



Full wwPDB EM Validation Report ⓘ

Dec 27, 2023 – 04:32 PM EST

PDB ID : 8UD9
EMDB ID : EMD-42148
Title : Structure of human constitutive 20S proteasome complexed with the inhibitor
TDI-8304
Authors : Hsu, H.-C.; Li, H.
Deposited on : 2023-09-28
Resolution : 2.04 Å(reported)
Based on initial model : 5LF3

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:

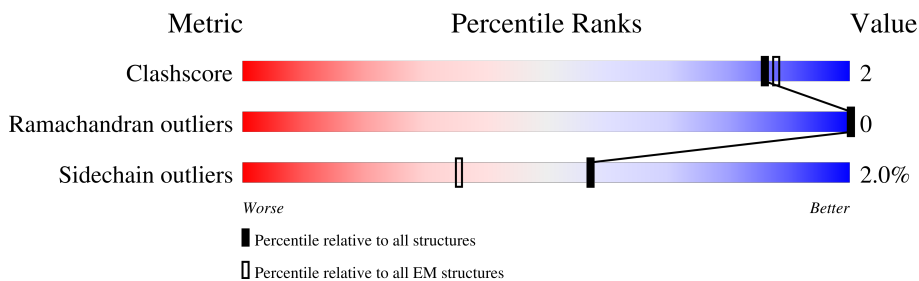
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.04 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.








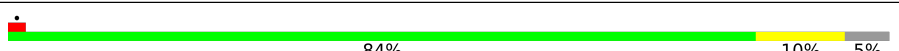
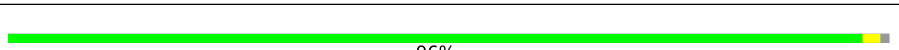
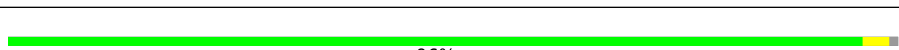
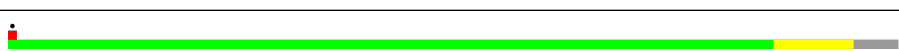

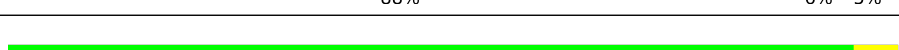
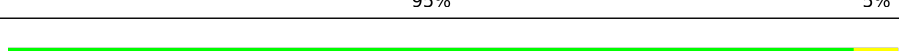
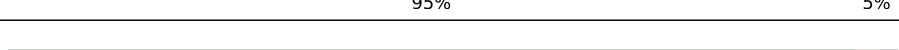
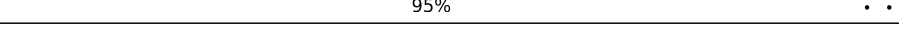
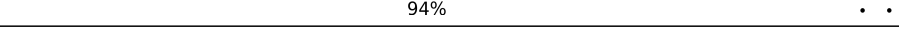
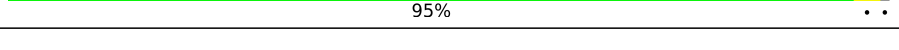
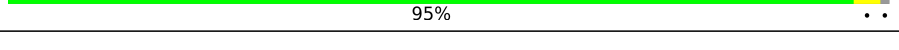

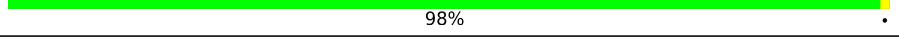
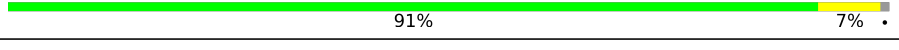
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	246	
1	O	246	
2	B	234	
2	P	234	
3	C	261	
3	Q	261	
4	D	248	
4	R	248	

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Mol	Chain	Length	Quality of chain
5	E	241	 89% 8%
5	S	241	 90% 7%
6	F	263	 84% 6% 10%
6	T	263	 85% 5% 10%
7	G	255	 85% 9% 5%
7	U	255	 84% 10% 5%
8	H	205	 96%
8	V	205	 96%
9	I	234	 86% 9% 5%
9	W	234	 88% 6% 5%
10	J	205	 95% 5%
10	X	205	 95% 5%
11	K	201	 95%
11	Y	201	 94%
12	L	204	 95%
12	Z	204	 95%
13	M	213	 89% 10%
13	a	213	 98%
14	N	219	 91% 7%
14	b	219	 97%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 49955 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	244	Total	C	N	O	S	0	0
			1903	1206	320	364	13		
1	O	244	Total	C	N	O	S	0	0
			1903	1206	320	364	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		
2	P	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	246	Total	C	N	O	S	0	0
			1941	1227	334	370	10		
3	Q	246	Total	C	N	O	S	0	0
			1941	1227	334	370	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	243	Total	C	N	O	S	0	0
			1923	1206	342	370	5		
4	R	243	Total	C	N	O	S	0	0
			1923	1206	342	370	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	235	1799	1130	296	362	11	0	0
5	S	235	1799	1130	296	362	11	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	237	1864	1167	335	351	11	0	0
6	T	237	1864	1167	335	351	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	241	1890	1198	322	359	11	0	0
7	U	241	1890	1198	322	359	11	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	202	1509	945	258	294	12	0	0
8	V	202	1509	945	258	294	12	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	222	1676	1055	285	324	12	0	0
9	W	222	1676	1055	285	324	12	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	204	1591	1013	265	294	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
11	Y	197	Total	C	N	O	S	0	0
			1575	1011	268	287	9		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
12	Z	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

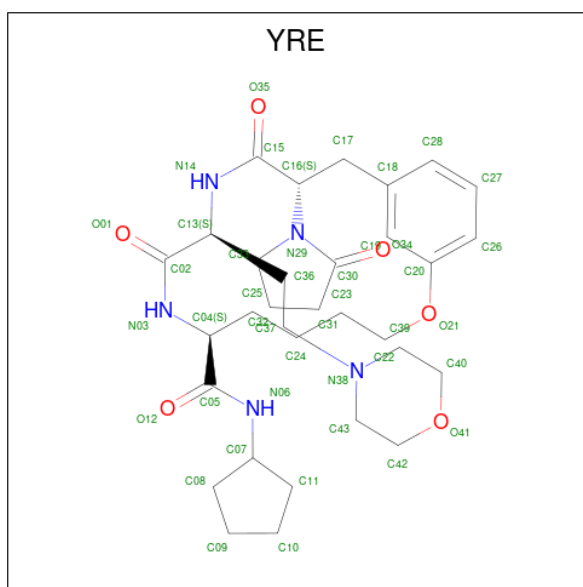
- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
13	a	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
14	b	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 15 is (7S,10S,13S)-N-cyclopentyl-10-[2-(morpholin-4-yl)ethyl]-9,12-dioxo-13-(2-oxopyrrolidin-1-yl)-2-oxa-8,11-diazabicyclo[13.3.1]nonadeca-1(19),15,17-triene-7-carboxamide (three-letter code: YRE) (formula: C₃₂H₄₇N₅O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
15	L	1	43	32	5	6	0
15	Z	1	43	32	5	6	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
16	A	39	39	39	0
16	B	19	19	19	0
16	C	37	37	37	0
16	D	26	26	26	0
16	E	27	27	27	0
16	F	32	32	32	0
16	G	31	31	31	0
16	H	46	46	46	0
16	I	48	48	48	0
16	J	43	43	43	0

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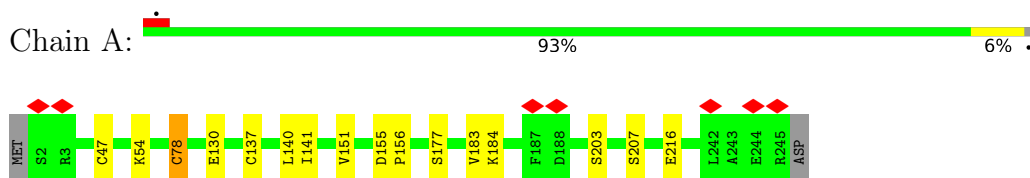
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Mol	Chain	Residues	Atoms		AltConf
16	K	45	Total 45	O 45	0
16	L	51	Total 51	O 51	0
16	M	44	Total 44	O 44	0
16	N	54	Total 54	O 54	0
16	O	32	Total 32	O 32	0
16	P	25	Total 25	O 25	0
16	Q	43	Total 43	O 43	0
16	R	30	Total 30	O 30	0
16	S	35	Total 35	O 35	0
16	T	39	Total 39	O 39	0
16	U	31	Total 31	O 31	0
16	V	48	Total 48	O 48	0
16	W	42	Total 42	O 42	0
16	X	47	Total 47	O 47	0
16	Y	38	Total 38	O 38	0
16	Z	52	Total 52	O 52	0
16	a	49	Total 49	O 49	0
16	b	67	Total 67	O 67	0

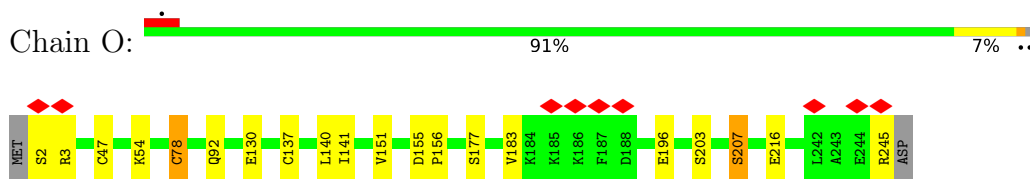
3 Residue-property plots [i](#)

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.

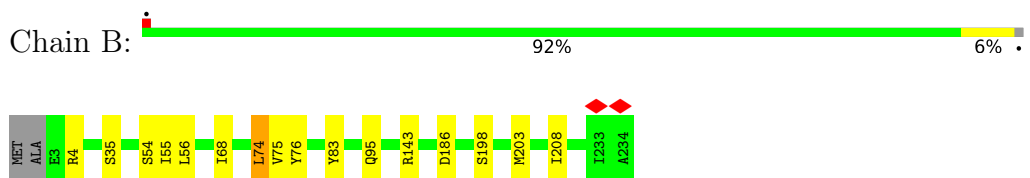
- Molecule 1: Proteasome subunit alpha type-6



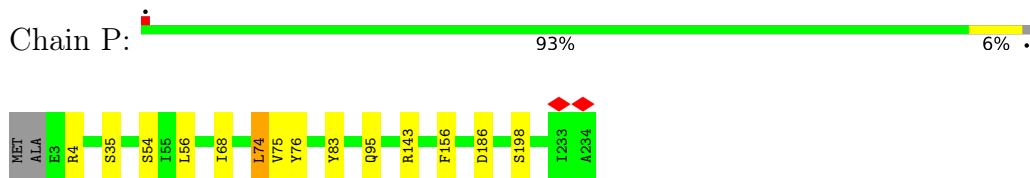
- Molecule 1: Proteasome subunit alpha type-6



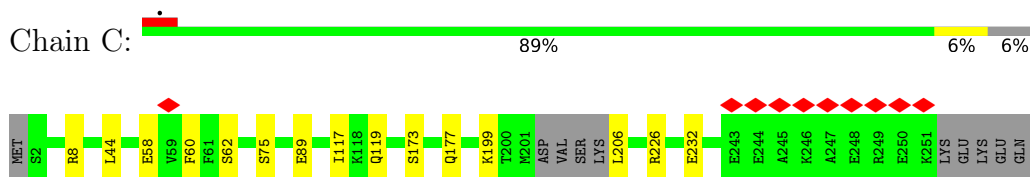
- Molecule 2: Proteasome subunit alpha type-2



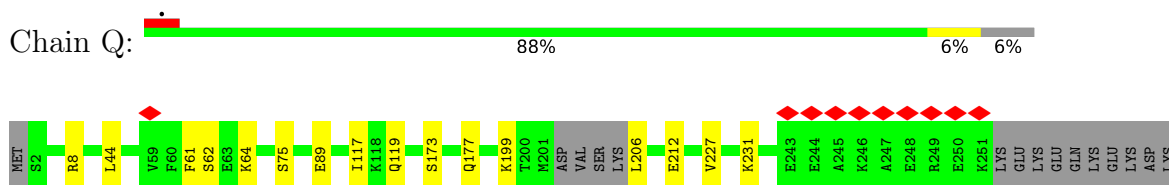
- Molecule 2: Proteasome subunit alpha type-2



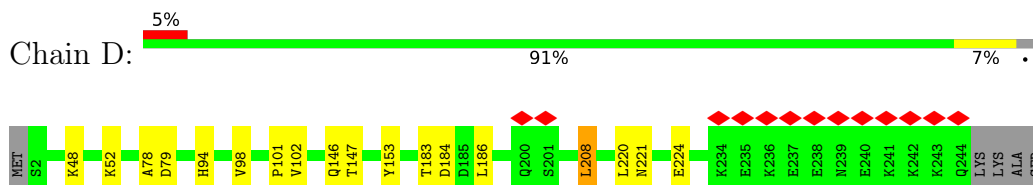
- Molecule 3: Proteasome subunit alpha type-4



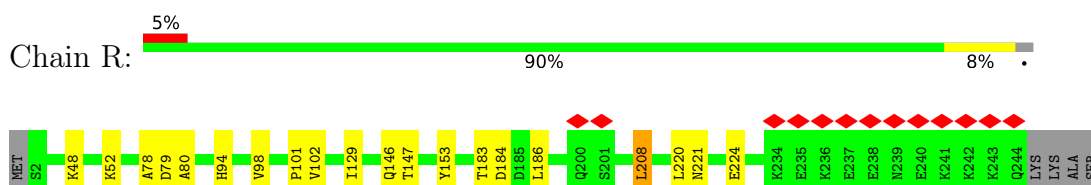
• Molecule 3: Proteasome subunit alpha type-4



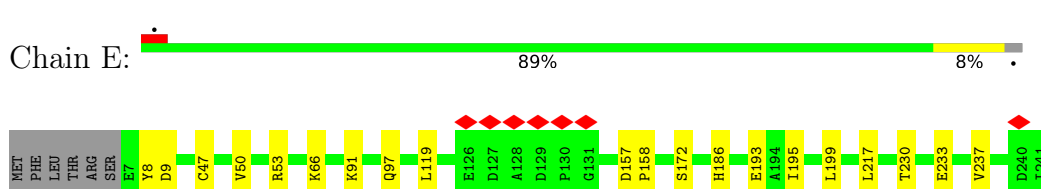
• Molecule 4: Proteasome subunit alpha type-7



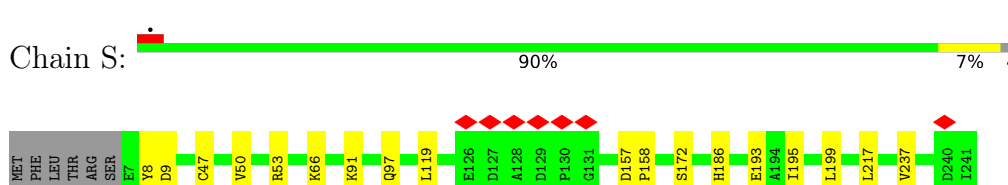
• Molecule 4: Proteasome subunit alpha type-7



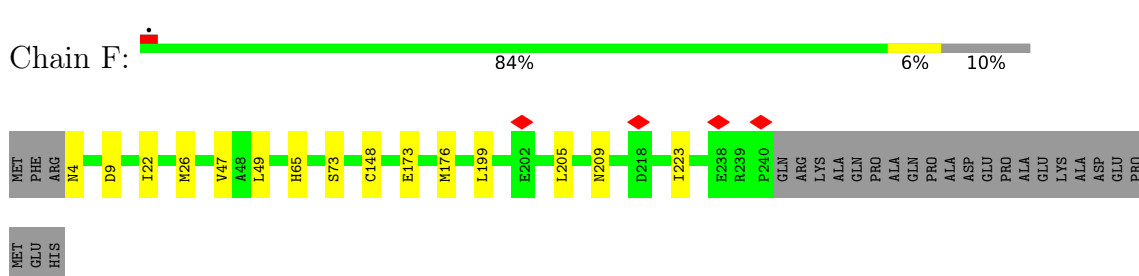
• Molecule 5: Proteasome subunit alpha type-5



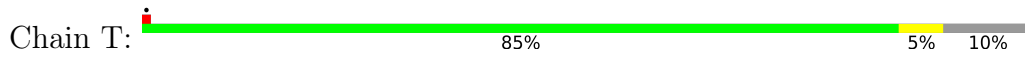
• Molecule 5: Proteasome subunit alpha type-5



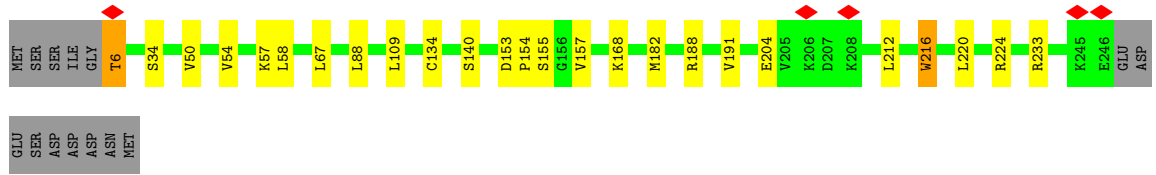
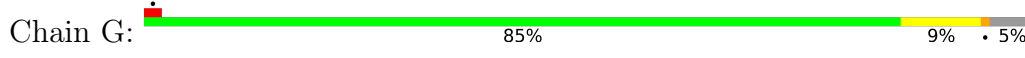
• Molecule 6: Proteasome subunit alpha type-1



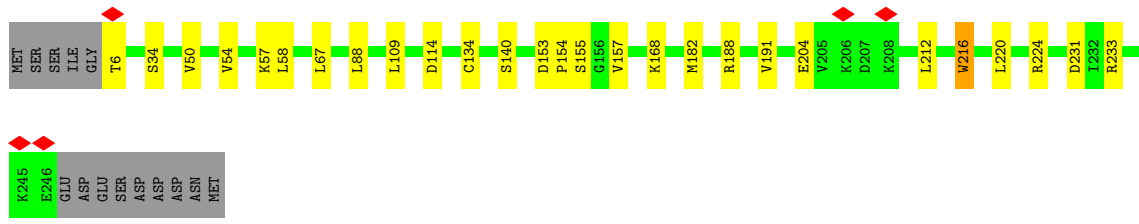
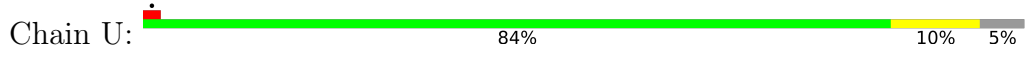
• Molecule 6: Proteasome subunit alpha type-1



• Molecule 7: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-3



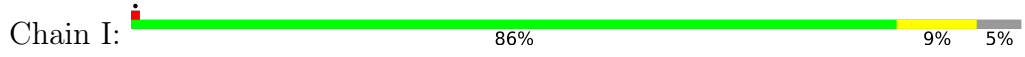
• Molecule 8: Proteasome subunit beta type-6




• Molecule 8: Proteasome subunit beta type-6

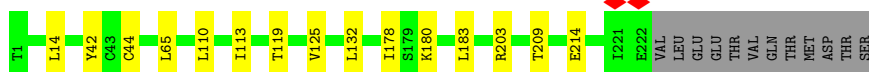


• Molecule 9: Proteasome subunit beta type-7



• Molecule 9: Proteasome subunit beta type-7

Chain W:  88% 6% 5%



- Molecule 10: Proteasome subunit beta type-3

Chain J:  95% 5%



- Molecule 10: Proteasome subunit beta type-3

Chain X:  95% 5%



- Molecule 11: Proteasome subunit beta type-2

Chain K:  95%



- Molecule 11: Proteasome subunit beta type-2

Chain Y:  94%



- Molecule 12: Proteasome subunit beta type-5

Chain L:  95%




- Molecule 12: Proteasome subunit beta type-5

Chain Z:  95%



- Molecule 13: Proteasome subunit beta type-1

Chain M:  89% 10%



- Molecule 13: Proteasome subunit beta type-1

Chain a:  98%



- Molecule 14: Proteasome subunit beta type-4

Chain N:  91% 7%



- Molecule 14: Proteasome subunit beta type-4

Chain b:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1250898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.576	Depositor
Minimum map value	-1.486	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	291.456, 291.456, 291.456	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YRE

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	0.29	0/1937	0.50	0/2617
1	O	0.29	0/1937	0.50	0/2617
2	B	0.29	0/1852	0.50	0/2507
2	P	0.29	0/1852	0.50	0/2507
3	C	0.28	0/1970	0.50	0/2651
3	Q	0.28	0/1970	0.50	0/2651
4	D	0.28	0/1949	0.53	0/2626
4	R	0.28	0/1949	0.53	0/2626
5	E	0.26	0/1827	0.47	0/2467
5	S	0.26	0/1827	0.47	0/2467
6	F	0.27	0/1899	0.54	0/2567
6	T	0.27	0/1899	0.54	0/2567
7	G	0.29	0/1925	0.50	0/2592
7	U	0.29	0/1925	0.50	0/2592
8	H	0.29	0/1535	0.53	0/2078
8	V	0.30	0/1535	0.53	0/2078
9	I	0.29	0/1703	0.53	0/2305
9	W	0.29	0/1703	0.52	0/2305
10	J	0.29	0/1620	0.52	0/2184
10	X	0.29	0/1620	0.52	0/2184
11	K	0.30	0/1611	0.52	0/2180
11	Y	0.30	0/1608	0.52	0/2174
12	L	0.29	0/1590	0.54	0/2147
12	Z	0.29	0/1590	0.54	0/2147
13	M	0.29	0/1673	0.53	0/2254
13	a	0.29	0/1673	0.53	0/2254
14	N	0.29	0/1720	0.55	0/2328
14	b	0.29	0/1720	0.55	0/2328
All	All	0.29	0/49619	0.52	0/67000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1903	0	1911	11	0
1	O	1903	0	1911	11	0
2	B	1813	0	1806	10	0
2	P	1813	0	1806	6	0
3	C	1941	0	1960	7	0
3	Q	1941	0	1960	7	0
4	D	1923	0	1952	9	0
4	R	1923	0	1952	10	0
5	E	1799	0	1779	11	0
5	S	1799	0	1779	10	0
6	F	1864	0	1852	10	0
6	T	1864	0	1852	7	0
7	G	1890	0	1874	12	0
7	U	1890	0	1874	12	0
8	H	1509	0	1473	3	0
8	V	1509	0	1473	4	0
9	I	1676	0	1698	13	0
9	W	1676	0	1698	11	0
10	J	1591	0	1609	7	0
10	X	1591	0	1609	8	0
11	K	1578	0	1580	3	0
11	Y	1575	0	1580	4	0
12	L	1559	0	1523	5	0
12	Z	1559	0	1523	5	0
13	M	1643	0	1640	12	0
13	a	1643	0	1640	0	0
14	N	1687	0	1666	9	0
14	b	1687	0	1666	0	0
15	L	43	0	0	0	0
15	Z	43	0	0	0	0
16	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	19	0	0	0	0
16	C	37	0	0	0	0
16	D	26	0	0	0	0
16	E	27	0	0	0	0
16	F	32	0	0	0	0
16	G	31	0	0	0	0
16	H	46	0	0	0	0
16	I	48	0	0	0	0
16	J	43	0	0	0	0
16	K	45	0	0	0	0
16	L	51	0	0	0	0
16	M	44	0	0	0	0
16	N	54	0	0	0	0
16	O	32	0	0	0	0
16	P	25	0	0	0	0
16	Q	43	0	0	0	0
16	R	30	0	0	0	0
16	S	35	0	0	0	0
16	T	39	0	0	0	0
16	U	31	0	0	0	0
16	V	48	0	0	0	0
16	W	42	0	0	0	0
16	X	47	0	0	0	0
16	Y	38	0	0	0	0
16	Z	52	0	0	0	0
16	a	49	0	0	0	0
16	b	67	0	0	0	0
All	All	49955	0	48646	184	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 2.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:221:ASN:ND2	4:R:224:GLU:OE2	2.27	0.67
4:D:221:ASN:ND2	4:D:224:GLU:OE2	2.27	0.66
5:E:91:LYS:HG2	5:E:119:LEU:HD11	1.78	0.66
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.77	0.65
5:S:91:LYS:HG2	5:S:119:LEU:HD11	1.79	0.63
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:147:THR:HG22	4:R:153:TYR:HB3	1.83	0.60
8:V:14:LEU:HD23	8:V:44:CYS:SG	2.41	0.60
4:D:147:THR:HG22	4:D:153:TYR:HB3	1.83	0.60
9:I:143:ARG:NH2	9:I:150:GLU:OE1	2.34	0.60
8:H:14:LEU:HD23	8:H:44:CYS:SG	2.42	0.60
1:O:54:LYS:NZ	1:O:216:GLU:OE2	2.24	0.59
1:A:130:GLU:OE1	1:A:130:GLU:N	2.33	0.58
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.35	0.58
1:A:183:VAL:HG21	2:B:56:LEU:HD23	1.86	0.57
6:F:199:LEU:HD11	6:F:205:LEU:HD23	1.86	0.56
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.88	0.56
1:A:54:LYS:NZ	1:A:216:GLU:OE2	2.26	0.56
3:C:119:GLN:NE2	4:D:79:ASP:OD1	2.34	0.55
7:G:54:VAL:O	7:G:54:VAL:HG23	2.08	0.54
6:F:49:LEU:HD21	6:F:199:LEU:HD21	1.89	0.54
6:T:199:LEU:HD11	6:T:205:LEU:HD23	1.89	0.54
7:U:54:VAL:HG23	7:U:54:VAL:O	2.08	0.54
1:O:130:GLU:OE1	1:O:130:GLU:N	2.33	0.54
9:I:203:ARG:NH2	10:J:155:GLU:OE1	2.38	0.53
7:U:212:LEU:O	7:U:233:ARG:NH1	2.41	0.53
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.89	0.53
2:B:75:VAL:HG22	2:B:76:TYR:H	1.74	0.53
7:G:212:LEU:O	7:G:233:ARG:NH1	2.41	0.53
2:P:75:VAL:HG22	2:P:76:TYR:H	1.74	0.53
5:S:9:ASP:N	5:S:9:ASP:OD1	2.41	0.53
5:E:199:LEU:HD21	5:E:217:LEU:HD12	1.90	0.52
5:E:9:ASP:N	5:E:9:ASP:OD1	2.41	0.52
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.89	0.52
9:W:214:GLU:OE2	10:X:198:ARG:NH1	2.42	0.52
1:O:183:VAL:HG21	2:P:56:LEU:HD23	1.90	0.52
4:D:183:THR:HG23	4:D:186:LEU:H	1.74	0.52
5:S:199:LEU:HD12	5:S:237:VAL:HG12	1.91	0.52
1:O:92:GLN:NE2	8:V:69:GLU:OE1	2.39	0.52
1:A:203:SER:O	1:A:207:SER:N	2.42	0.52
1:O:203:SER:O	1:O:207:SER:N	2.43	0.52
11:Y:1:MET:HG2	11:Y:134:TYR:H	1.76	0.51
5:S:199:LEU:HD21	5:S:217:LEU:HD12	1.92	0.51
5:E:199:LEU:HD12	5:E:237:VAL:HG12	1.92	0.51
9:I:214:GLU:OE2	10:J:198:ARG:NH1	2.43	0.51
4:R:183:THR:HG23	4:R:186:LEU:H	1.75	0.51
7:U:109:LEU:HD13	7:U:140:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:THR:N	13:M:26:ASP:OD1	2.35	0.50
7:G:50:VAL:HG23	7:G:67:LEU:HD21	1.94	0.50
6:F:49:LEU:HD21	6:F:199:LEU:CD2	2.41	0.50
14:N:142:GLY:HA2	14:N:176:LEU:HD21	1.94	0.50
12:Z:20:ALA:CB	12:Z:31:VAL:HG21	2.41	0.50
9:W:203:ARG:NH1	10:X:162:HIS:HB3	2.27	0.50
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.94	0.50
1:A:183:VAL:HG23	2:B:55:ILE:CD1	2.42	0.49
3:C:44:LEU:HD12	3:C:44:LEU:C	2.32	0.49
5:E:195:ILE:HG23	5:E:217:LEU:HD11	1.95	0.49
9:I:203:ARG:NH1	10:J:162:HIS:HB3	2.27	0.49
3:Q:44:LEU:C	3:Q:44:LEU:HD12	2.32	0.49
4:R:94:HIS:CG	4:R:102:VAL:HG12	2.47	0.49
5:S:50:VAL:HG11	5:S:66:LYS:HB2	1.95	0.49
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.93	0.49
14:N:144:TYR:HB2	9:W:132:LEU:HD23	1.94	0.49
7:U:50:VAL:HG23	7:U:67:LEU:HD21	1.94	0.49
5:S:186:HIS:NE2	5:S:193:GLU:OE2	2.45	0.49
9:W:203:ARG:NH2	10:X:155:GLU:OE1	2.38	0.49
4:D:94:HIS:CG	4:D:102:VAL:HG12	2.48	0.49
7:G:109:LEU:HD13	7:G:140:SER:HB2	1.93	0.49
5:E:50:VAL:HG11	5:E:66:LYS:HB2	1.95	0.49
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.95	0.48
3:Q:61:PHE:CZ	3:Q:227:VAL:HG23	2.48	0.48
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.95	0.48
9:I:113:ILE:HG12	9:I:119:THR:HG22	1.96	0.47
5:S:195:ILE:HG23	5:S:217:LEU:HD11	1.97	0.47
9:W:113:ILE:HG12	9:W:119:THR:HG22	1.95	0.47
1:A:78:CYS:CB	1:A:140:LEU:HD23	2.45	0.47
12:L:133:VAL:HG21	11:Y:137:PHE:HB3	1.96	0.47
3:C:226:ARG:NH1	3:C:232:GLU:OE2	2.40	0.47
11:K:137:PHE:HB3	12:Z:133:VAL:HG21	1.96	0.47
1:O:2:SER:OG	1:O:3:ARG:N	2.44	0.47
1:O:78:CYS:CB	1:O:140:LEU:HD23	2.45	0.47
6:T:22:ILE:O	6:T:26:MET:HG2	2.14	0.47
6:F:22:ILE:O	6:F:26:MET:HG2	2.15	0.47
9:W:110:LEU:HD21	9:W:125:VAL:HG22	1.97	0.47
13:M:152:GLN:O	13:M:170:ARG:NH2	2.48	0.47
4:D:208:LEU:HD22	4:D:220:LEU:HD22	1.97	0.46
9:I:110:LEU:HD21	9:I:125:VAL:HG22	1.97	0.46
4:R:208:LEU:HD22	4:R:220:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:74:GLU:OE1	14:N:83:TYR:N	2.48	0.46
3:C:89:GLU:HG2	3:C:117:ILE:HD13	1.98	0.46
3:Q:89:GLU:HG2	3:Q:117:ILE:HD13	1.98	0.46
6:T:176:MET:HE1	7:U:58:LEU:HA	1.98	0.46
5:E:186:HIS:NE2	5:E:193:GLU:OE2	2.45	0.46
2:B:68:ILE:HD11	2:B:74:LEU:HD22	1.97	0.45
2:P:68:ILE:HD11	2:P:74:LEU:HD22	1.97	0.45
13:M:28:ARG:NE	13:M:191:ASP:OD2	2.43	0.45
14:N:124:TYR:O	14:N:131:ALA:HA	2.16	0.45
7:U:188:ARG:O	7:U:191:VAL:HG12	2.17	0.45
13:M:145:LEU:HD11	13:M:182:ALA:HB2	1.98	0.45
7:G:6:THR:O	7:G:6:THR:OG1	2.32	0.44
3:C:58:GLU:OE2	3:C:60:PHE:N	2.48	0.44
14:N:51:LEU:C	14:N:51:LEU:HD23	2.38	0.44
9:W:14:LEU:HB3	9:W:44:CYS:SG	2.58	0.44
2:B:76:TYR:HB3	2:B:83:TYR:CD1	2.53	0.44
7:G:188:ARG:O	7:G:191:VAL:HG12	2.17	0.44
6:F:176:MET:HE1	7:G:58:LEU:HA	2.00	0.44
2:P:76:TYR:HB3	2:P:83:TYR:CD1	2.53	0.44
3:Q:8:ARG:NH2	5:S:8:TYR:HB3	2.33	0.43
3:C:8:ARG:NH2	5:E:8:TYR:HB3	2.33	0.43
13:M:148:LEU:HD13	13:M:148:LEU:O	2.18	0.43
9:W:178:ILE:HG12	9:W:183:LEU:HD12	1.99	0.43
10:X:30:ILE:HD12	10:X:35:VAL:HG21	1.99	0.43
7:G:216:TRP:CH2	7:G:220:LEU:HD11	2.54	0.43
9:I:9:LYS:NZ	9:I:147:GLU:OE2	2.46	0.43
13:M:125:ASP:OD1	13:M:129:SER:N	2.50	0.43
1:A:183:VAL:HG23	2:B:55:ILE:HD11	1.99	0.43
10:J:45:MET:O	10:J:71:LEU:HD21	2.19	0.43
7:U:88:LEU:HD12	7:U:134:CYS:SG	2.58	0.43
6:F:173:GLU:HG3	7:G:58:LEU:HD21	2.00	0.43
7:G:88:LEU:HD12	7:G:134:CYS:SG	2.58	0.43
9:I:178:ILE:HG12	9:I:183:LEU:HD12	1.99	0.43
1:O:78:CYS:HB3	1:O:140:LEU:HD23	2.01	0.43
1:A:78:CYS:HB3	1:A:140:LEU:HD23	2.00	0.43
12:L:35:ILE:N	12:L:43:GLY:O	2.45	0.43
9:I:14:LEU:HB3	9:I:44:CYS:SG	2.58	0.43
11:Y:46:CYS:SG	11:Y:53:THR:HG23	2.59	0.43
11:K:46:CYS:SG	11:K:53:THR:HG23	2.59	0.42
12:L:20:ALA:CB	12:L:31:VAL:HG21	2.49	0.42
3:Q:119:GLN:HG3	4:R:78:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:98:VAL:HG12	4:R:98:VAL:O	2.19	0.42
5:S:157:ASP:HB2	5:S:158:PRO:CD	2.49	0.42
6:F:49:LEU:HD12	6:F:209:ASN:O	2.19	0.42
5:E:97:GLN:HG3	12:L:65:ILE:HG13	2.01	0.42
9:I:42:TYR:CE1	9:I:183:LEU:HD11	2.54	0.42
12:Z:3:THR:HB	12:Z:44:THR:HG21	2.02	0.42
2:B:95:GLN:HG3	9:I:65:LEU:HG	2.01	0.42
3:C:119:GLN:HG3	4:D:78:ALA:HB1	2.00	0.42
2:P:95:GLN:HG3	9:W:65:LEU:HG	2.01	0.42
5:S:97:GLN:HG3	12:Z:65:ILE:HG13	2.01	0.42
7:U:216:TRP:CH2	7:U:220:LEU:HD11	2.54	0.42
10:X:116:THR:HG22	10:X:116:THR:O	2.20	0.42
5:E:157:ASP:HB2	5:E:158:PRO:CD	2.49	0.42
9:W:42:TYR:CE1	9:W:183:LEU:HD11	2.54	0.42
1:A:155:ASP:HB2	1:A:156:PRO:CD	2.50	0.42
4:D:98:VAL:HG12	4:D:98:VAL:O	2.19	0.42
10:X:45:MET:O	10:X:71:LEU:HD21	2.19	0.42
10:J:116:THR:O	10:J:116:THR:HG22	2.19	0.42
13:M:63:THR:OG1	14:N:94:ARG:NH2	2.39	0.42
13:M:191:ASP:O	13:M:192:ALA:HB2	2.18	0.42
6:T:173:GLU:HG3	7:U:58:LEU:HD21	2.00	0.42
8:V:14:LEU:HD11	8:V:179:ILE:HD12	2.01	0.42
9:I:209:THR:HG21	10:J:168:SER:HB3	2.01	0.42
1:O:155:ASP:HB2	1:O:156:PRO:CD	2.50	0.42
6:T:26:MET:HE1	6:T:148:CYS:HB3	2.00	0.42
10:J:30:ILE:HD12	10:J:35:VAL:HG21	2.02	0.41
4:R:147:THR:HG22	4:R:153:TYR:CB	2.48	0.41
2:B:75:VAL:HG22	2:B:76:TYR:N	2.35	0.41
9:W:209:THR:HG21	10:X:168:SER:HB3	2.01	0.41
8:H:14:LEU:HD11	8:H:179:ILE:HD12	2.00	0.41
2:P:75:VAL:HG22	2:P:76:TYR:N	2.35	0.41
2:B:203:MET:HE3	2:B:208:ILE:HD13	2.03	0.41
6:F:26:MET:HE1	6:F:148:CYS:HB3	2.02	0.41
3:Q:64:LYS:N	3:Q:212:GLU:OE2	2.50	0.41
6:T:157:ARG:HE	6:T:176:MET:HE2	1.85	0.41
5:E:230:THR:OG1	5:E:233:GLU:OE1	2.30	0.41
6:F:65:HIS:CE1	6:F:223:ILE:HD12	2.56	0.41
13:M:14:ALA:HA	13:M:22:ILE:O	2.20	0.41
13:M:198:VAL:HG22	13:M:203:ILE:HG12	2.02	0.41
14:N:25:ASP:HA	14:N:187:PHE:HA	2.03	0.41
1:O:196:GLU:OE2	1:O:245:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:65:HIS:CE1	6:T:223:ILE:HD12	2.55	0.41
6:F:47:VAL:O	6:F:47:VAL:HG23	2.21	0.41
1:A:184:LYS:HG3	2:B:55:ILE:HD13	2.03	0.40
4:D:147:THR:HG22	4:D:153:TYR:CB	2.48	0.40
7:G:153:ASP:HB2	7:G:154:PRO:CD	2.51	0.40
14:N:15:LYS:HD2	14:N:135:PRO:HA	2.04	0.40
7:G:155:SER:OG	7:G:157:VAL:HG23	2.21	0.40
13:M:13:LEU:HD13	13:M:149:LEU:HD11	2.02	0.40
10:X:65:GLN:OE1	11:Y:86:ARG:NH2	2.54	0.40
9:I:45:GLY:HA3	9:I:52:THR:HG21	2.02	0.40
11:K:45:LEU:N	11:K:45:LEU:HD12	2.37	0.40
7:U:54:VAL:O	7:U:54:VAL:CG2	2.70	0.40
7:U:153:ASP:HB2	7:U:154:PRO:CD	2.51	0.40
7:U:155:SER:OG	7:U:157:VAL:HG23	2.22	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	242/246 (98%)	241 (100%)	1 (0%)	0	100	100
1	O	242/246 (98%)	240 (99%)	2 (1%)	0	100	100
2	B	230/234 (98%)	227 (99%)	3 (1%)	0	100	100
2	P	230/234 (98%)	227 (99%)	3 (1%)	0	100	100
3	C	242/261 (93%)	238 (98%)	4 (2%)	0	100	100
3	Q	242/261 (93%)	238 (98%)	4 (2%)	0	100	100
4	D	241/248 (97%)	236 (98%)	5 (2%)	0	100	100
4	R	241/248 (97%)	235 (98%)	6 (2%)	0	100	100
5	E	233/241 (97%)	226 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	233/241 (97%)	226 (97%)	7 (3%)	0	100	100
6	F	235/263 (89%)	233 (99%)	2 (1%)	0	100	100
6	T	235/263 (89%)	232 (99%)	3 (1%)	0	100	100
7	G	239/255 (94%)	237 (99%)	2 (1%)	0	100	100
7	U	239/255 (94%)	237 (99%)	2 (1%)	0	100	100
8	H	200/205 (98%)	196 (98%)	4 (2%)	0	100	100
8	V	200/205 (98%)	196 (98%)	4 (2%)	0	100	100
9	I	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
9	W	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
10	J	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	X	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
11	K	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	Y	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
12	L	199/204 (98%)	197 (99%)	2 (1%)	0	100	100
12	Z	199/204 (98%)	197 (99%)	2 (1%)	0	100	100
13	M	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
13	a	210/213 (99%)	207 (99%)	3 (1%)	0	100	100
14	N	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
14	b	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
All	All	6204/6458 (96%)	6097 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	204 (98%)	4 (2%)	57	53
1	O	208/210 (99%)	203 (98%)	5 (2%)	49	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	190/191 (100%)	183 (96%)	7 (4%)	34	27
2	P	190/191 (100%)	182 (96%)	8 (4%)	30	22
3	C	206/221 (93%)	200 (97%)	6 (3%)	42	35
3	Q	206/221 (93%)	199 (97%)	7 (3%)	37	30
4	D	207/211 (98%)	201 (97%)	6 (3%)	42	35
4	R	207/211 (98%)	201 (97%)	6 (3%)	42	35
5	E	197/203 (97%)	194 (98%)	3 (2%)	65	62
5	S	197/203 (97%)	194 (98%)	3 (2%)	65	62
6	F	203/224 (91%)	200 (98%)	3 (2%)	65	62
6	T	203/224 (91%)	199 (98%)	4 (2%)	55	50
7	G	199/212 (94%)	191 (96%)	8 (4%)	31	24
7	U	199/212 (94%)	189 (95%)	10 (5%)	24	16
8	H	155/159 (98%)	154 (99%)	1 (1%)	86	87
8	V	155/159 (98%)	154 (99%)	1 (1%)	86	87
9	I	183/195 (94%)	182 (100%)	1 (0%)	88	89
9	W	183/195 (94%)	182 (100%)	1 (0%)	88	89
10	J	173/174 (99%)	172 (99%)	1 (1%)	86	87
10	X	173/174 (99%)	173 (100%)	0	100	100
11	K	168/171 (98%)	166 (99%)	2 (1%)	71	70
11	Y	168/171 (98%)	166 (99%)	2 (1%)	71	70
12	L	156/159 (98%)	155 (99%)	1 (1%)	86	87
12	Z	156/159 (98%)	155 (99%)	1 (1%)	86	87
13	M	177/178 (99%)	174 (98%)	3 (2%)	60	57
13	a	177/178 (99%)	174 (98%)	3 (2%)	60	57
14	N	179/181 (99%)	176 (98%)	3 (2%)	60	57
14	b	179/181 (99%)	176 (98%)	3 (2%)	60	57
All	All	5202/5378 (97%)	5099 (98%)	103 (2%)	57	50

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	CYS
1	A	78	CYS

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Mol	Chain	Res	Type
1	A	137	CYS
1	A	177	SER
2	B	4	ARG
2	B	35	SER
2	B	54	SER
2	B	74	LEU
2	B	143	ARG
2	B	186	ASP
2	B	198	SER
3	C	62	SER
3	C	75	SER
3	C	173	SER
3	C	177	GLN
3	C	199	LYS
3	C	206	LEU
4	D	48	LYS
4	D	52	LYS
4	D	101	PRO
4	D	146	GLN
4	D	184	ASP
4	D	208	LEU
5	E	47	CYS
5	E	53	ARG
5	E	172	SER
6	F	4	ASN
6	F	9	ASP
6	F	73	SER
7	G	6	THR
7	G	34	SER
7	G	57	LYS
7	G	168	LYS
7	G	182	MET
7	G	204	GLU
7	G	216	TRP
7	G	224	ARG
8	H	48	SER
9	I	180	LYS
10	J	135	ASP
11	K	18	ASP
11	K	185	LYS
12	L	197	GLU
13	M	99	ARG

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Mol	Chain	Res	Type
13	M	125	ASP
13	M	136	LYS
14	N	94	ARG
14	N	100	ARG
14	N	216	SER
1	O	47	CYS
1	O	78	CYS
1	O	137	CYS
1	O	177	SER
1	O	207	SER
2	P	4	ARG
2	P	35	SER
2	P	54	SER
2	P	74	LEU
2	P	143	ARG
2	P	156	PHE
2	P	186	ASP
2	P	198	SER
3	Q	62	SER
3	Q	75	SER
3	Q	173	SER
3	Q	177	GLN
3	Q	199	LYS
3	Q	206	LEU
3	Q	231	LYS
4	R	48	LYS
4	R	52	LYS
4	R	101	PRO
4	R	146	GLN
4	R	184	ASP
4	R	208	LEU
5	S	47	CYS
5	S	53	ARG
5	S	172	SER
6	T	4	ASN
6	T	9	ASP
6	T	73	SER
6	T	239	ARG
7	U	6	THR
7	U	34	SER
7	U	57	LYS
7	U	114	ASP

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Mol	Chain	Res	Type
7	U	168	LYS
7	U	182	MET
7	U	204	GLU
7	U	216	TRP
7	U	224	ARG
7	U	231	ASP
8	V	48	SER
9	W	180	LYS
11	Y	18	ASP
11	Y	185	LYS
12	Z	197	GLU
13	a	99	ARG
13	a	125	ASP
13	a	136	LYS
14	b	94	ARG
14	b	100	ARG
14	b	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	167	ASN
4	D	154	HIS
7	G	225	HIS
3	Q	167	ASN
4	R	154	HIS
7	U	225	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	YRE	Z	301	-	47,47,47	0.91	3 (6%)	62,63,63	1.27	5 (8%)
15	YRE	L	301	-	47,47,47	1.04	3 (6%)	62,63,63	1.50	7 (11%)

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	YRE	Z	301	-	-	15/45/70/70	0/4/5/5
15	YRE	L	301	-	-	18/45/70/70	0/4/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	YRE	C30-N29	2.85	1.38	1.34
15	Z	301	YRE	C30-N29	2.84	1.38	1.34
15	Z	301	YRE	C05-N06	2.33	1.39	1.34
15	L	301	YRE	C05-N06	2.30	1.39	1.34
15	L	301	YRE	C17-C16	2.16	1.58	1.54
15	Z	301	YRE	C17-C16	2.12	1.58	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	YRE	C40-C39-N38	5.48	118.41	110.10
15	L	301	YRE	C16-N29-C30	5.04	128.36	122.83
15	Z	301	YRE	C16-N29-C30	4.94	128.25	122.83
15	L	301	YRE	C33-N29-C30	-4.41	110.61	113.42
15	Z	301	YRE	C33-N29-C30	-4.26	110.70	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	YRE	C18-C17-C16	3.33	121.19	113.25
15	L	301	YRE	C18-C17-C16	3.31	121.15	113.25
15	L	301	YRE	C42-C43-N38	3.24	115.02	110.10
15	Z	301	YRE	C17-C16-N29	2.88	115.62	112.65
15	L	301	YRE	C17-C16-N29	2.84	115.58	112.65
15	L	301	YRE	C43-N38-C39	2.18	113.74	108.83
15	Z	301	YRE	C36-C37-N38	-2.11	106.99	113.93

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	301	YRE	C15-C16-N29-C30
15	L	301	YRE	C17-C16-N29-C30
15	L	301	YRE	C17-C16-N29-C33
15	L	301	YRE	C13-C36-C37-N38
15	Z	301	YRE	C15-C16-N29-C30
15	Z	301	YRE	C17-C16-N29-C30
15	Z	301	YRE	C17-C16-N29-C33
15	L	301	YRE	C36-C37-N38-C43
15	L	301	YRE	C26-C20-O21-C22
15	Z	301	YRE	C26-C20-O21-C22
15	L	301	YRE	C19-C20-O21-C22
15	Z	301	YRE	C19-C20-O21-C22
15	L	301	YRE	O21-C22-C23-C24
15	Z	301	YRE	O21-C22-C23-C24
15	Z	301	YRE	C23-C24-C25-C04
15	L	301	YRE	C23-C24-C25-C04
15	Z	301	YRE	C16-C17-C18-C19
15	L	301	YRE	C16-C17-C18-C19
15	Z	301	YRE	C16-C17-C18-C28
15	L	301	YRE	C36-C37-N38-C39
15	L	301	YRE	C16-C17-C18-C28
15	Z	301	YRE	O35-C15-C16-C17
15	L	301	YRE	O35-C15-C16-C17
15	L	301	YRE	C22-C23-C24-C25
15	L	301	YRE	C23-C22-O21-C20
15	Z	301	YRE	C22-C23-C24-C25
15	L	301	YRE	N14-C15-C16-C17
15	Z	301	YRE	C23-C22-O21-C20
15	Z	301	YRE	N14-C15-C16-C17
15	L	301	YRE	C15-C16-N29-C33

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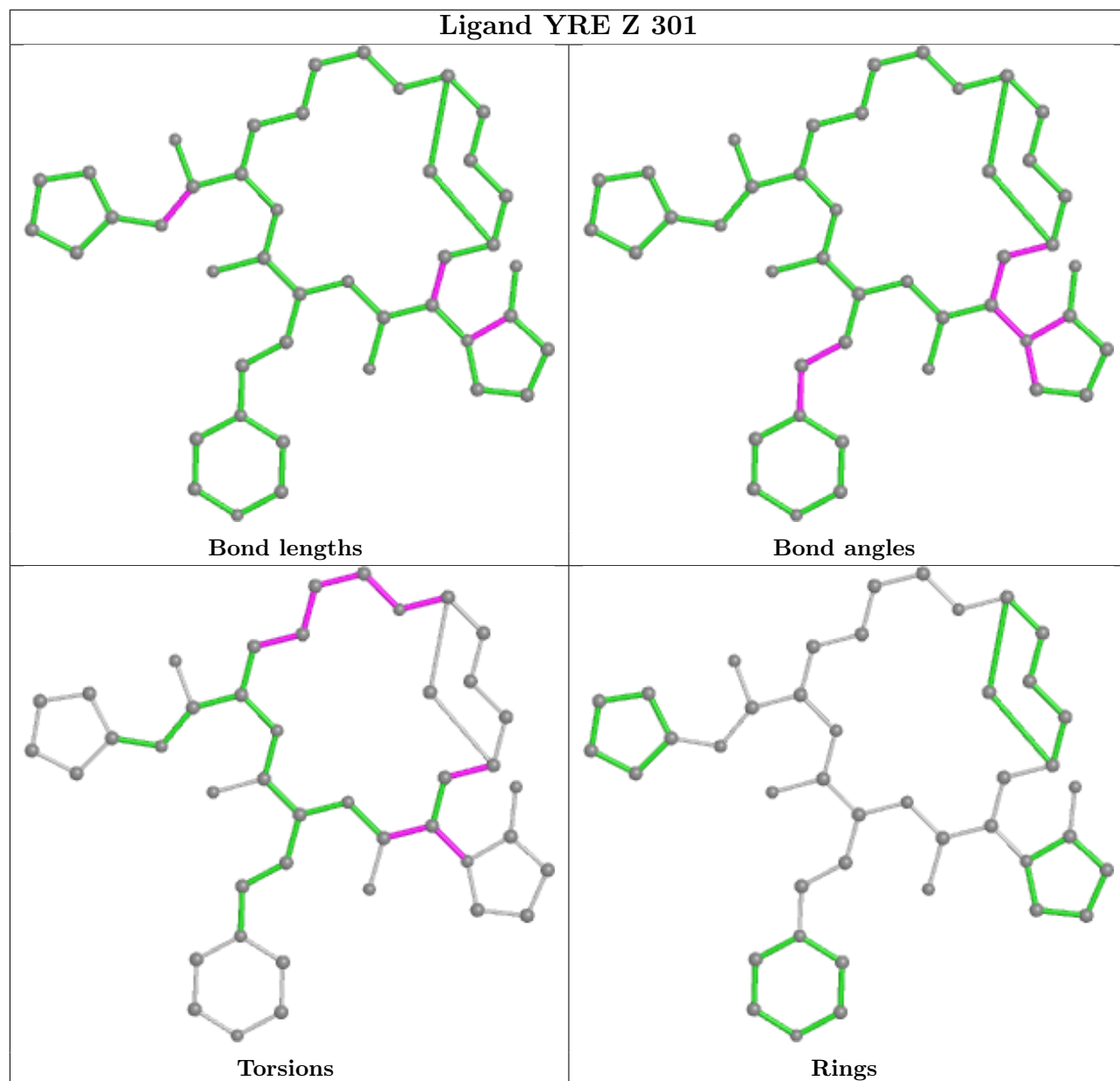
Continued from previous page...

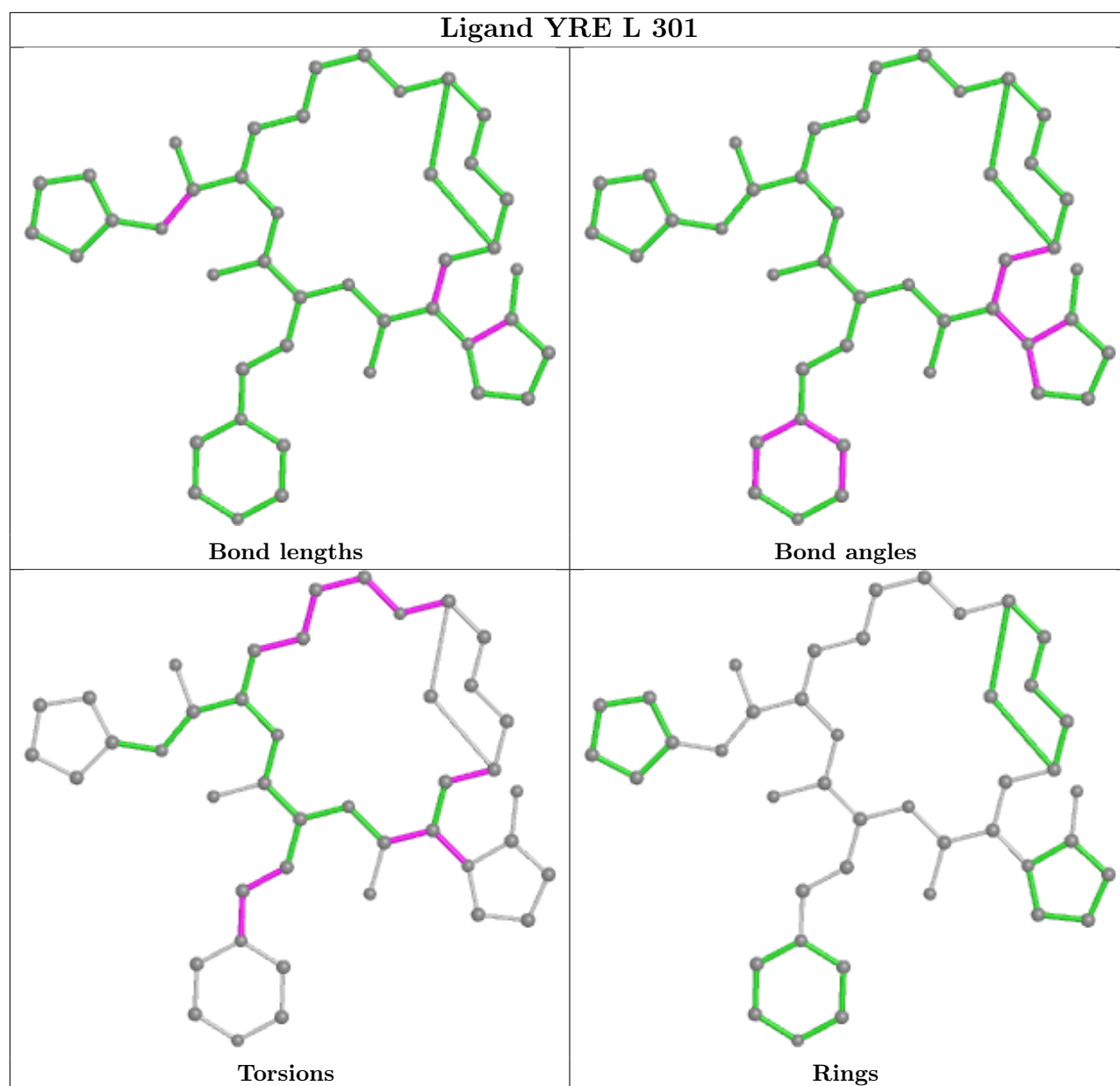
Mol	Chain	Res	Type	Atoms
15	Z	301	YRE	C15-C16-N29-C33
15	L	301	YRE	O35-C15-C16-N29
15	Z	301	YRE	O35-C15-C16-N29

There are no ring outliers.

No monomer is involved in short contacts.

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.

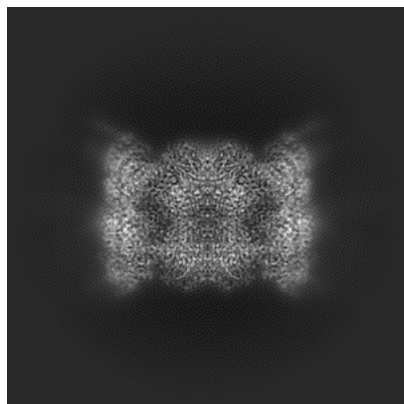
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42148. These allow visual inspection of the internal detail of the map and identification of artifacts.

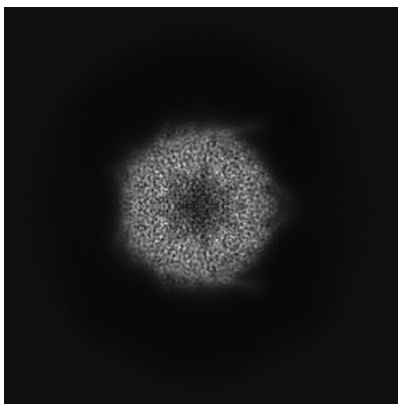
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

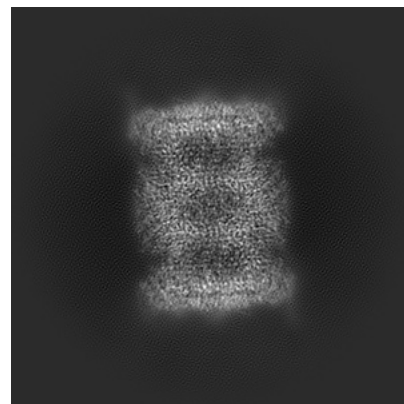
6.1.1 Primary map



X

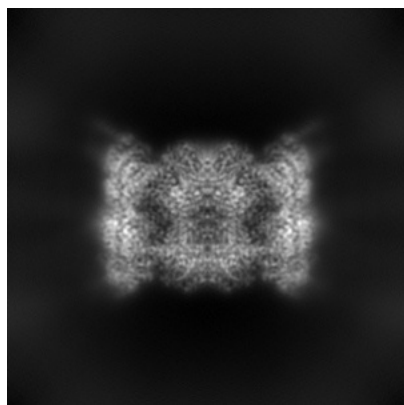


Y

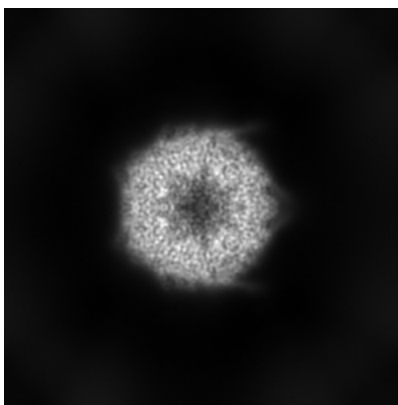


Z

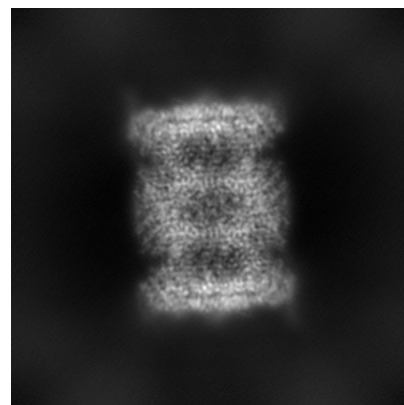
6.1.2 Raw map



X



Y

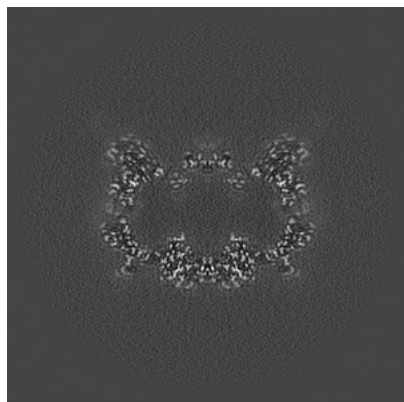


Z

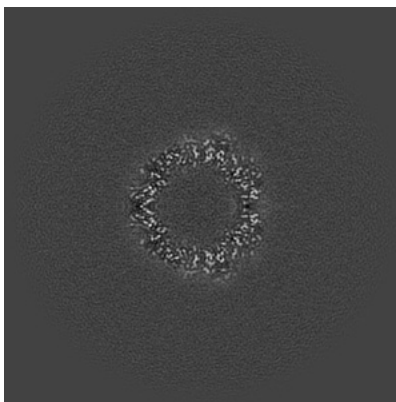
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

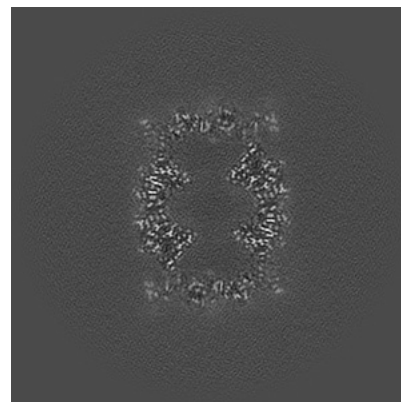
6.2.1 Primary map



X Index: 176

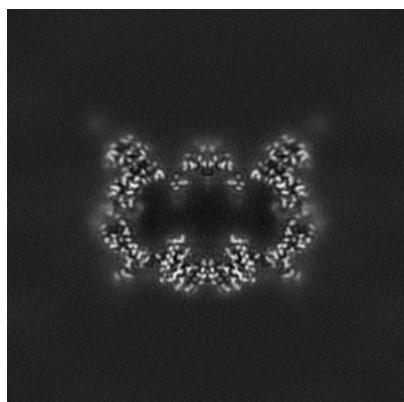


Y Index: 176

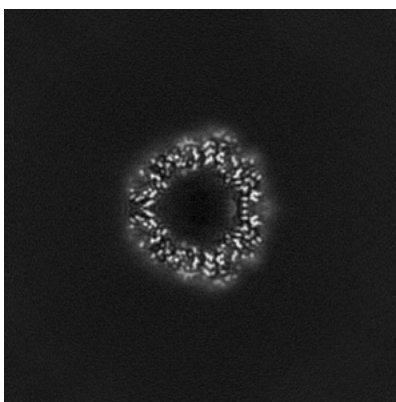


Z Index: 176

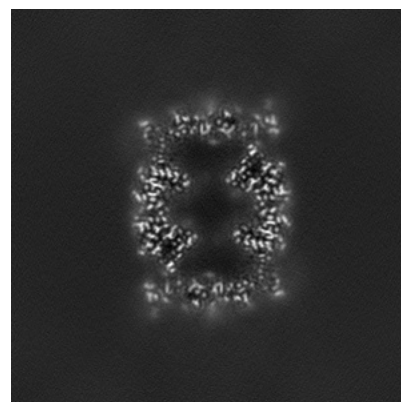
6.2.2 Raw map



X Index: 176



Y Index: 176

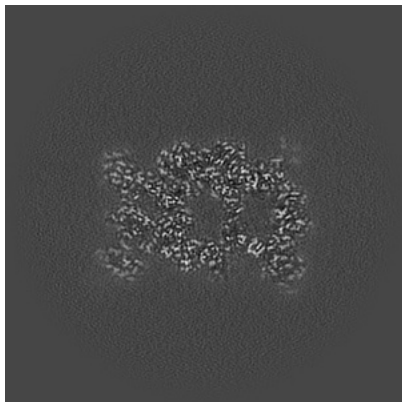


Z Index: 176

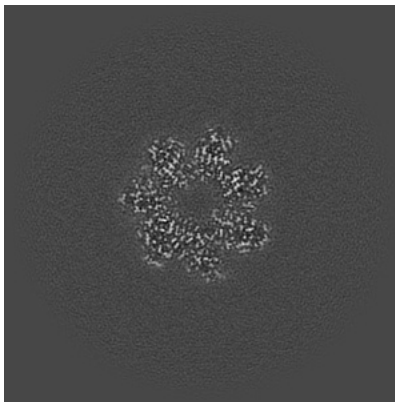
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

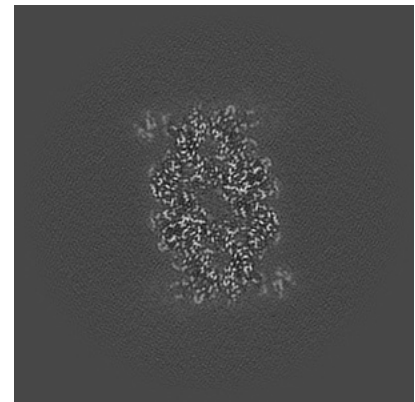
6.3.1 Primary map



X Index: 149

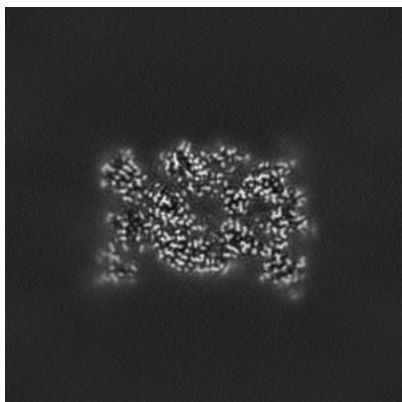


Y Index: 156

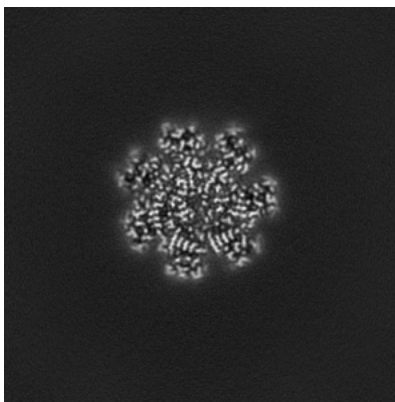


Z Index: 138

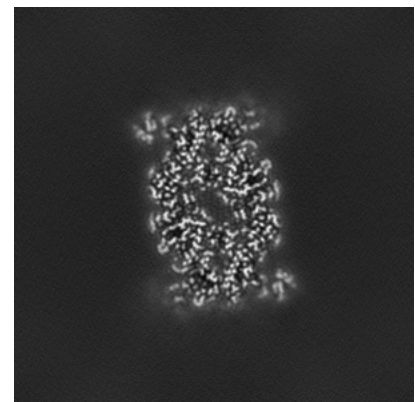
6.3.2 Raw map



X Index: 144



Y Index: 105

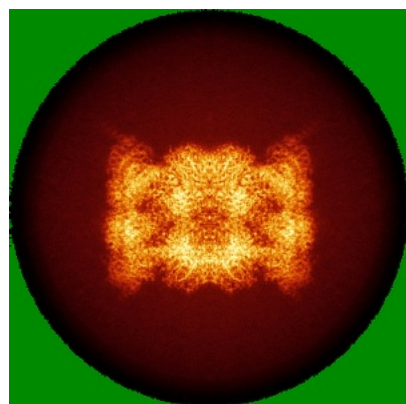


Z Index: 138

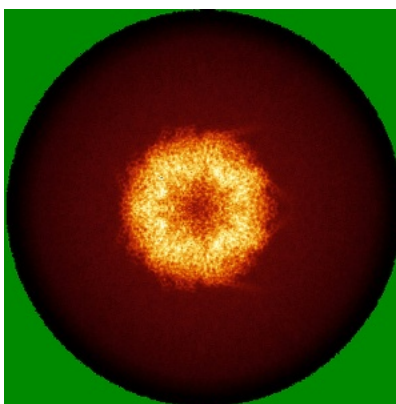
The images above show the largest variance slices of the map in three orthogonal directions.

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

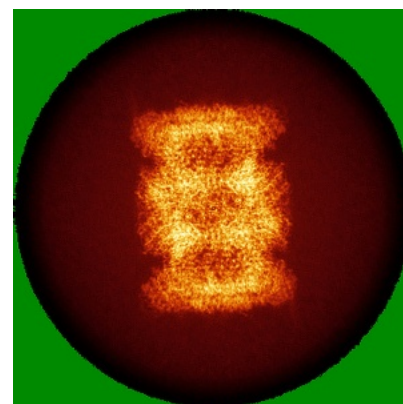
6.4.1 Primary map



X

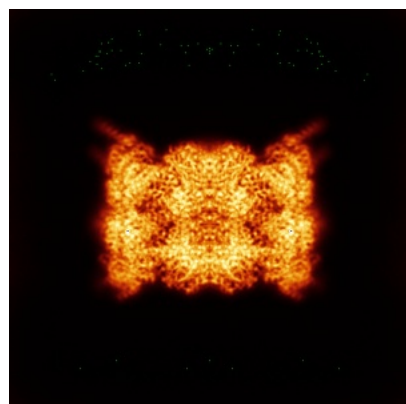


Y

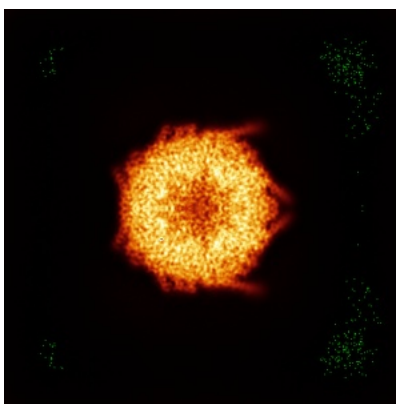


Z

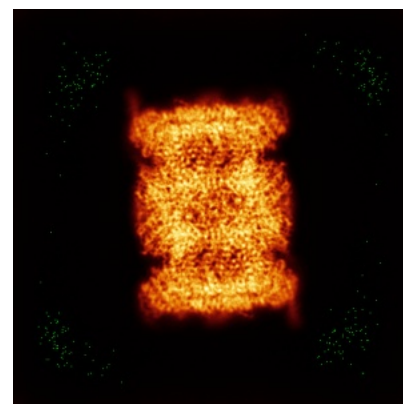
6.4.2 Raw map



X



Y

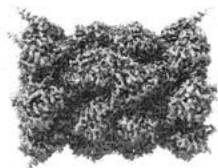


Z

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

6.5 Orthogonal surface views [i](#)

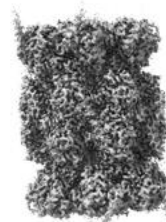
6.5.1 Primary map



X



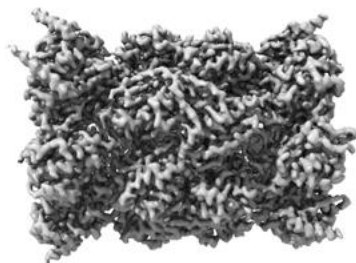
Y



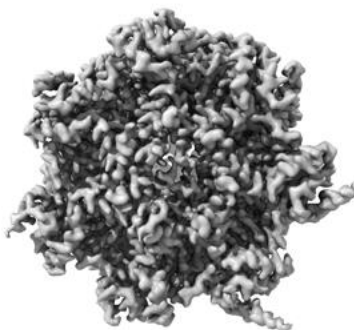
Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

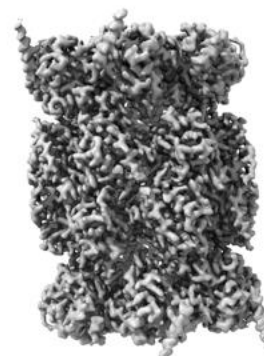
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

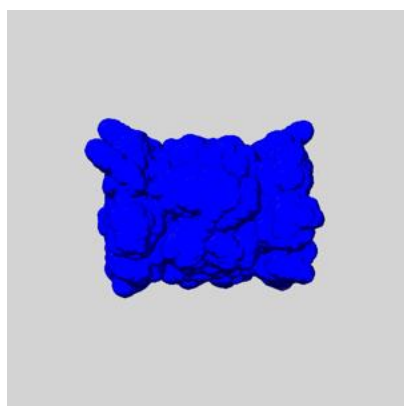
6.6 Mask visualisation [i](#)

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

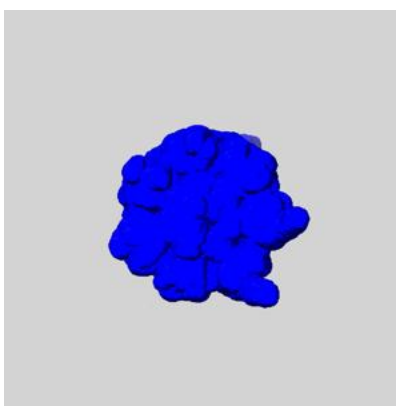
A mask typically either:

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

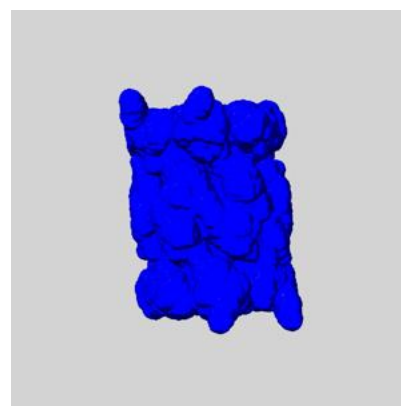
6.6.1 emd_42148_msk_1.map [i](#)



X



Y

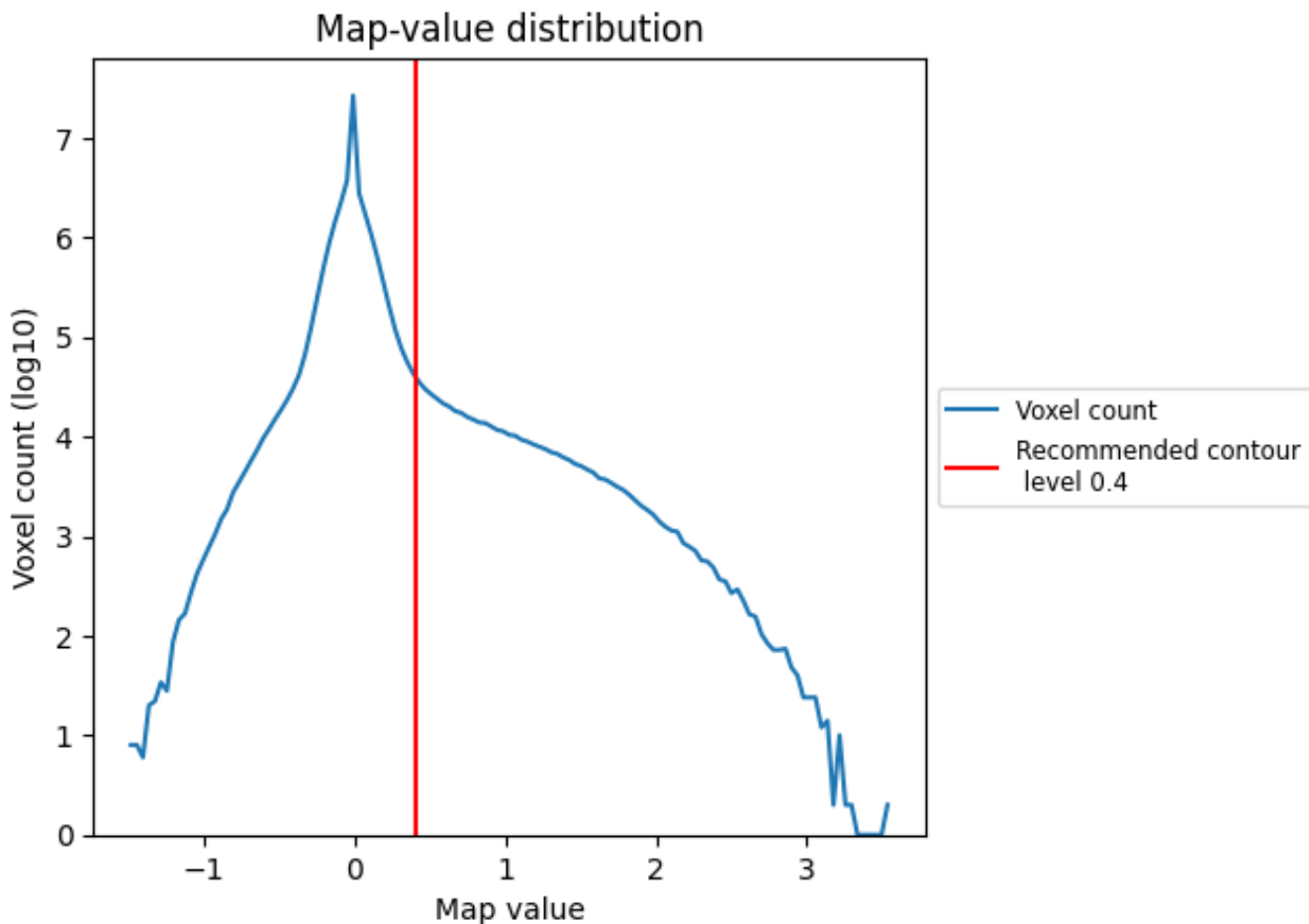


Z

7 Map analysis [i](#)

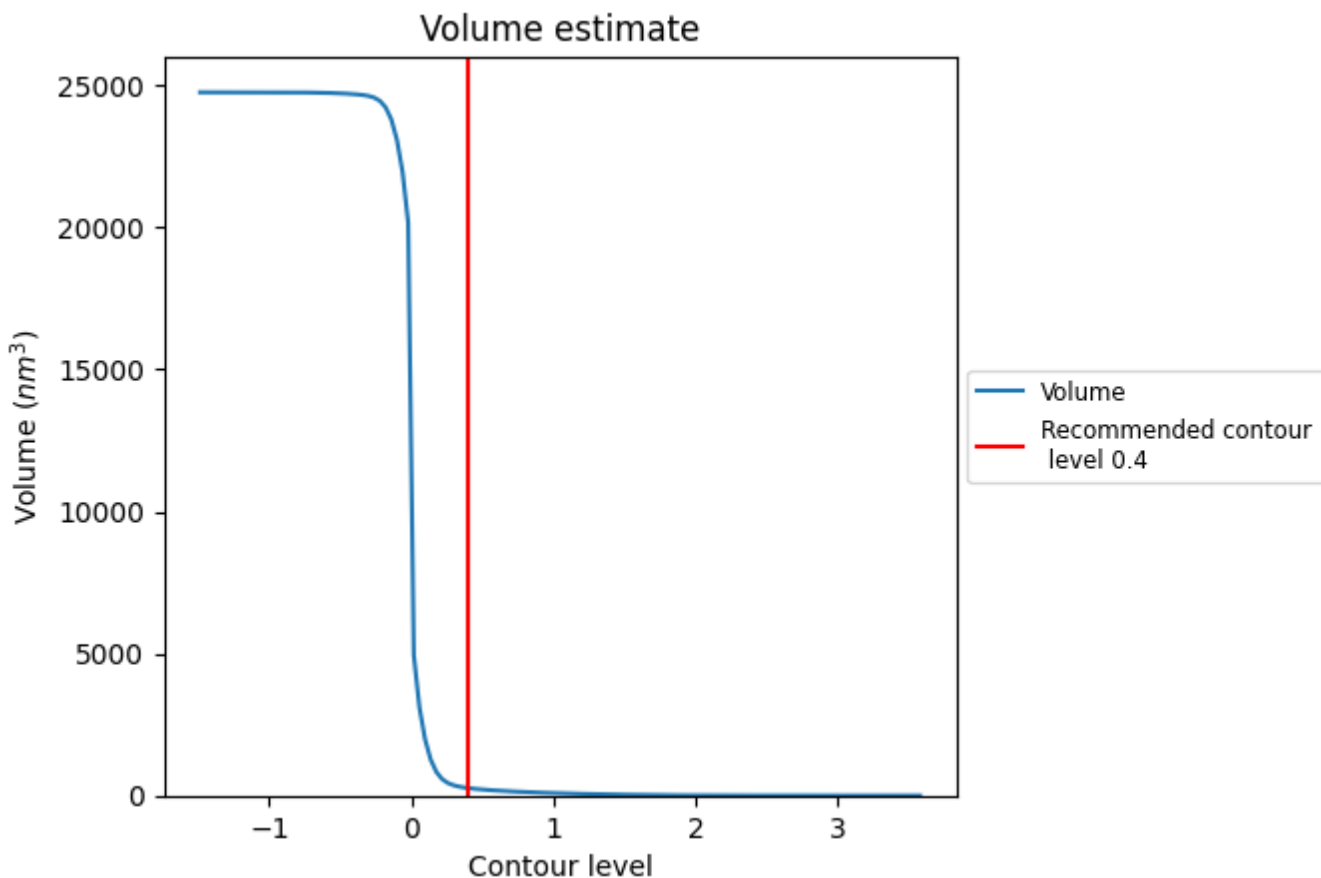
This section contains the results of statistical analysis of the map.

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.

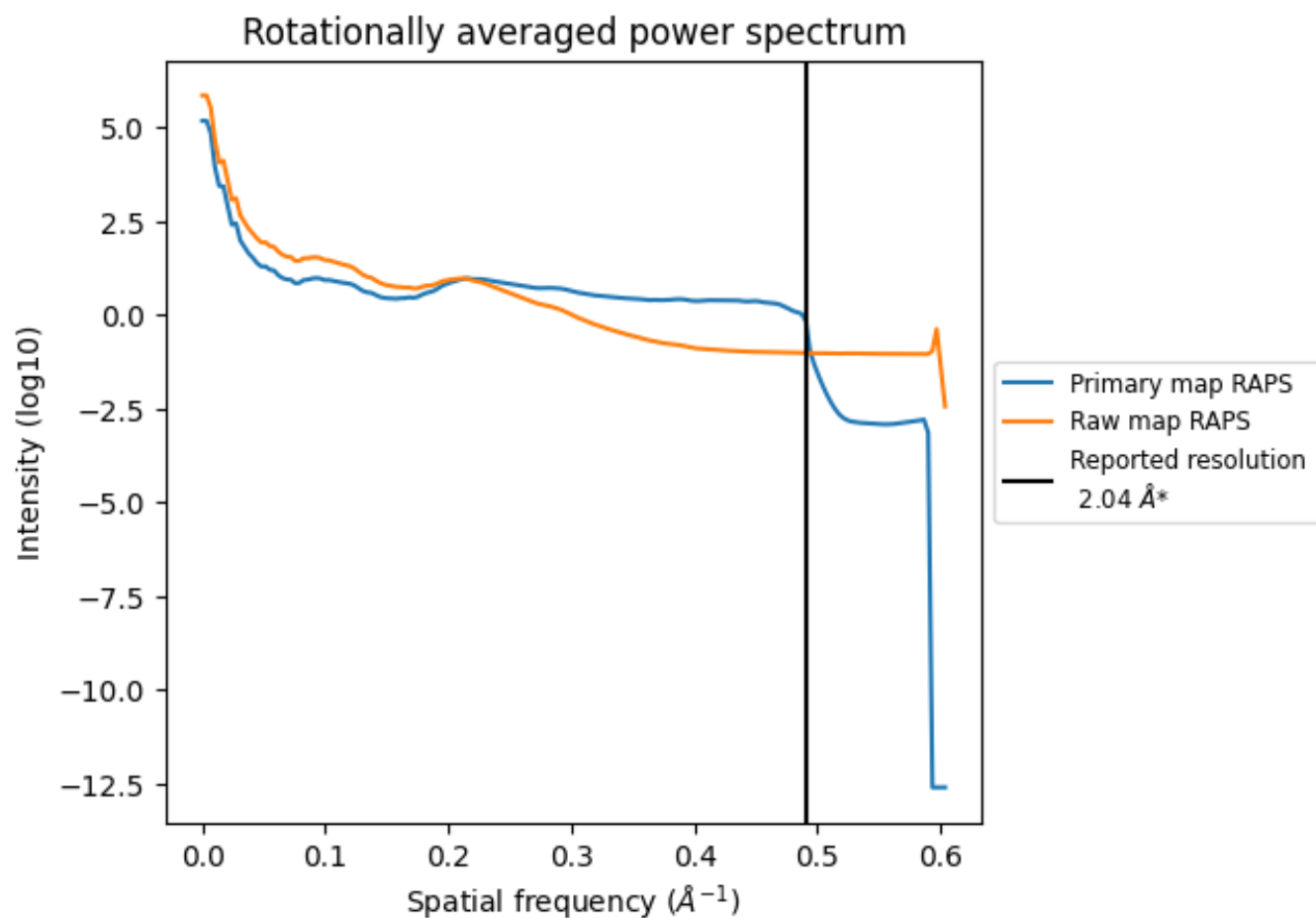
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm³; this corresponds to an approximate mass of 237 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](#)

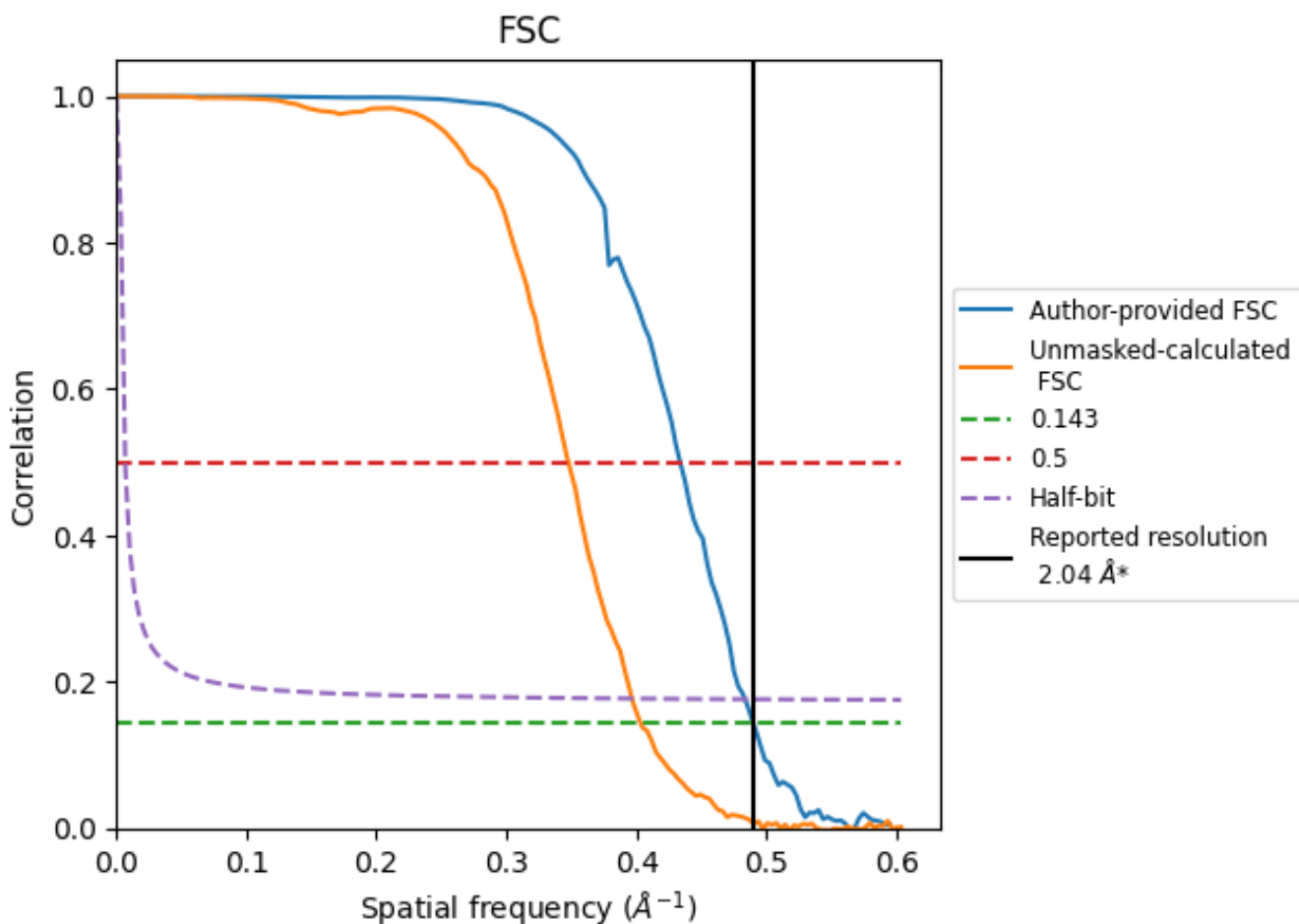


*Reported resolution corresponds to spatial frequency of 0.490 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.490 Å⁻¹

8.2 Resolution estimates [i](#)

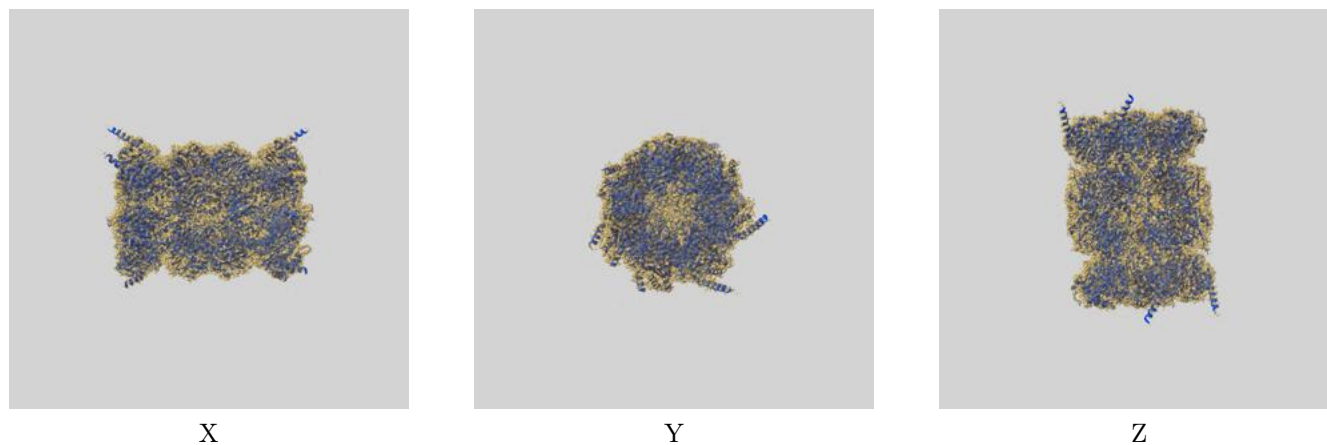
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.31	2.07
Unmasked-calculated*	2.48	2.88	2.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.48 differs from the reported value 2.04 by more than 10 %

9 Map-model fit [i](#)

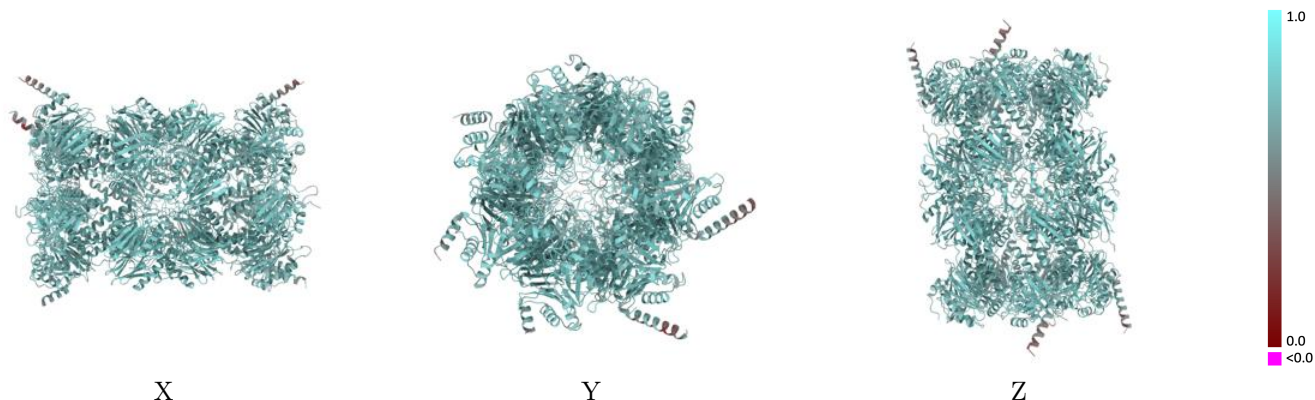
This section contains information regarding the fit between EMDB map EMD-42148 and PDB model 8UD9. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



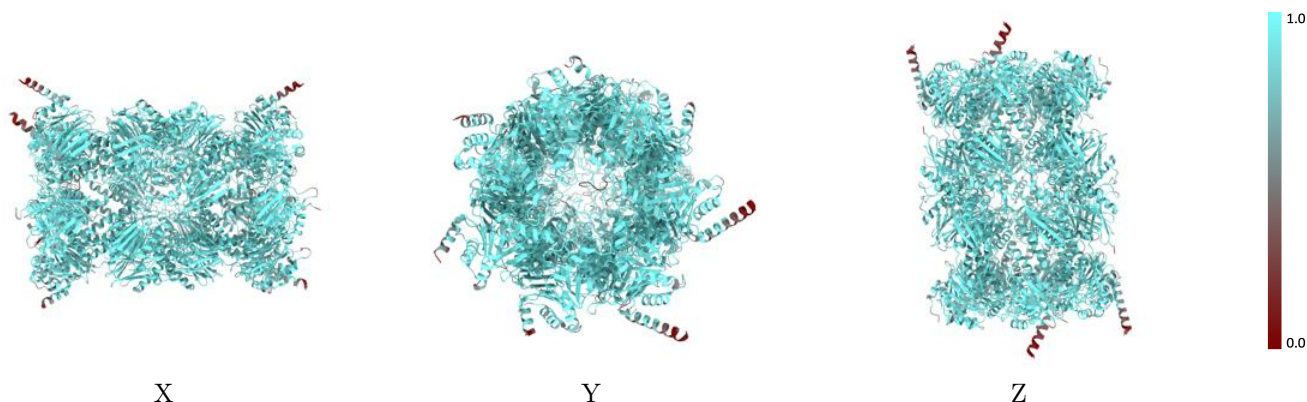
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



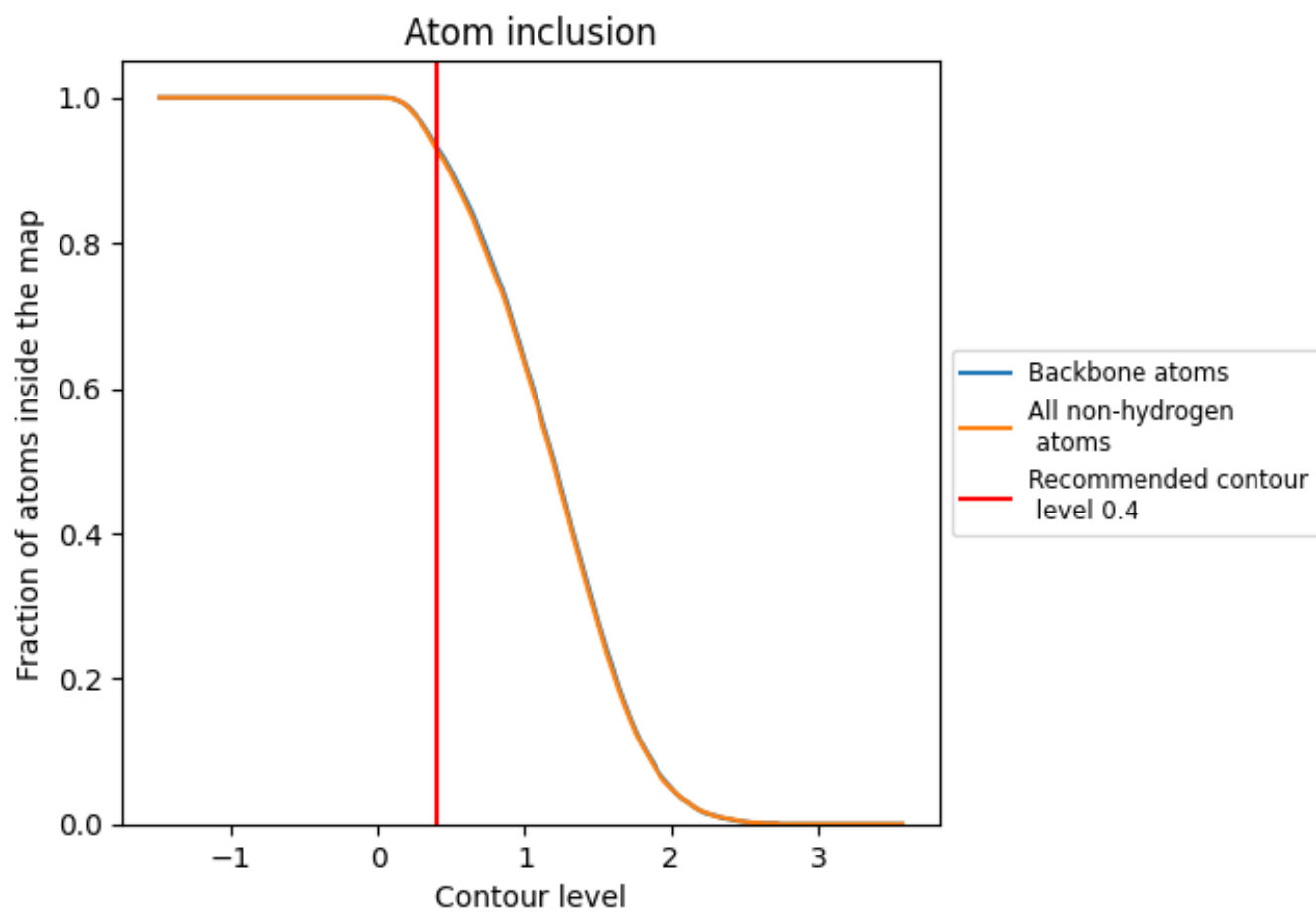
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.7320
A	 0.9110	 0.7200
B	 0.9220	 0.7260
C	 0.8990	 0.7090
D	 0.8800	 0.6960
E	 0.9160	 0.7170
F	 0.9190	 0.7150
G	 0.9030	 0.7170
H	 0.9640	 0.7580
I	 0.9490	 0.7450
J	 0.9730	 0.7590
K	 0.9680	 0.7550
L	 0.9700	 0.7550
M	 0.9580	 0.7520
N	 0.9620	 0.7500
O	 0.9070	 0.7180
P	 0.9220	 0.7250
Q	 0.9000	 0.7090
R	 0.8780	 0.6980
S	 0.9150	 0.7180
T	 0.9210	 0.7170
U	 0.9030	 0.7160
V	 0.9630	 0.7580
W	 0.9490	 0.7440
X	 0.9730	 0.7590
Y	 0.9680	 0.7540
Z	 0.9700	 0.7540
a	 0.9570	 0.7510
b	 0.9620	 0.7490

