



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 03:29 AM EST

PDB ID : 6AVO
EMDB ID : EMD-7010
Title : Cryo-EM structure of human immunoproteasome with a novel noncompetitive inhibitor that selectively inhibits activated lymphocytes
Authors : Li, H.; Santos, R.; Bai, L.
Deposited on : 2017-09-04
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

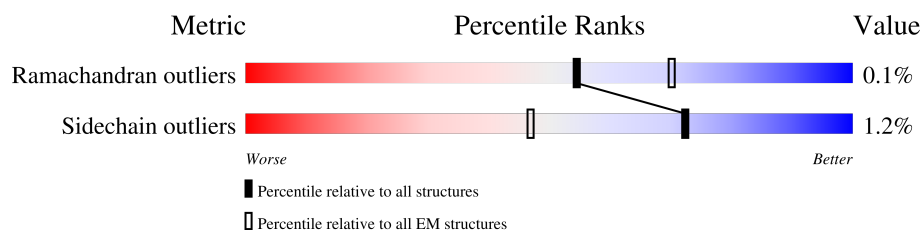
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)
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	199	98%
1	F	199	99%
2	B	234	91% 6%
2	E	234	91% 6%
3	C	204	98%
3	D	204	98%
4	G	263	87% 11%
4	L	263	87% 11%
5	H	241	96%

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Mol	Chain	Length	Quality of chain
5	M	241	
6	I	248	
6	N	248	
7	J	255	
7	Q	255	
8	K	246	
8	R	246	
9	O	261	
9	Z	261	
10	P	234	
10	b	234	
11	S	213	
11	X	213	
12	T	201	
12	V	201	
13	U	205	
13	Y	205	
14	W	219	
14	a	219	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47715 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 beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		
1	F	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		

- Molecule 2 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		
2	E	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		

- Molecule 3 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		
3	D	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	234	Total	C	N	O	S	1	0
			1817	1140	324	342	11		
4	L	234	Total	C	N	O	S	3	0
			1841	1153	332	345	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	233	Total	C	N	O	S	0	0
			1753	1100	289	353	11		
5	M	233	Total	C	N	O	S	0	0
			1748	1100	292	345	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	232	Total	C	N	O	S	2	0
			1749	1092	312	340	5		
6	N	232	Total	C	N	O	S	0	0
			1754	1098	309	342	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	239	Total	C	N	O	S	4	0
			1888	1198	325	353	12		
7	Q	239	Total	C	N	O	S	1	0
			1851	1175	314	350	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	240	Total	C	N	O	S	2	0
			1850	1172	313	352	13		
8	R	240	Total	C	N	O	S	1	0
			1817	1149	304	350	14		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	240	Total	C	N	O	S	2	0
			1843	1168	313	351	11		
9	Z	240	Total	C	N	O	S	2	0
			1860	1182	320	347	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	230	Total	C	N	O	S	0	0
			1741	1111	293	331	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	230	Total	C	N	O	S	3	0
			1788	1145	301	336	6		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	213	Total	C	N	O	S	1	0
			1642	1041	280	310	11		
11	X	213	Total	C	N	O	S	2	0
			1636	1038	277	310	11		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	196	Total	C	N	O	S	2	0
			1567	1006	266	285	10		
12	V	196	Total	C	N	O	S	3	0
			1581	1015	270	286	10		

- Molecule 13 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	204	Total	C	N	O	S	2	0
			1599	1018	267	295	19		
13	Y	204	Total	C	N	O	S	2	0
			1604	1022	268	294	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	216	Total	C	N	O	S	1	0
			1692	1067	291	322	12		
14	a	216	Total	C	N	O	S	1	0
			1684	1062	290	320	12		

- Molecule 15 is N 1 -{2-[(1,1'-biphenyl)-3-carbonyl]amino}ethyl}-N 4 -tert-butyl-N 2 -(3-phenylpropanoyl)-L-aspartamide (three-letter code: BZ7) (formula: C₃₂H₃₈N₄O₄).

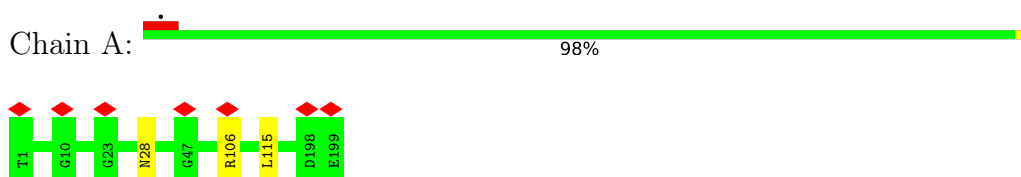


Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total 40	C 32	N 4	O 4	0
15	D	1	Total 40	C 32	N 4	O 4	0

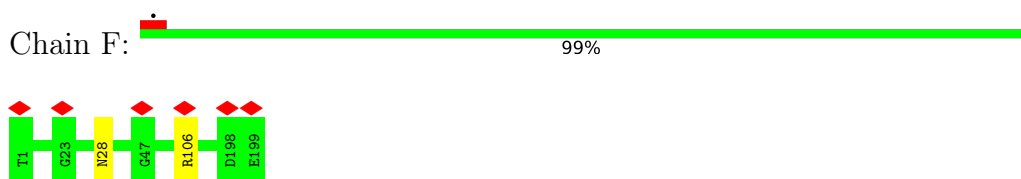
3 Residue-property plots [i](#)

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.

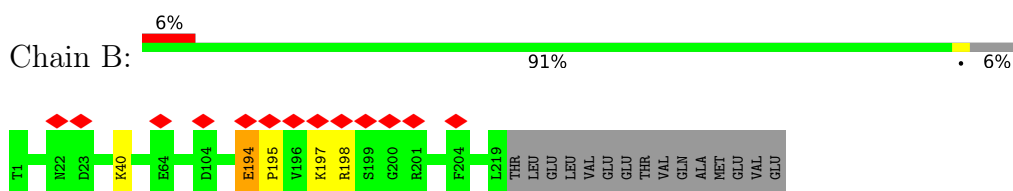
- Molecule 1: Proteasome subunit beta type-9



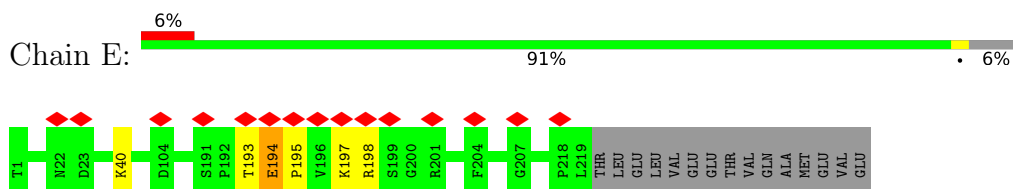
- Molecule 1: Proteasome subunit beta type-9



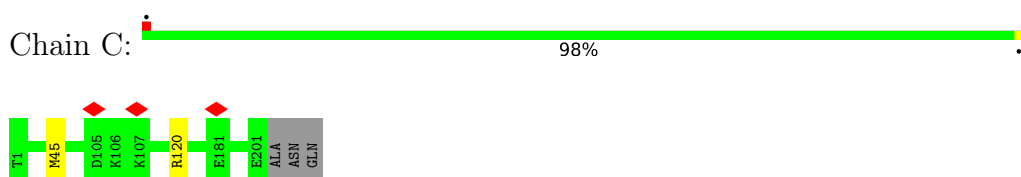
- Molecule 2: Proteasome subunit beta type-10



- Molecule 2: Proteasome subunit beta type-10

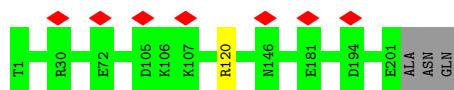


- Molecule 3: Proteasome subunit beta type-8




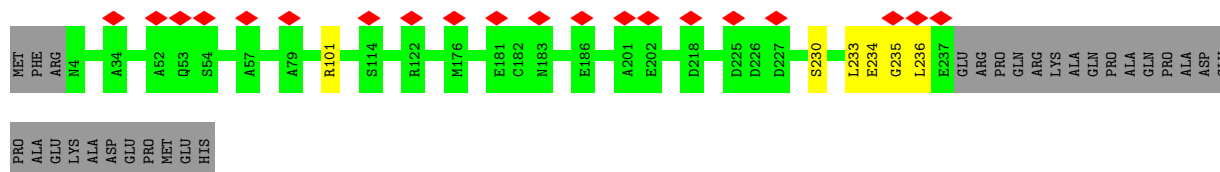
- Molecule 3: Proteasome subunit beta type-8

Chain D:  98%




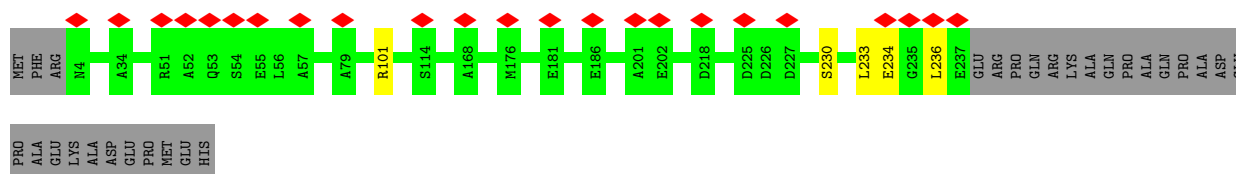
- Molecule 4: Proteasome subunit alpha type-1

Chain G:  87% 11%



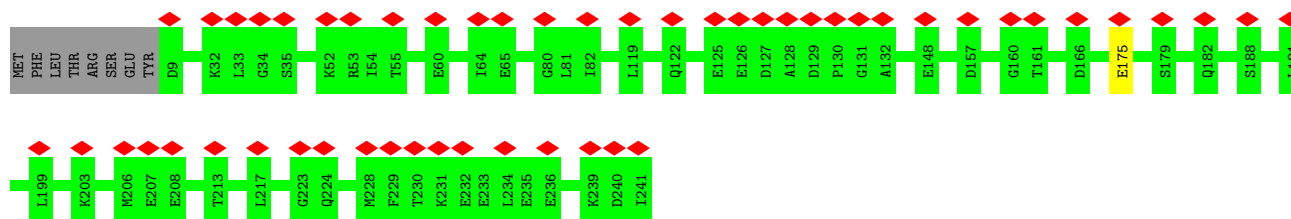
- Molecule 4: Proteasome subunit alpha type-1

Chain L:  87% 11%



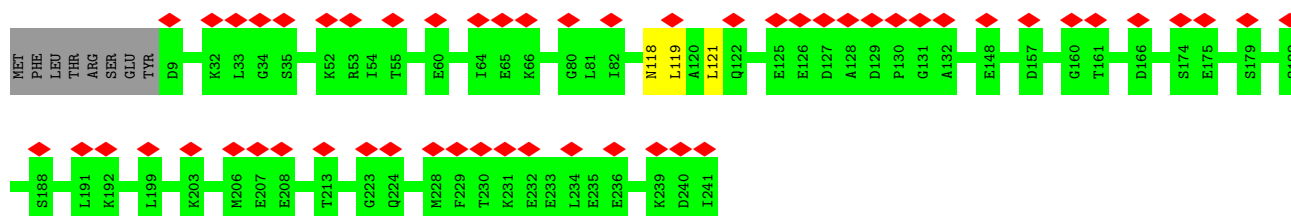
- Molecule 5: Proteasome subunit alpha type-5

Chain H:  96%

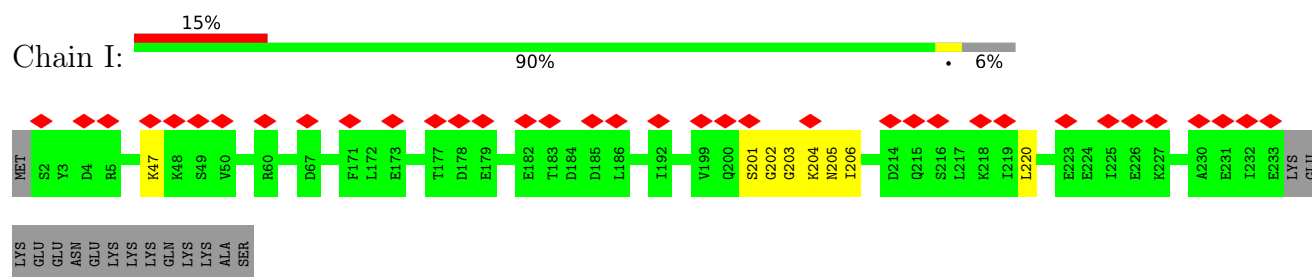


- Molecule 5: Proteasome subunit alpha type-5

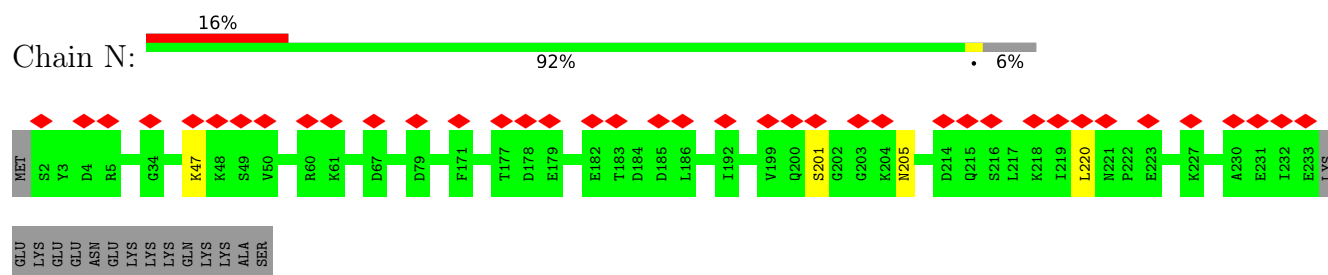
Chain M:  95%



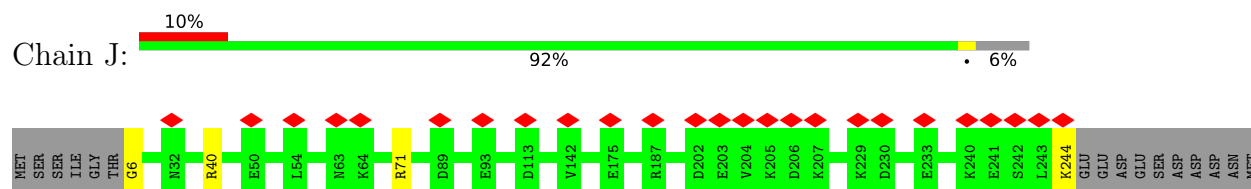
- Molecule 6: Proteasome subunit alpha type-7



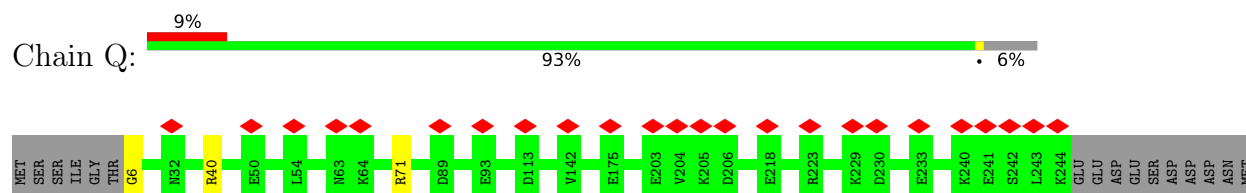
- Molecule 6: Proteasome subunit alpha type-7



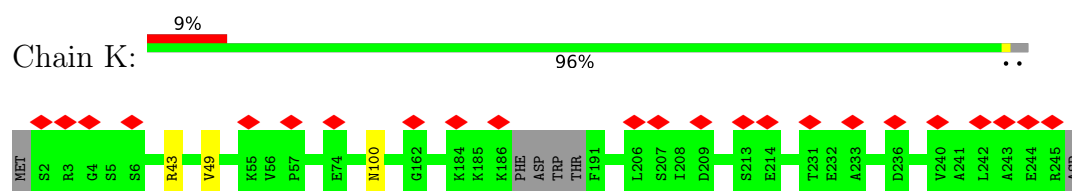
- Molecule 7: Proteasome subunit alpha type-3



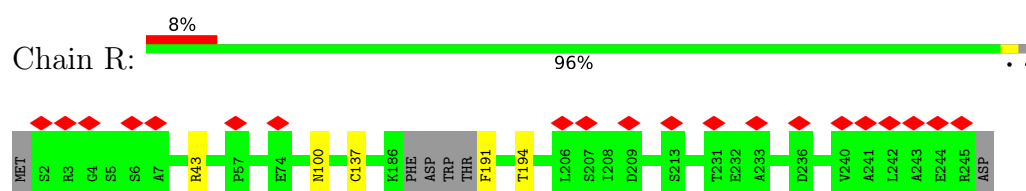
- Molecule 7: Proteasome subunit alpha type-3



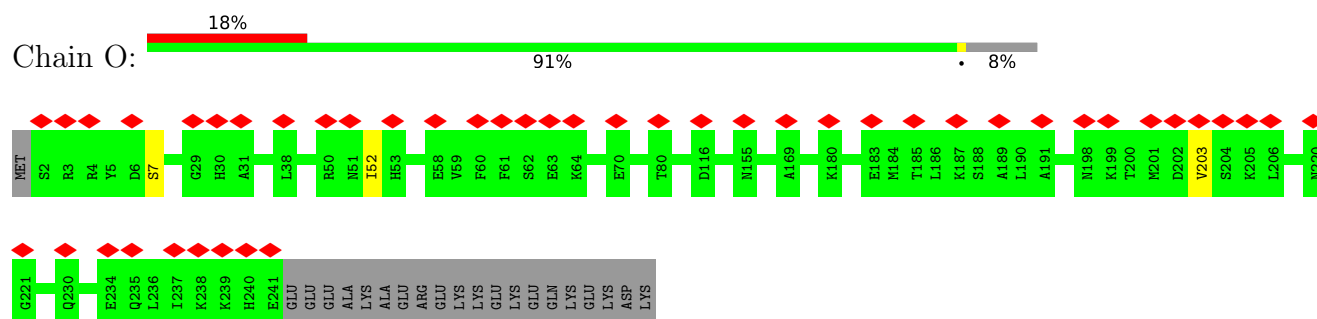
- Molecule 8: Proteasome subunit alpha type-6



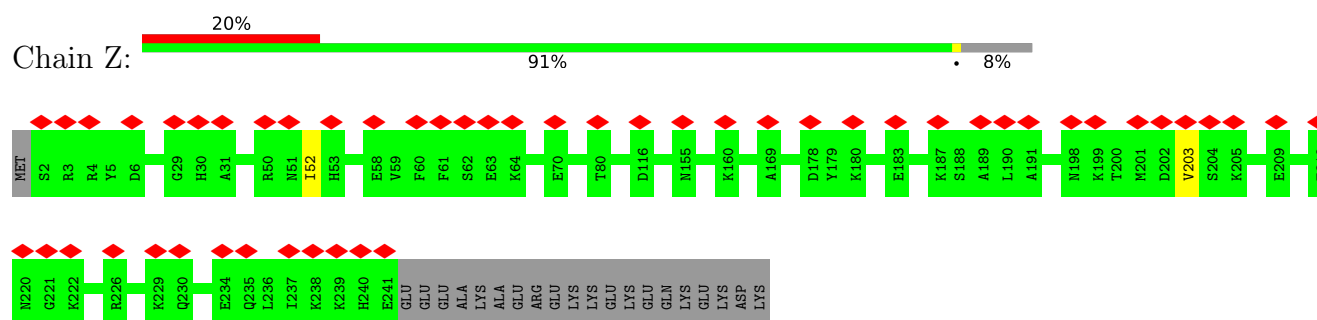
- Molecule 8: Proteasome subunit alpha type-6



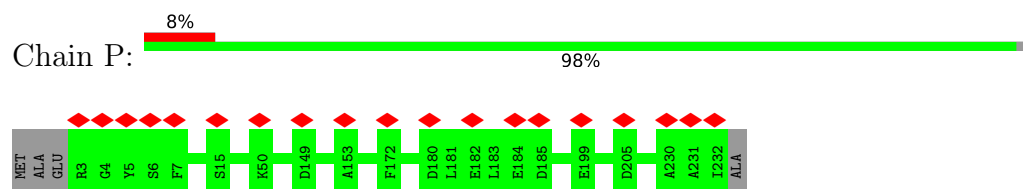
- Molecule 9: Proteasome subunit alpha type-4



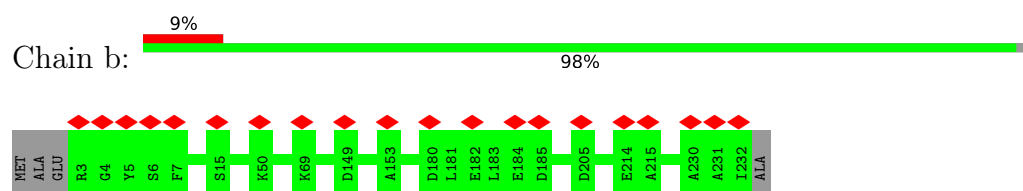
- Molecule 9: Proteasome subunit alpha type-4



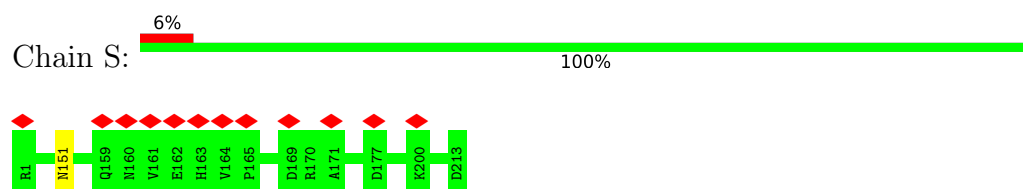
- Molecule 10: Proteasome subunit alpha type-2



- Molecule 10: Proteasome subunit alpha type-2

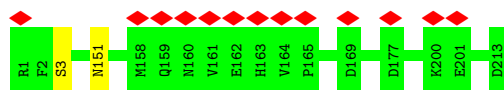


- Molecule 11: Proteasome subunit beta type-1

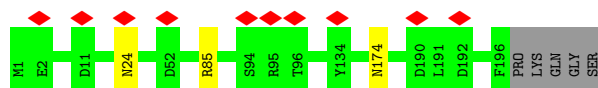


- Molecule 11: Proteasome subunit beta type-1

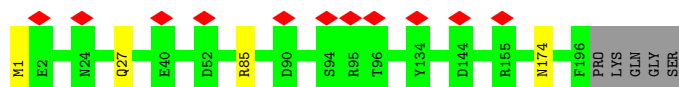




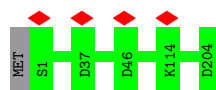
- Molecule 12: Proteasome subunit beta type-2



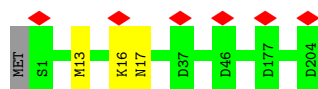
- Molecule 12: Proteasome subunit beta type-2



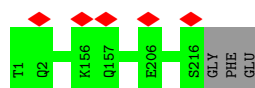
- Molecule 13: Proteasome subunit beta type-3



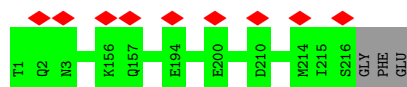
- Molecule 13: Proteasome subunit beta type-3



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0383	Depositor
Map size (\AA)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BZ7

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	0.46	0/1521	0.53	0/2062
1	F	0.47	0/1521	0.53	0/2062
2	B	0.44	0/1635	0.55	0/2222
2	E	0.44	0/1635	0.55	0/2222
3	C	0.48	0/1596	0.54	0/2152
3	D	0.48	0/1596	0.54	0/2152
4	G	0.41	0/1853	0.52	0/2510
4	L	0.41	0/1882	0.53	0/2548
5	H	0.37	0/1780	0.51	0/2412
5	M	0.37	0/1775	0.51	0/2401
6	I	0.41	0/1780	0.55	0/2422
6	N	0.40	0/1779	0.52	0/2420
7	J	0.44	0/1935	0.52	0/2605
7	Q	0.45	0/1889	0.52	0/2549
8	K	0.45	0/1886	0.53	0/2549
8	R	0.45	0/1850	0.52	0/2507
9	O	0.41	0/1879	0.52	0/2544
9	Z	0.41	0/1896	0.53	0/2562
10	P	0.46	0/1778	0.52	0/2419
10	b	0.46	0/1833	0.51	0/2489
11	S	0.46	0/1675	0.56	0/2257
11	X	0.46	0/1672	0.56	0/2257
12	T	0.44	0/1606	0.55	0/2174
12	V	0.44	0/1620	0.54	0/2191
13	U	0.46	0/1630	0.56	0/2197
13	Y	0.46	0/1639	0.54	0/2208
14	W	0.49	0/1728	0.56	0/2339
14	a	0.49	0/1720	0.56	0/2330
All	All	0.44	0/48589	0.53	0/65762

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
6	I	0	8
6	N	0	2
7	J	0	1
7	Q	0	1
9	O	0	2
9	Z	0	2
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	201	SER	Peptide
6	I	202	GLY	Peptide
6	I	203	GLY	Peptide
6	I	204	LYS	Peptide
6	I	205	ASN	Peptide
6	I	220	LEU	Peptide
6	I	47	LYS	Peptide
7	J	6	GLY	Peptide
6	N	220	LEU	Peptide
6	N	47	LYS	Peptide
9	O	203	VAL	Peptide
9	O	52	ILE	Peptide
7	Q	6	GLY	Peptide
9	Z	203	VAL	Peptide
9	Z	52	ILE	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
1	F	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
2	B	217/234 (93%)	183 (84%)	32 (15%)	2 (1%)	17	54
2	E	217/234 (93%)	184 (85%)	31 (14%)	2 (1%)	17	54
3	C	199/204 (98%)	179 (90%)	20 (10%)	0	100	100
3	D	199/204 (98%)	180 (90%)	19 (10%)	0	100	100
4	G	233/263 (89%)	214 (92%)	18 (8%)	1 (0%)	34	70
4	L	235/263 (89%)	217 (92%)	18 (8%)	0	100	100
5	H	231/241 (96%)	209 (90%)	22 (10%)	0	100	100
5	M	231/241 (96%)	210 (91%)	21 (9%)	0	100	100
6	I	232/248 (94%)	203 (88%)	28 (12%)	1 (0%)	34	70
6	N	230/248 (93%)	204 (89%)	26 (11%)	0	100	100
7	J	241/255 (94%)	222 (92%)	19 (8%)	0	100	100
7	Q	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
8	K	238/246 (97%)	218 (92%)	20 (8%)	0	100	100
8	R	237/246 (96%)	215 (91%)	21 (9%)	1 (0%)	34	70
9	O	240/261 (92%)	223 (93%)	17 (7%)	0	100	100
9	Z	240/261 (92%)	223 (93%)	17 (7%)	0	100	100
10	P	228/234 (97%)	211 (92%)	17 (8%)	0	100	100
10	b	231/234 (99%)	214 (93%)	17 (7%)	0	100	100
11	S	212/213 (100%)	188 (89%)	24 (11%)	0	100	100
11	X	213/213 (100%)	189 (89%)	24 (11%)	0	100	100
12	T	196/201 (98%)	179 (91%)	17 (9%)	0	100	100
12	V	196/201 (98%)	177 (90%)	19 (10%)	0	100	100
13	U	204/205 (100%)	190 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	204/205 (100%)	189 (93%)	14 (7%)	1 (0%)	29	66
14	W	215/219 (98%)	190 (88%)	25 (12%)	0	100	100
14	a	215/219 (98%)	190 (88%)	25 (12%)	0	100	100
All	All	6166/6446 (96%)	5586 (91%)	572 (9%)	8 (0%)	54	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	I	206	ILE
8	R	194	THR
2	B	195	PRO
2	E	195	PRO
4	G	235	GLY
2	E	194	GLU
2	B	194	GLU
13	Y	17	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/153 (100%)	150 (98%)	3 (2%)	55	75
1	F	153/153 (100%)	151 (99%)	2 (1%)	69	82
2	B	171/185 (92%)	167 (98%)	4 (2%)	50	72
2	E	171/185 (92%)	166 (97%)	5 (3%)	42	67
3	C	164/166 (99%)	162 (99%)	2 (1%)	71	84
3	D	164/166 (99%)	163 (99%)	1 (1%)	86	92
4	G	194/224 (87%)	188 (97%)	6 (3%)	40	65
4	L	198/224 (88%)	193 (98%)	5 (2%)	47	70
5	H	188/203 (93%)	187 (100%)	1 (0%)	88	94
5	M	187/203 (92%)	184 (98%)	3 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	I	175/211 (83%)	175 (100%)	0	100	100
6	N	178/211 (84%)	176 (99%)	2 (1%)	73	85
7	J	199/212 (94%)	196 (98%)	3 (2%)	65	81
7	Q	192/212 (91%)	190 (99%)	2 (1%)	76	86
8	K	201/210 (96%)	197 (98%)	4 (2%)	55	75
8	R	192/210 (91%)	188 (98%)	4 (2%)	53	74
9	O	191/221 (86%)	189 (99%)	2 (1%)	76	86
9	Z	194/221 (88%)	194 (100%)	0	100	100
10	P	176/191 (92%)	176 (100%)	0	100	100
10	b	185/191 (97%)	185 (100%)	0	100	100
11	S	175/178 (98%)	174 (99%)	1 (1%)	86	92
11	X	175/178 (98%)	172 (98%)	3 (2%)	60	78
12	T	166/171 (97%)	163 (98%)	3 (2%)	59	77
12	V	167/171 (98%)	161 (96%)	6 (4%)	35	63
13	U	173/174 (99%)	173 (100%)	0	100	100
13	Y	175/174 (101%)	172 (98%)	3 (2%)	60	78
14	W	180/181 (99%)	180 (100%)	0	100	100
14	a	178/181 (98%)	178 (100%)	0	100	100
All	All	5015/5360 (94%)	4950 (99%)	65 (1%)	72	82

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	106	ARG
1	A	115	LEU
2	B	40	LYS
2	B	194	GLU
2	B	197	LYS
2	B	198	ARG
3	C	45	MET
3	C	120	ARG
3	D	120	ARG
2	E	40	LYS
2	E	193	THR
2	E	194	GLU

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Mol	Chain	Res	Type
2	E	197	LYS
2	E	198	ARG
1	F	28	ASN
1	F	106	ARG
4	G	101[A]	ARG
4	G	101[B]	ARG
4	G	230	SER
4	G	233	LEU
4	G	234	GLU
4	G	236	LEU
5	H	175	GLU
7	J	40	ARG
7	J	71	ARG
7	J	244	LYS
8	K	43	ARG
8	K	49[A]	VAL
8	K	49[B]	VAL
8	K	100	ASN
4	L	101	ARG
4	L	230	SER
4	L	233	LEU
4	L	234	GLU
4	L	236	LEU
5	M	118	ASN
5	M	119	LEU
5	M	121	LEU
6	N	201	SER
6	N	205	ASN
9	O	7[A]	SER
9	O	7[B]	SER
7	Q	40	ARG
7	Q	71	ARG
8	R	43	ARG
8	R	100	ASN
8	R	137	CYS
8	R	191	PHE
11	S	151	ASN
12	T	24	ASN
12	T	85	ARG
12	T	174	ASN
12	V	1[A]	MET
12	V	1[B]	MET

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Mol	Chain	Res	Type
12	V	27[A]	GLN
12	V	27[B]	GLN
12	V	85	ARG
12	V	174	ASN
11	X	3[A]	SER
11	X	3[B]	SER
11	X	151	ASN
13	Y	13[A]	MET
13	Y	13[B]	MET
13	Y	16	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	38	HIS
1	A	81	ASN
2	B	9	GLN
2	B	114	HIS
2	B	145	ASN
2	B	152	GLN
2	B	203	HIS
3	C	38	ASN
3	D	38	ASN
2	E	9	GLN
2	E	66	HIS
2	E	114	HIS
2	E	145	ASN
2	E	152	GLN
1	F	28	ASN
1	F	38	HIS
1	F	81	ASN
4	G	65	HIS
5	H	99	HIS
5	H	155	HIS
5	H	221	GLN
7	J	97	ASN
7	J	110	HIS
8	K	100	ASN
5	M	98	ASN
5	M	99	HIS
5	M	155	HIS

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Mol	Chain	Res	Type
5	M	221	GLN
9	O	40	ASN
9	O	109	GLN
9	O	198	ASN
9	O	240	HIS
10	P	101	GLN
10	P	108	GLN
10	P	139	ASN
7	Q	97	ASN
7	Q	110	HIS
7	Q	143	ASN
8	R	53	GLN
8	R	100	ASN
8	R	128	ASN
11	S	108	ASN
11	S	131	GLN
11	S	157	ASN
11	S	163	HIS
12	T	8	GLN
12	T	55	GLN
12	T	63	ASN
12	T	132	HIS
12	T	174	ASN
13	U	92	ASN
12	V	8	GLN
12	V	63	ASN
12	V	132	HIS
12	V	174	ASN
14	W	69	GLN
14	W	89	HIS
14	W	162	GLN
14	W	213	HIS
11	X	108	ASN
11	X	131	GLN
11	X	151	ASN
11	X	163	HIS
13	Y	32	GLN
13	Y	92	ASN
13	Y	168	GLN
9	Z	40	ASN
9	Z	109	GLN
9	Z	198	ASN

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Mol	Chain	Res	Type
9	Z	240	HIS
14	a	81	HIS
14	a	89	HIS
14	a	213	HIS
10	b	101	GLN
10	b	108	GLN
10	b	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	BZ7	C	301	-	42,42,42	2.71	14 (33%)	56,56,56	1.22	3 (5%)
15	BZ7	D	301	-	42,42,42	2.72	14 (33%)	56,56,56	1.22	3 (5%)

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	BZ7	C	301	-	-	16/37/37/37	0/3/3/3
15	BZ7	D	301	-	-	16/37/37/37	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	BZ7	CAE-CAD	6.75	1.53	1.38
15	D	301	BZ7	CAE-CAD	6.74	1.53	1.38
15	D	301	BZ7	CAB-CAC	6.66	1.53	1.38
15	D	301	BZ7	CG-ND2	6.64	1.45	1.34
15	C	301	BZ7	CAB-CAC	6.64	1.53	1.38
15	C	301	BZ7	CG-ND2	6.62	1.45	1.34
15	D	301	BZ7	CAF-CAA	5.72	1.53	1.38
15	C	301	BZ7	CAF-CAA	5.70	1.53	1.38
15	D	301	BZ7	C-NAN	5.49	1.45	1.33
15	D	301	BZ7	CAI-N	5.47	1.45	1.34
15	C	301	BZ7	C-NAN	5.46	1.45	1.33
15	C	301	BZ7	CAI-N	5.45	1.45	1.34
15	D	301	BZ7	CBA-NAZ	5.34	1.45	1.33
15	C	301	BZ7	CBA-NAZ	5.34	1.45	1.33
15	D	301	BZ7	CAA-CAB	-3.24	1.32	1.38
15	C	301	BZ7	CAA-CAB	-3.22	1.32	1.38
15	C	301	BZ7	CAD-CAC	-3.11	1.32	1.38
15	D	301	BZ7	CAD-CAC	-3.11	1.32	1.38
15	D	301	BZ7	CAF-CAE	-2.25	1.32	1.38
15	D	301	BZ7	O-C	-2.24	1.18	1.23
15	C	301	BZ7	O-C	-2.23	1.19	1.23
15	C	301	BZ7	CAF-CAE	-2.21	1.32	1.38
15	D	301	BZ7	OB-BA	-2.16	1.18	1.23
15	C	301	BZ7	OD1-CG	-2.15	1.18	1.23
15	C	301	BZ7	OAK-CAI	-2.15	1.18	1.23
15	C	301	BZ7	OB-BA	-2.14	1.18	1.23
15	D	301	BZ7	OAK-CAI	-2.14	1.18	1.23
15	D	301	BZ7	OD1-CG	-2.11	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	301	BZ7	CAS-ND2-CG	-5.59	119.97	126.32
15	C	301	BZ7	CAS-ND2-CG	-5.59	119.97	126.32
15	D	301	BZ7	CB-CG-ND2	3.24	120.01	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	301	BZ7	CB-CG-ND2	3.20	119.96	116.00
15	C	301	BZ7	CAH-CAI-N	2.41	120.01	115.83
15	D	301	BZ7	CAH-CAI-N	2.39	119.97	115.83

There are no chirality outliers.

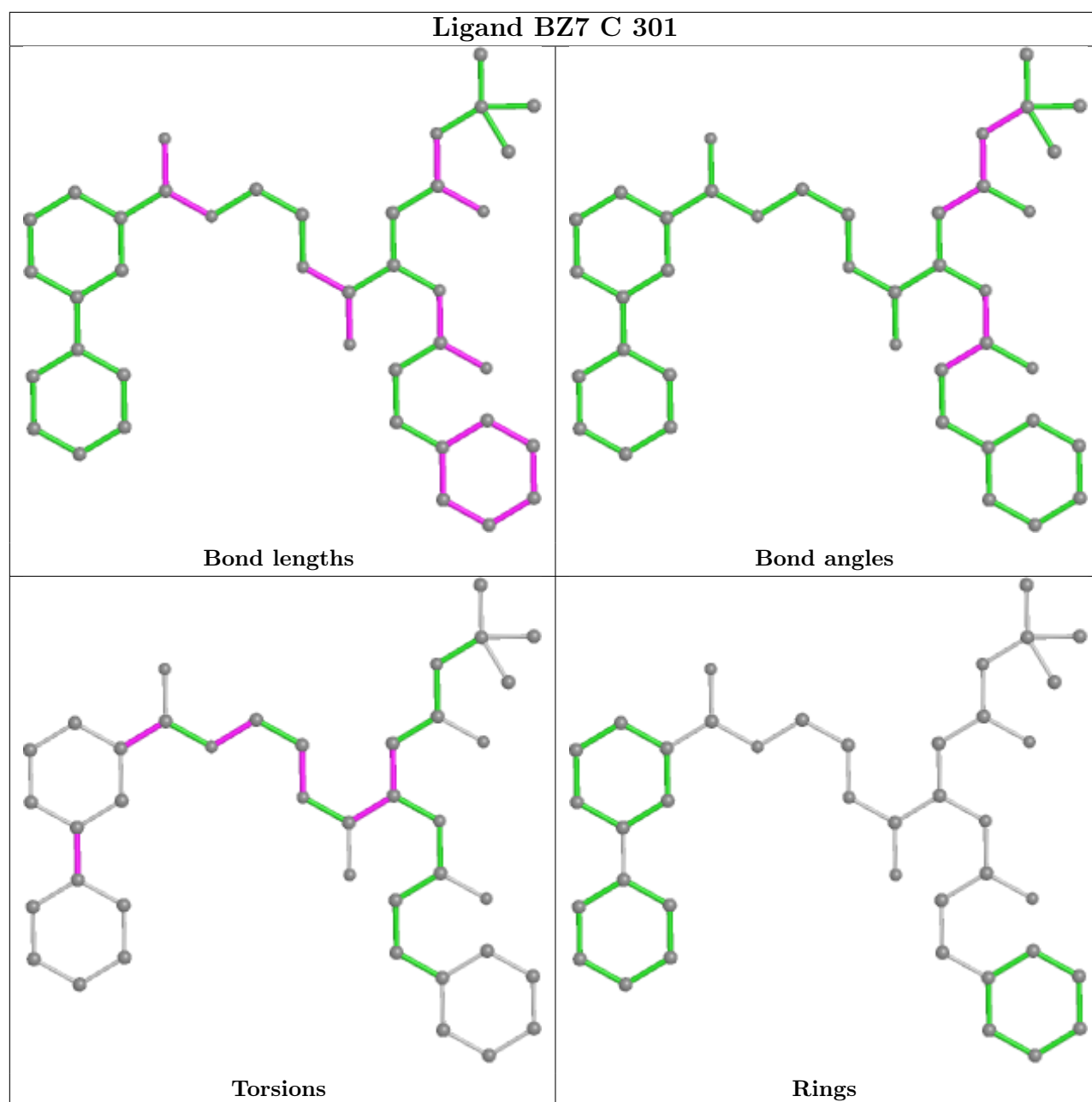
All (32) torsion outliers are listed below:

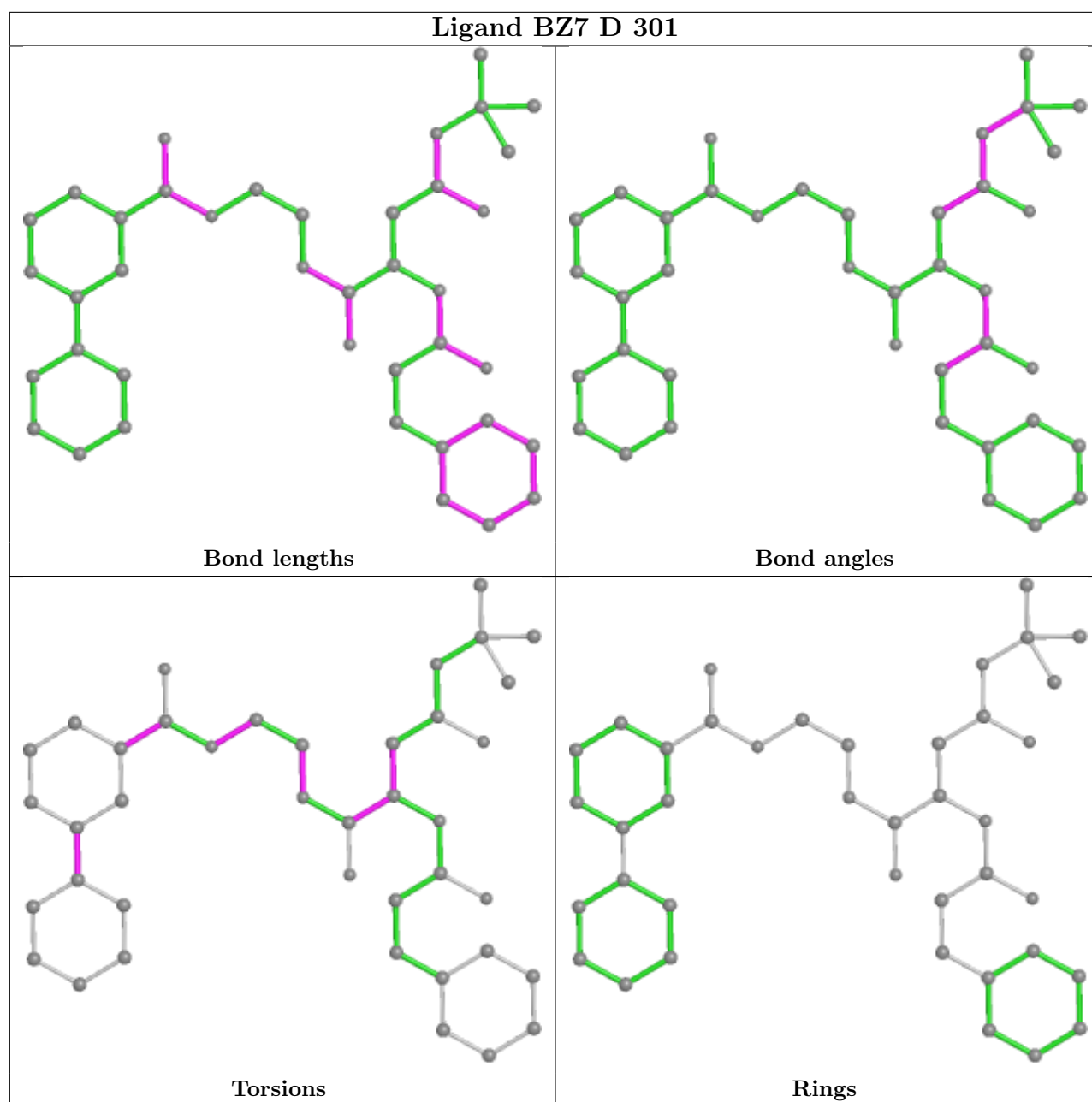
Mol	Chain	Res	Type	Atoms
15	C	301	BZ7	CBF-CBG-CBI-CBJ
15	C	301	BZ7	CBF-CBG-CBI-CBN
15	C	301	BZ7	CBH-CBG-CBI-CBJ
15	C	301	BZ7	CBH-CBG-CBI-CBN
15	D	301	BZ7	CBF-CBG-CBI-CBJ
15	D	301	BZ7	CBF-CBG-CBI-CBN
15	D	301	BZ7	CBH-CBG-CBI-CBJ
15	D	301	BZ7	CBH-CBG-CBI-CBN
15	D	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	NAZ-CBA-CBC-CBD
15	C	301	BZ7	OBB-CBA-CBC-CBD
15	D	301	BZ7	NAZ-CBA-CBC-CBD
15	D	301	BZ7	OBB-CBA-CBC-CBD
15	C	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	CAX-CAY-NAZ-CBA
15	D	301	BZ7	CAX-CAY-NAZ-CBA
15	C	301	BZ7	N-CA-CB-CG
15	D	301	BZ7	N-CA-CB-CG
15	C	301	BZ7	C-CA-CB-CG
15	D	301	BZ7	C-CA-CB-CG
15	D	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-CB
15	C	301	BZ7	O-C-CA-CB
15	D	301	BZ7	NAN-C-CA-CB
15	C	301	BZ7	NAN-C-CA-CB

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.

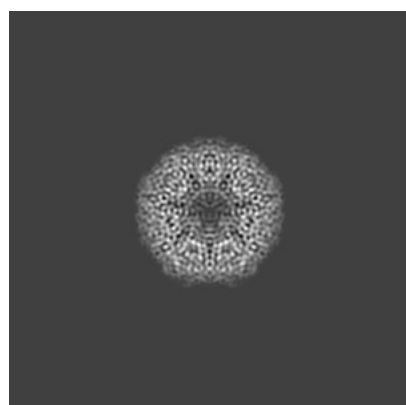
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7010. These allow visual inspection of the internal detail of the map and identification of artifacts.

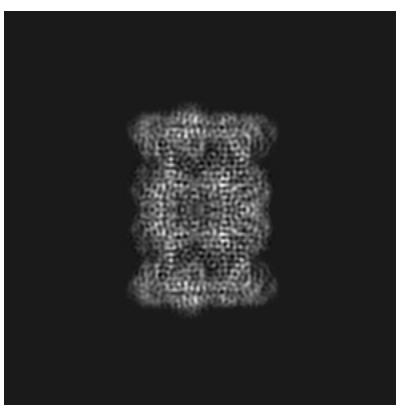
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

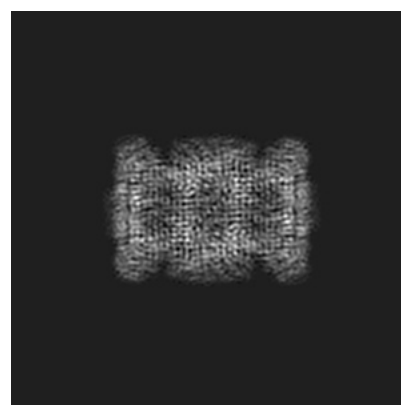
6.1.1 Primary map



X



Y

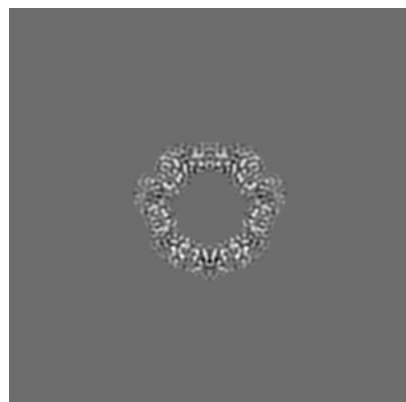


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

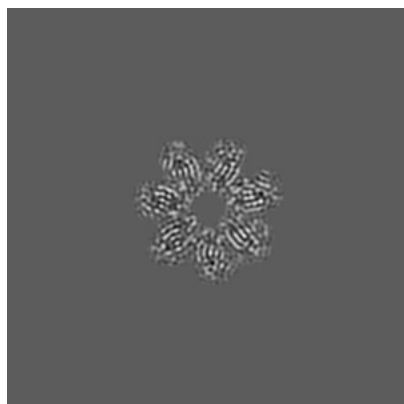


Z Index: 128

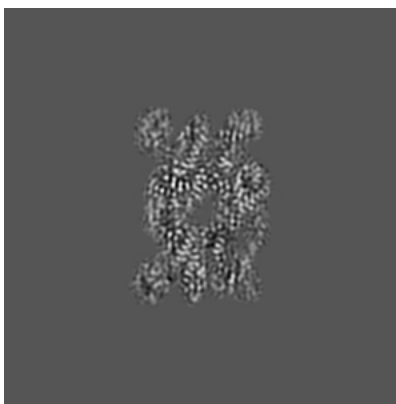
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 106

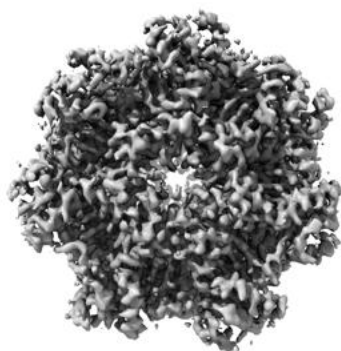


Z Index: 105

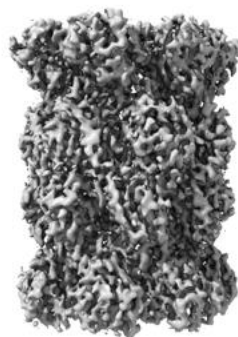
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

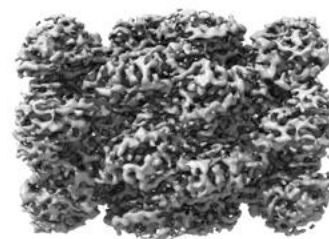
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0383. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

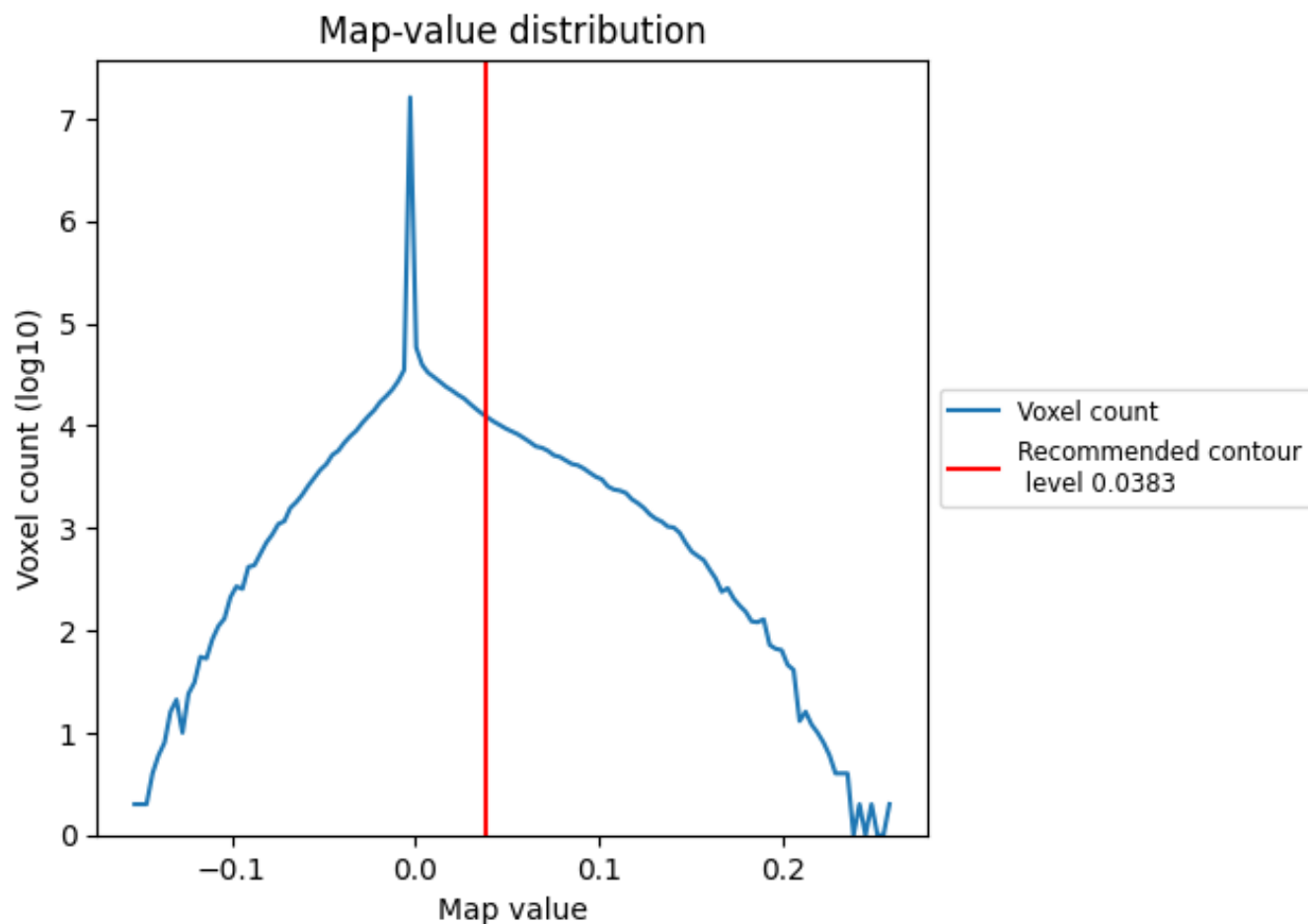
6.5 Mask visualisation

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

7 Map analysis [i](#)

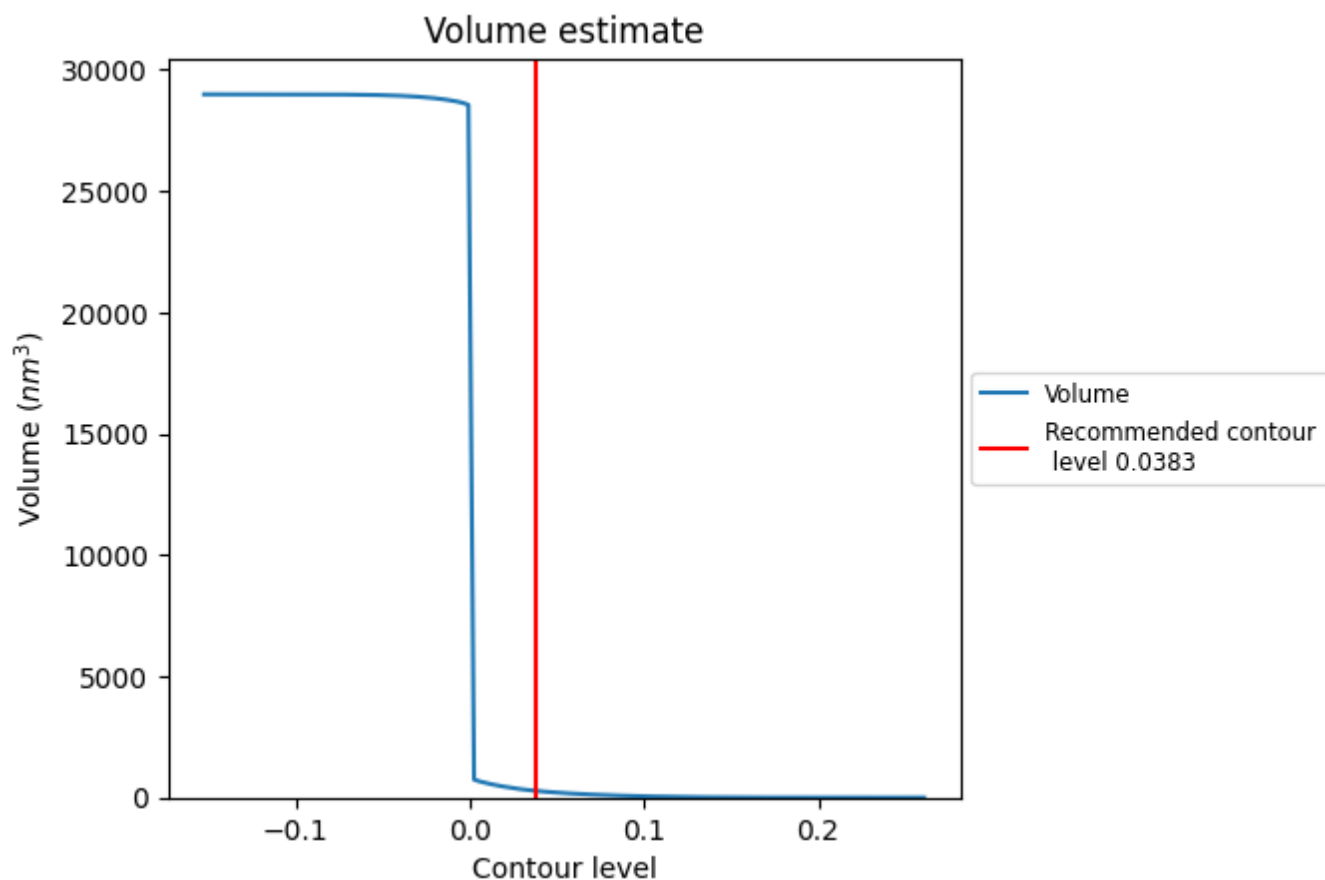
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

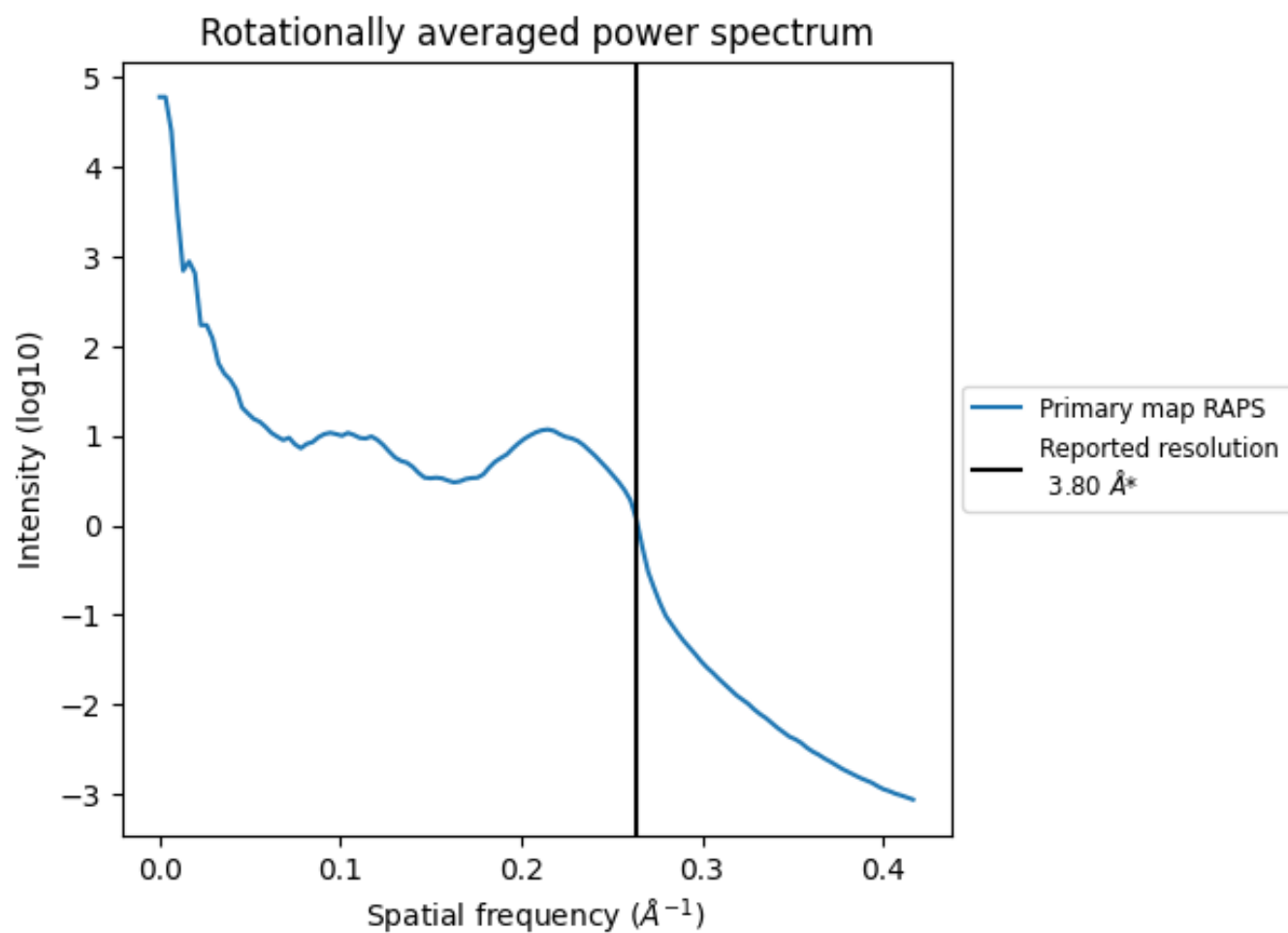
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 247 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

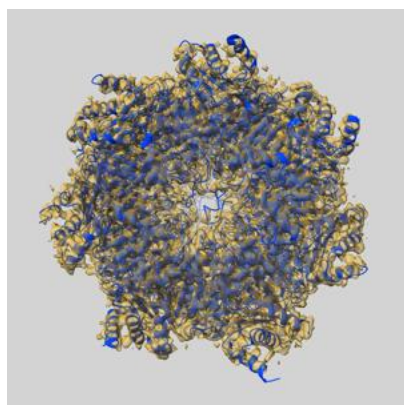
8 Fourier-Shell correlation

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

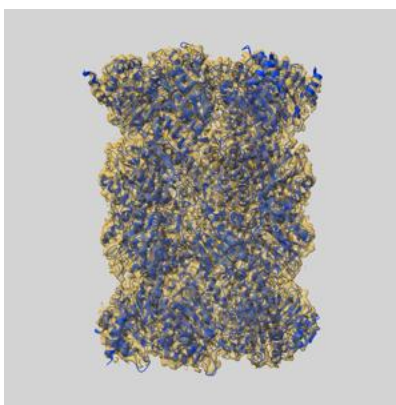
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7010 and PDB model 6AVO. Per-residue inclusion information can be found in section 3 on page 8.

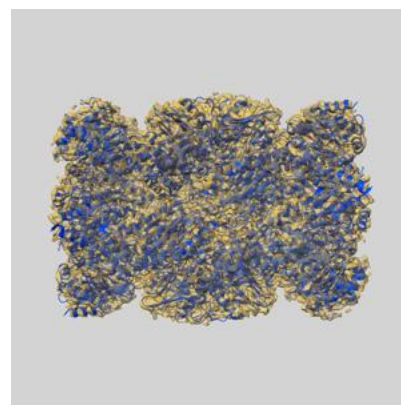
9.1 Map-model overlay [i](#)



X



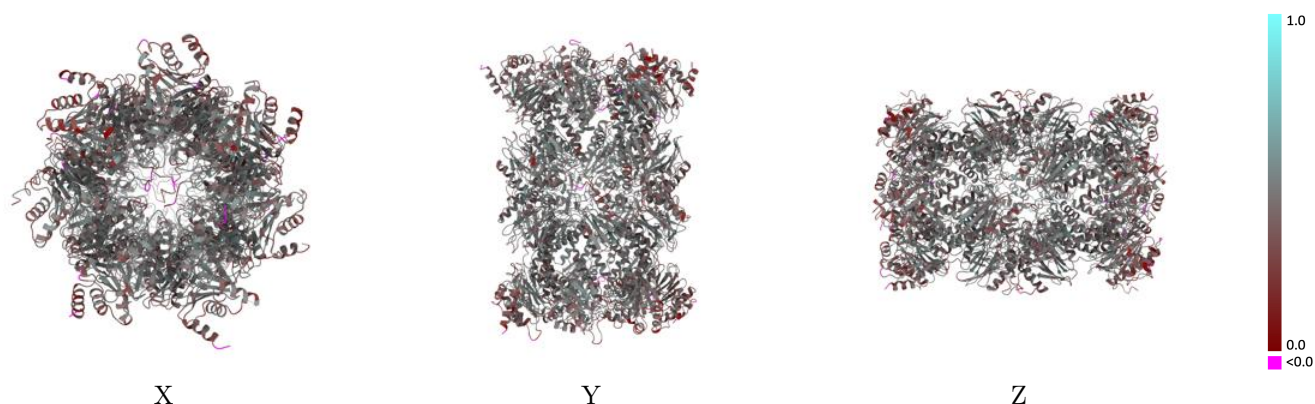
Y



Z

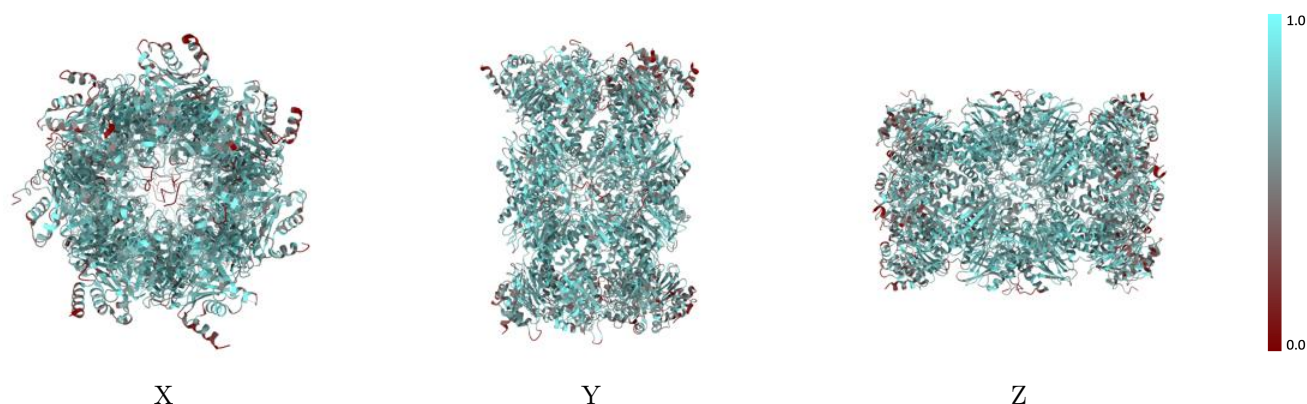
The images above show the 3D surface view of the map at the recommended contour level 0.0383 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



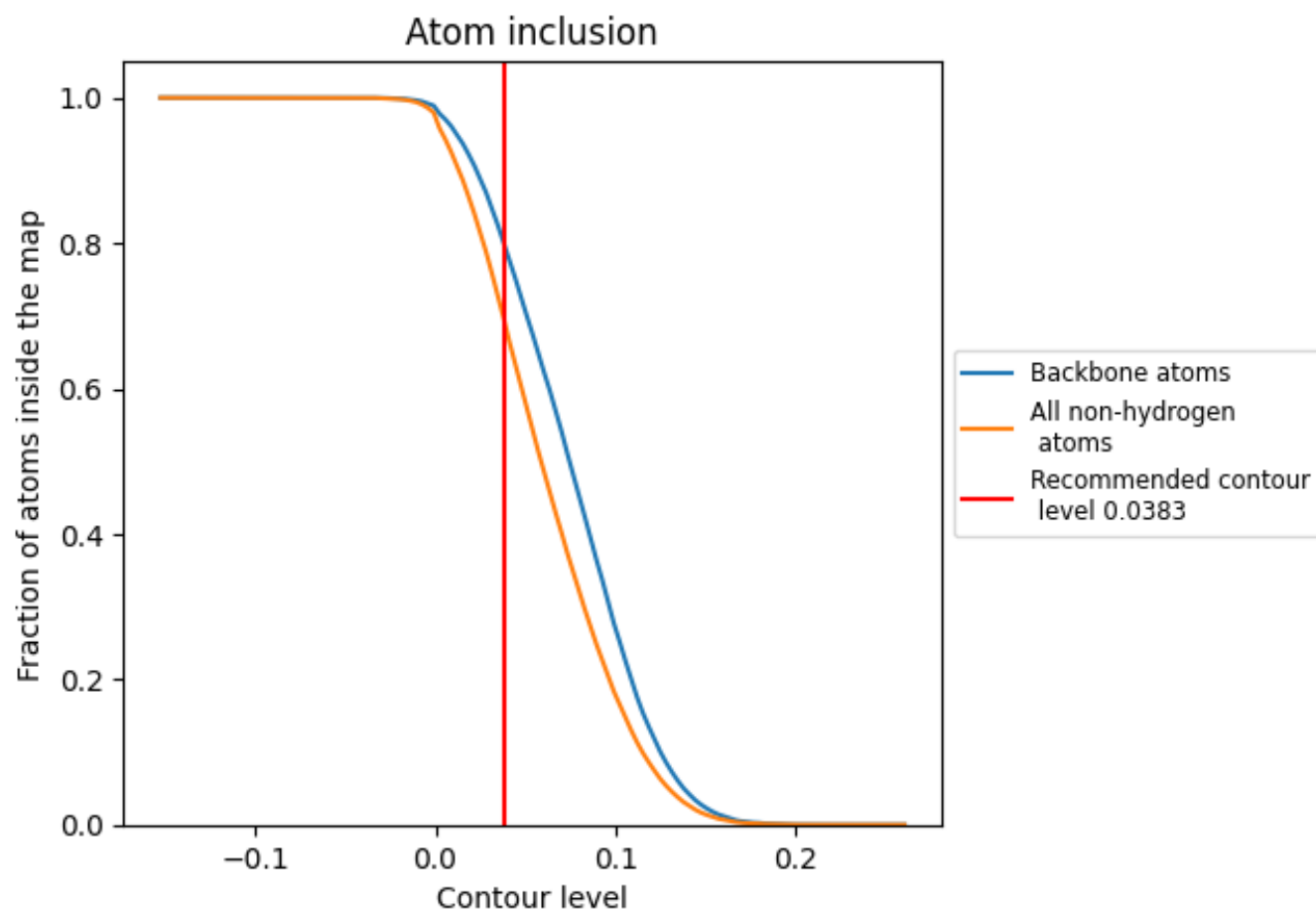
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0383).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.0383) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6936	 0.4320
A	 0.7411	 0.4580
B	 0.7108	 0.4360
C	 0.7815	 0.4510
D	 0.7667	 0.4470
E	 0.7025	 0.4390
F	 0.7425	 0.4620
G	 0.6808	 0.4290
H	 0.5671	 0.3760
I	 0.6378	 0.4060
J	 0.6767	 0.4190
K	 0.6812	 0.4260
L	 0.6804	 0.4280
M	 0.5699	 0.3790
N	 0.6327	 0.4050
O	 0.6119	 0.4020
P	 0.6975	 0.4290
Q	 0.6766	 0.4190
R	 0.6957	 0.4290
S	 0.7252	 0.4570
T	 0.7247	 0.4380
U	 0.7598	 0.4650
V	 0.7262	 0.4410
W	 0.7605	 0.4620
X	 0.7265	 0.4590
Y	 0.7452	 0.4630
Z	 0.6114	 0.3960
a	 0.7655	 0.4620
b	 0.6980	 0.4300

