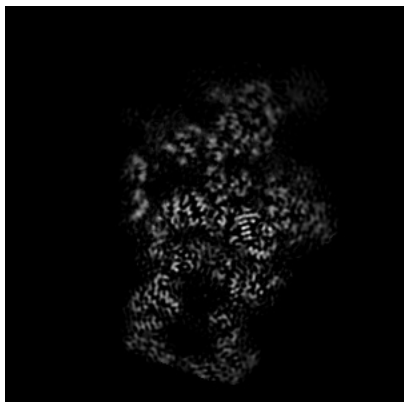


Z Index: 170

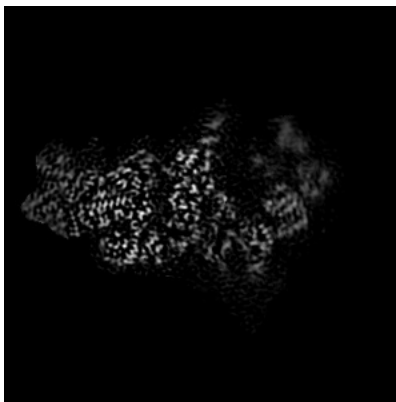
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

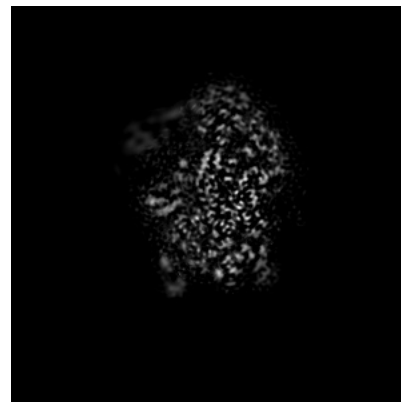
### 6.3.1 Primary map



X Index: 175



Y Index: 193

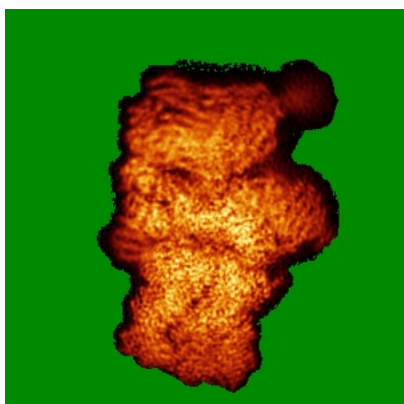


Z Index: 162

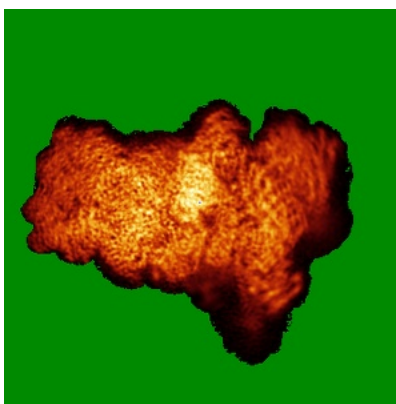
The images above show the largest variance slices of the map in three orthogonal directions.

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

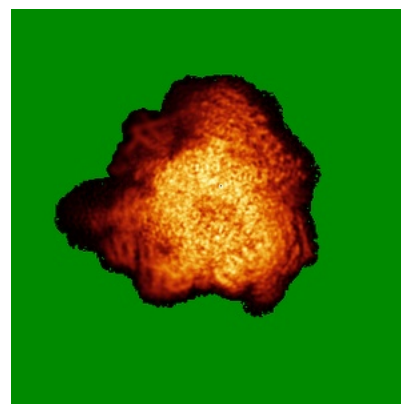
### 6.4.1 Primary map



X



Y



Z

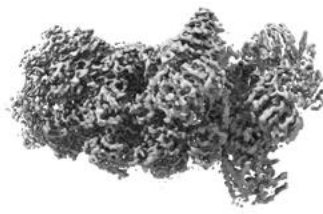
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

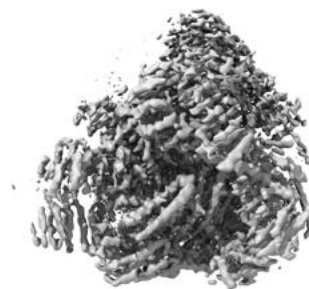
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

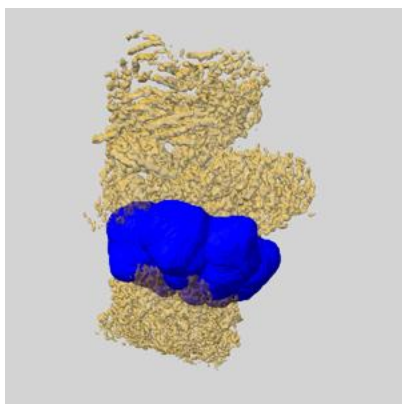
## 6.6 Mask visualisation [i](#)

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

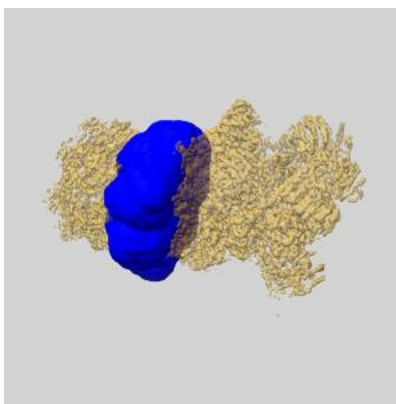
A mask typically either:

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

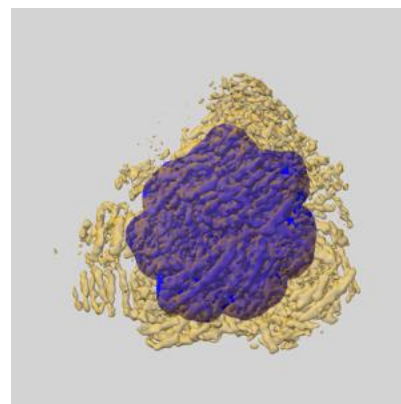
### 6.6.1 emd\_9044\_msk\_1.map [i](#)



X

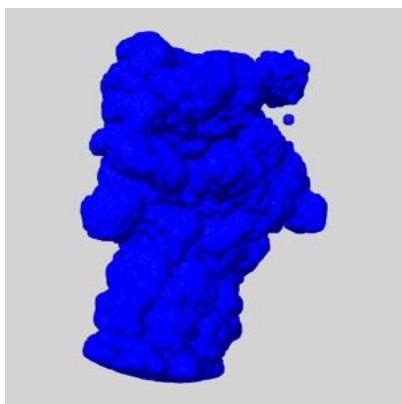


Y

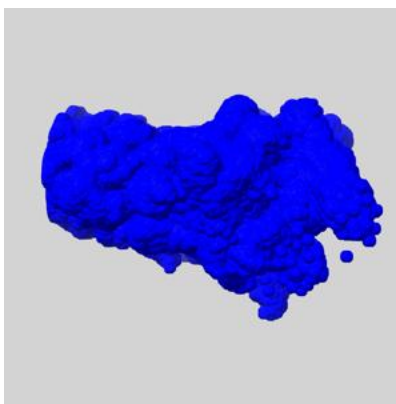


Z

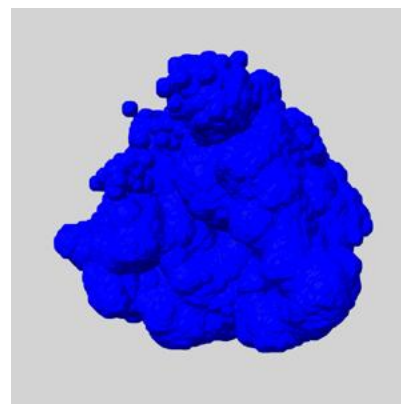
### 6.6.2 emd\_9044\_msk\_2.map [i](#)



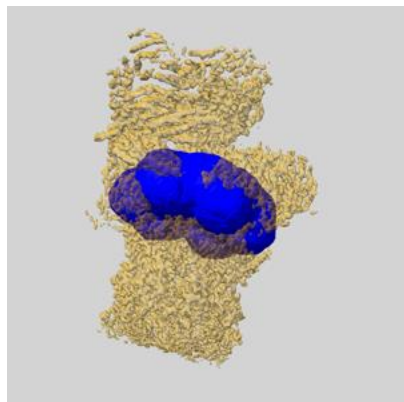
X



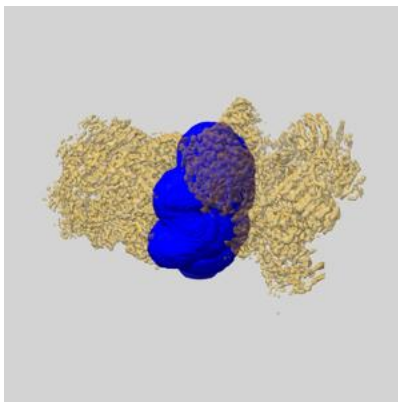
Y



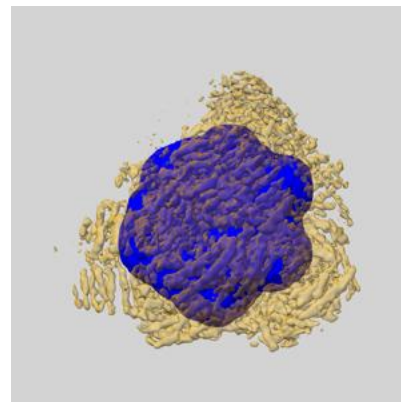
Z

6.6.3 emd\_9044\_msk\_3.map [i](#)

X



Y

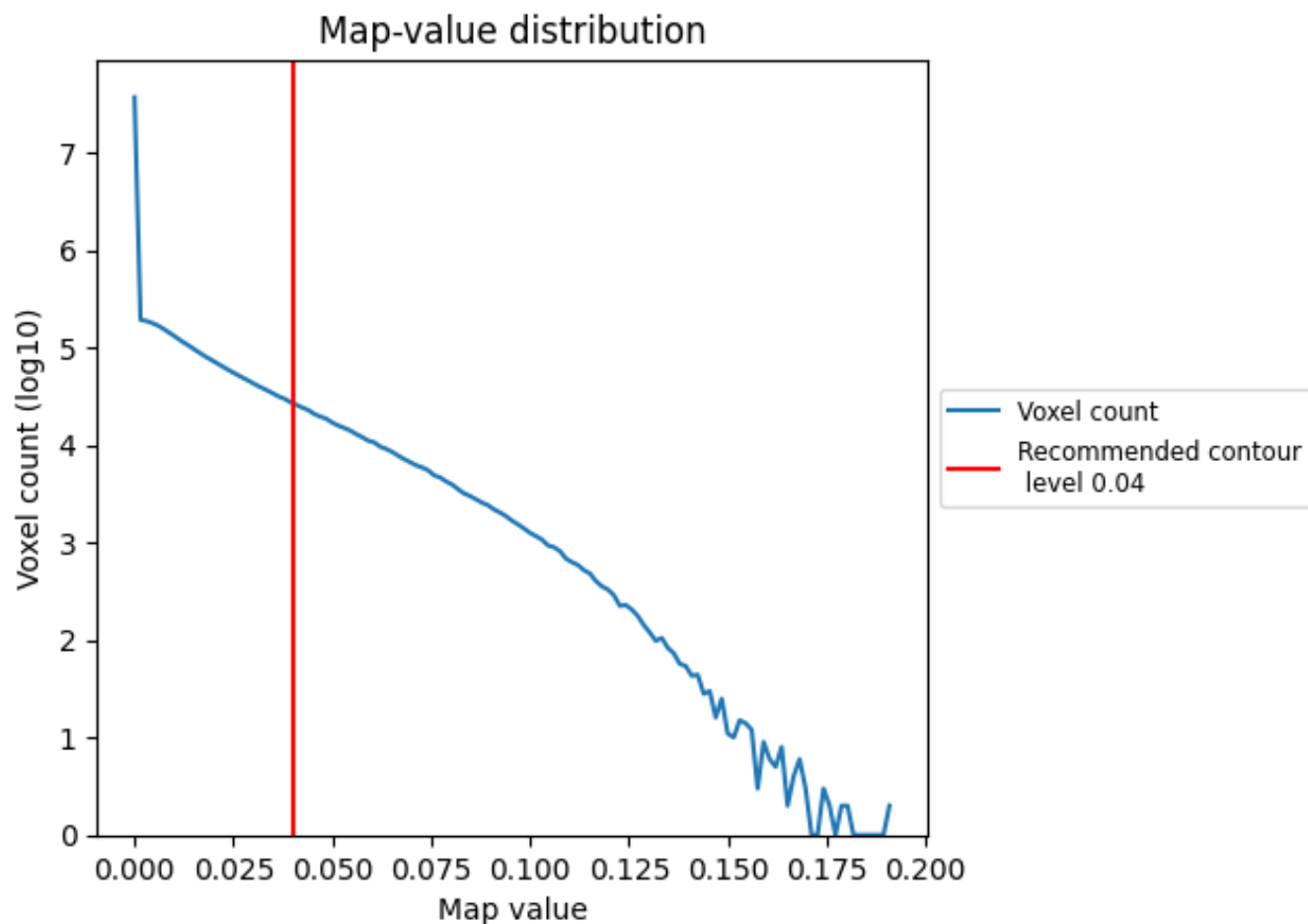


Z

## 7 Map analysis [i](#)

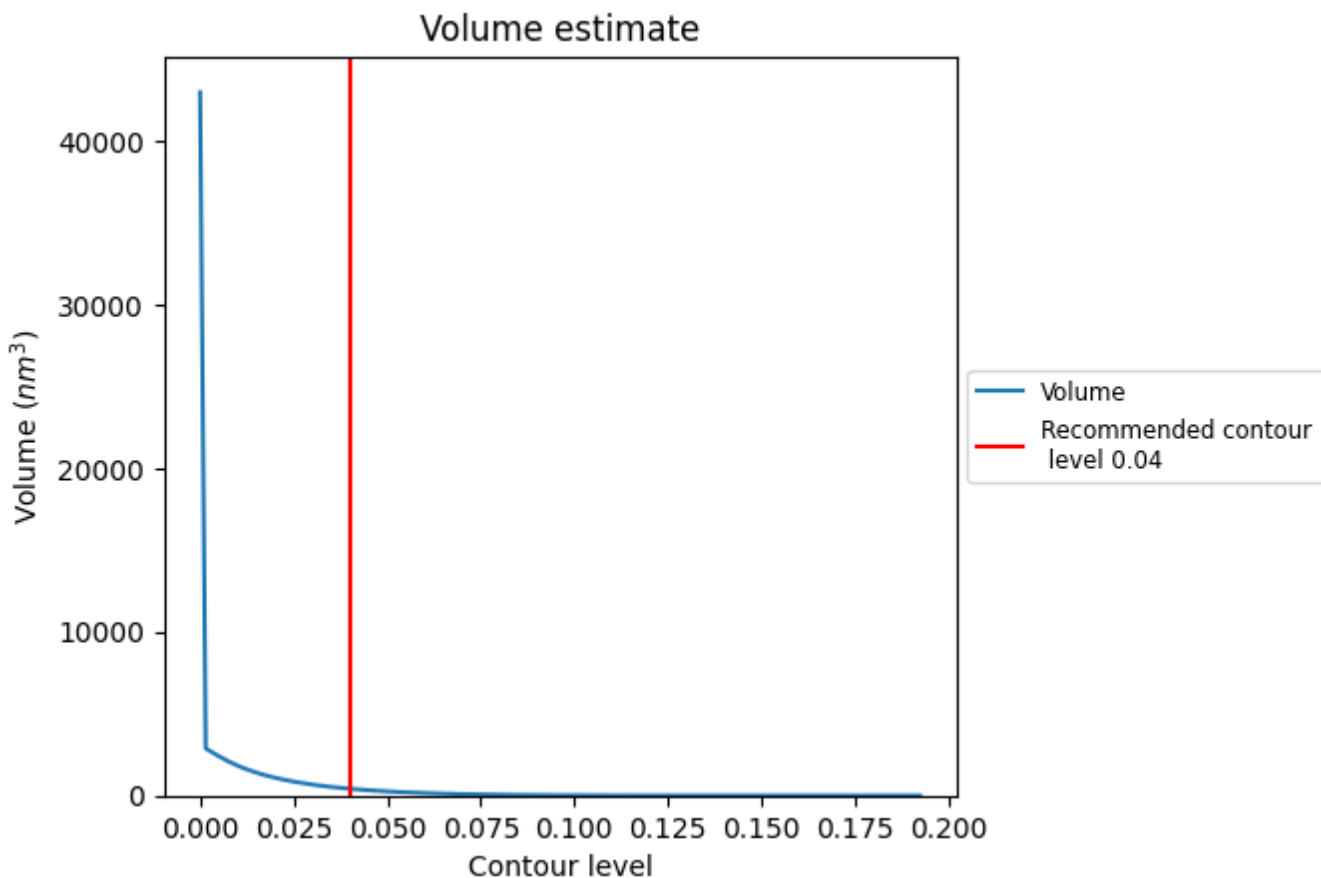
This section contains the results of statistical analysis of the map.

### 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.

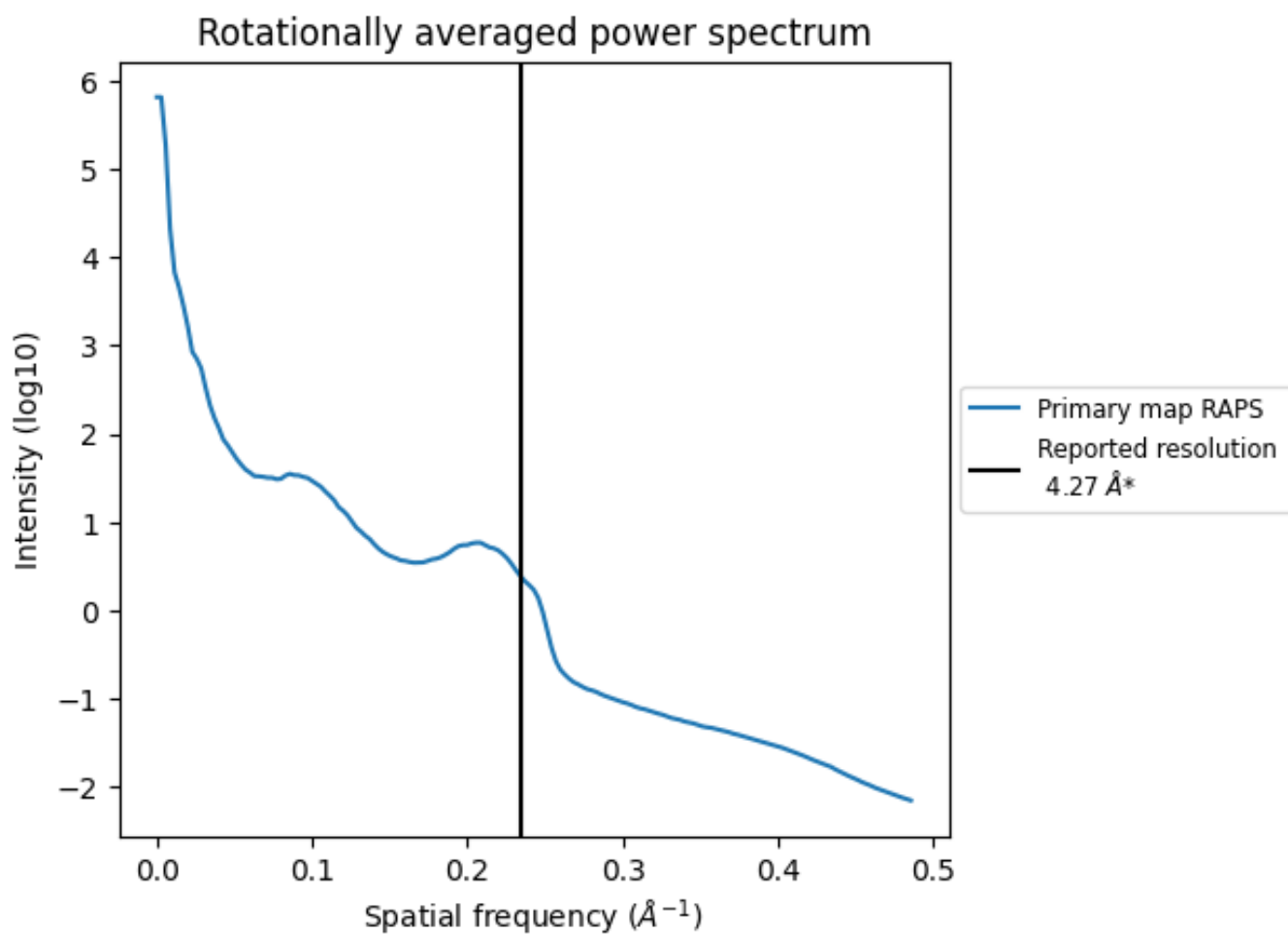
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 416 nm<sup>3</sup>; this corresponds to an approximate mass of 375 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.234 \text{\AA}^{-1}$



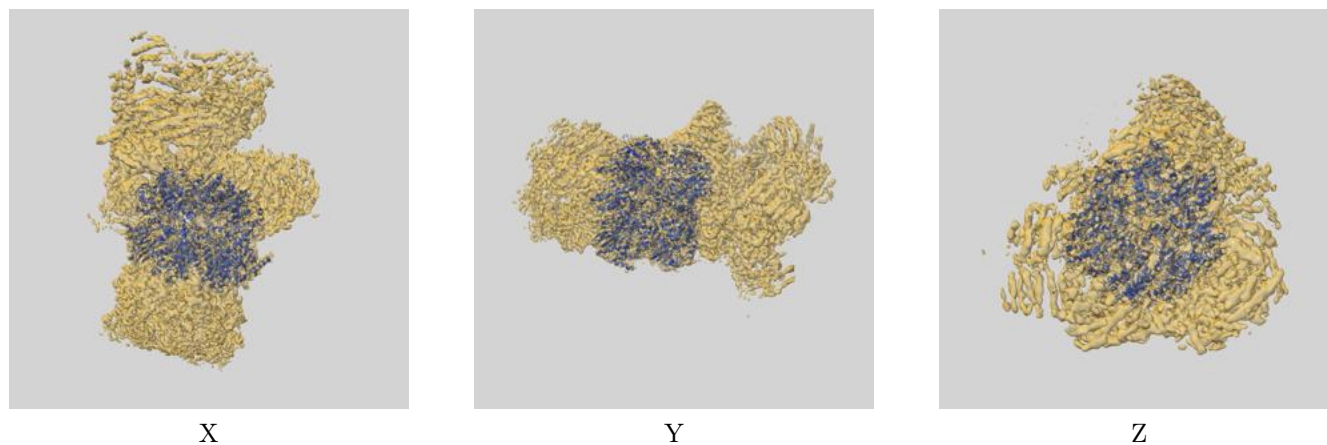
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

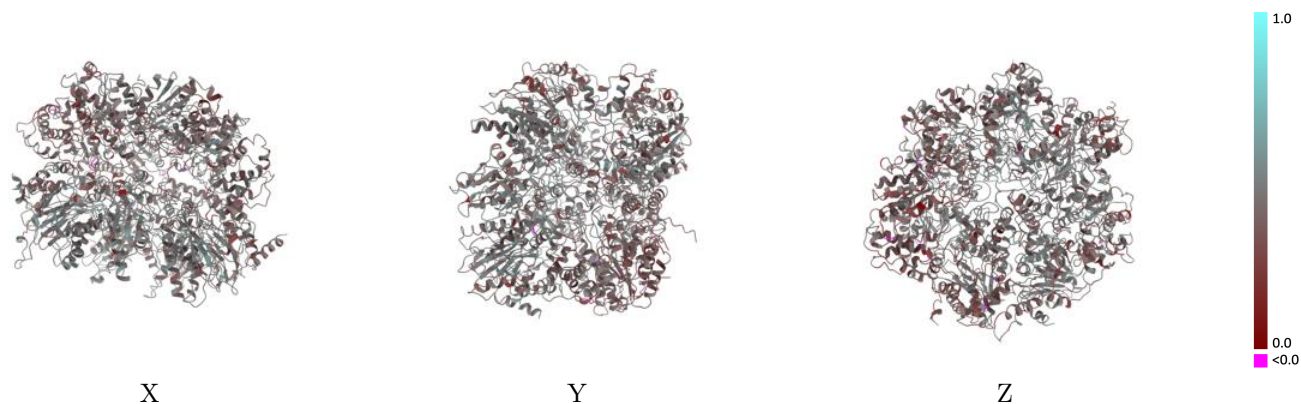
This section contains information regarding the fit between EMDB map EMD-9044 and PDB model 6EF2. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



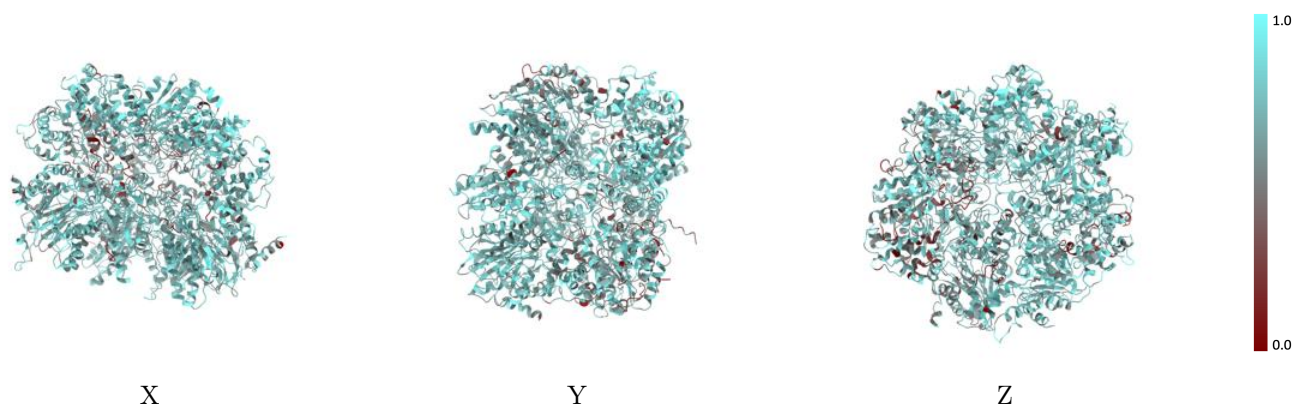
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



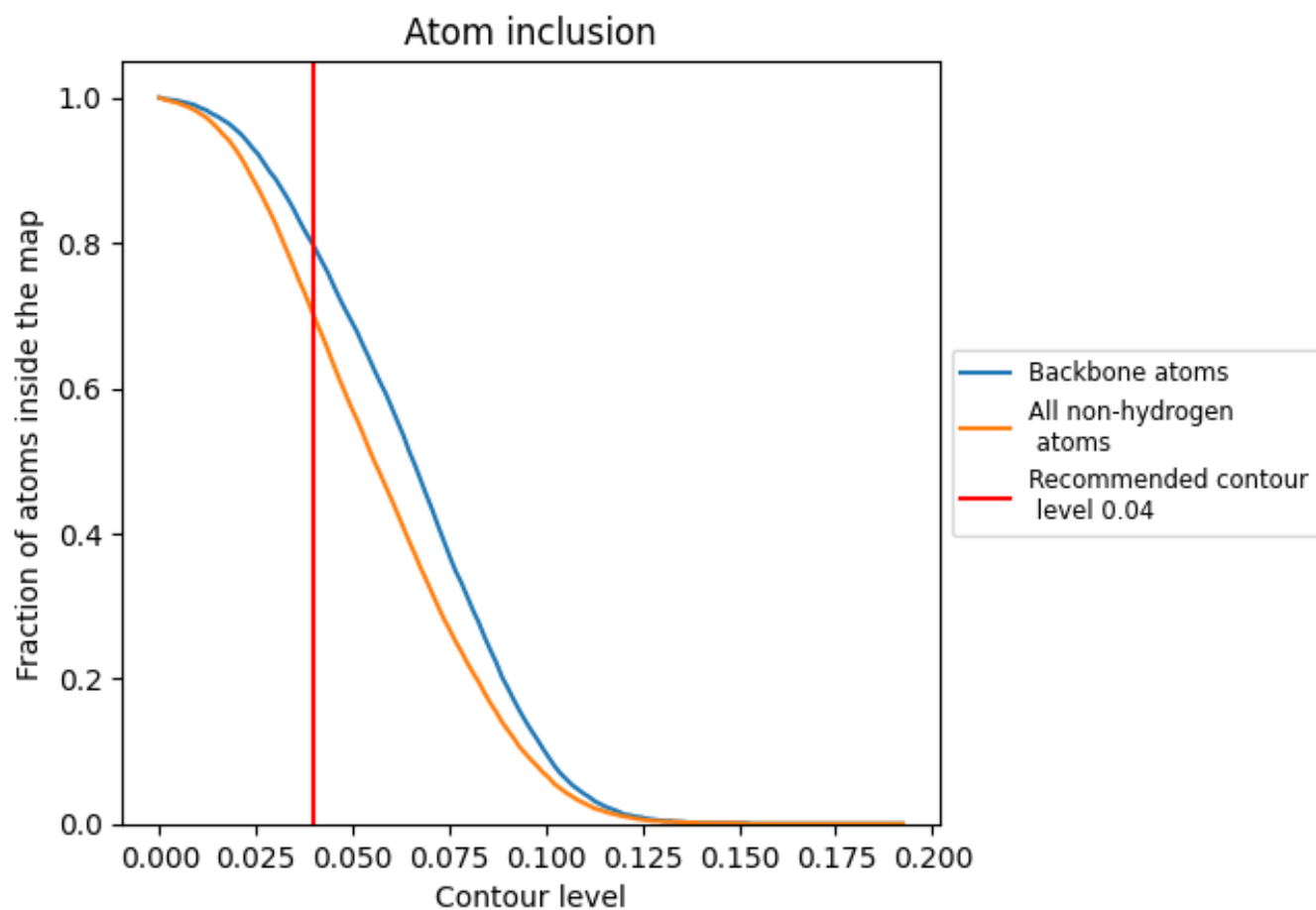
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.4300
A	 0.7210	 0.4440
B	 0.7410	 0.4620
C	 0.6850	 0.4570
D	 0.6850	 0.4350
E	 0.7210	 0.4520
F	 0.7490	 0.4570
G	 0.7370	 0.4620
H	 0.6730	 0.4090
I	 0.7490	 0.4340
J	 0.7310	 0.4250
K	 0.7270	 0.4180
L	 0.5760	 0.3740
M	 0.6120	 0.3720
s	 0.6350	 0.4620

