



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 10:42 AM UTC

PDB ID : 6QM7 / pdb_00006qm7
EMDB ID : EMD-4590
Title : Leishmania tarentolae proteasome 20S subunit complexed with GSK3494245
Authors : Rowland, P.; Goswami, P.
Deposited on : 2019-02-01
Resolution : 2.80 Å(reported)
Based on initial model : 4R3O

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

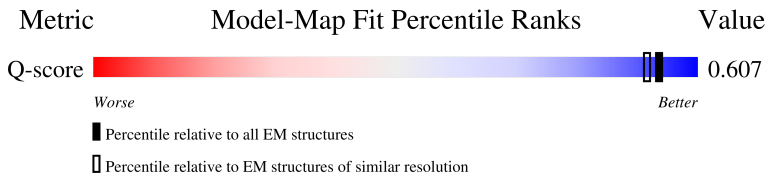
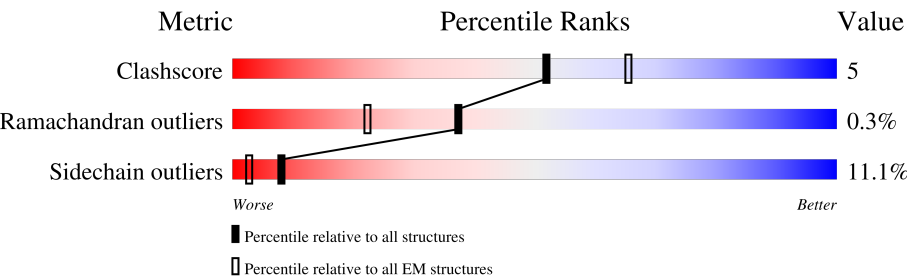
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.



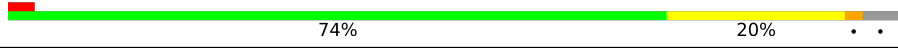
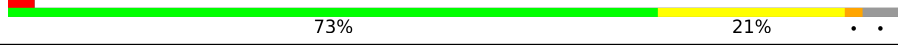
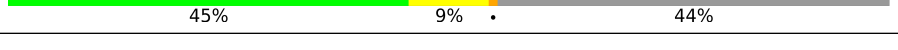
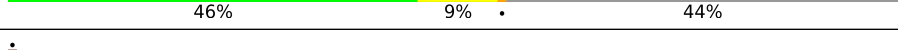
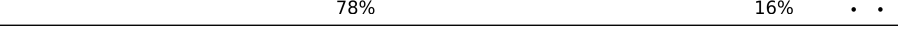
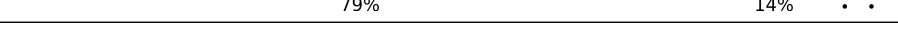
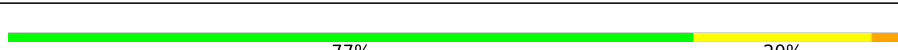
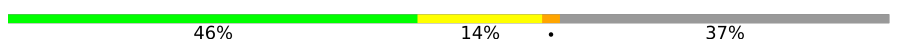
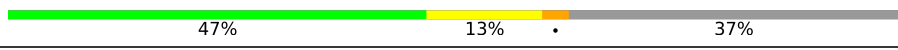
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	250	81%15%..
1	O	250	80%17%..
2	B	231	81%16%..
2	P	231	82%16%..

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Mol	Chain	Length	Quality of chain
3	C	285	
3	Q	285	
4	D	248	
4	R	248	
5	E	344	
5	S	344	
6	F	428	
6	T	428	
7	G	238	
7	U	238	
8	H	283	
8	V	283	
9	I	254	
9	W	254	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	302	
12	Z	302	
13	M	339	
13	a	339	
14	N	220	
14	b	220	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49518 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 alpha1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		
1	O	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		

- Molecule 2 is a protein called Proteasome alpha2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		
2	P	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		

- Molecule 3 is a protein called Proteasome alpha3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		
3	Q	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		

- Molecule 4 is a protein called Proteasome alpha4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		
4	R	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		

- Molecule 5 is a protein called Proteasome alpha5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		
5	S	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		

- Molecule 6 is a protein called Proteasome alpha6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		
6	T	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		

- Molecule 7 is a protein called Proteasome alpha7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		
7	U	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		

- Molecule 8 is a protein called Proteasome beta1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		
8	V	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		

- Molecule 9 is a protein called Proteasome beta2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	W	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- Molecule 10 is a protein called Proteasome beta3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome beta4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	Y	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- Molecule 12 is a protein called Proteasome beta5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total	C	N	O	S	0	0
			1579	998	277	297	7		
12	Z	202	Total	C	N	O	S	0	0
			1579	998	277	297	7		

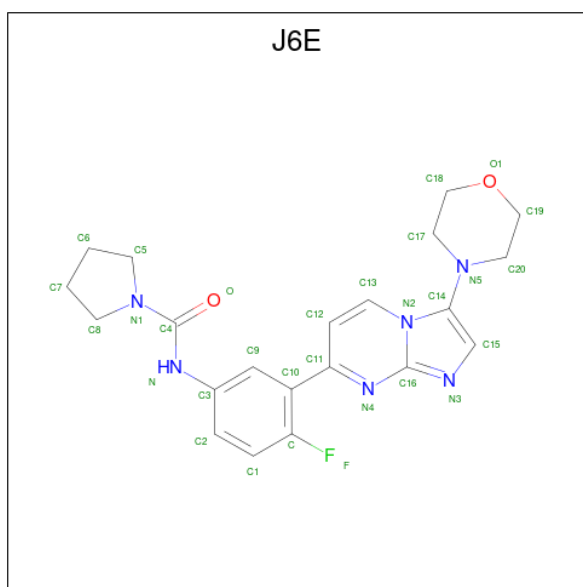
- Molecule 13 is a protein called Proteasome beta6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	a	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

- Molecule 14 is a protein called Proteasome beta7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		
14	b	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		

- Molecule 15 is {N}-[4-fluoranyl-3-(3-morpholin-4-ylimidazo[1,2-a]pyrimidin-7-yl)phenyl]pyrrolidine-1-carboxamide (CCD ID: J6E) (formula: C₂₁H₂₃FN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			30	21	1	6	2	
15	Z	1	Total	C	F	N	O	0
			30	21	1	6	2	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	A	9	Total	O	0
			9	9	
16	B	9	Total	O	0
			9	9	
16	C	8	Total	O	0
			8	8	
16	D	6	Total	O	0
			6	6	
16	E	8	Total	O	0
			8	8	
16	F	8	Total	O	0
			8	8	
16	G	12	Total	O	0
			12	12	
16	H	21	Total	O	0
			21	21	
16	I	7	Total	O	0
			7	7	
16	J	15	Total	O	0
			15	15	

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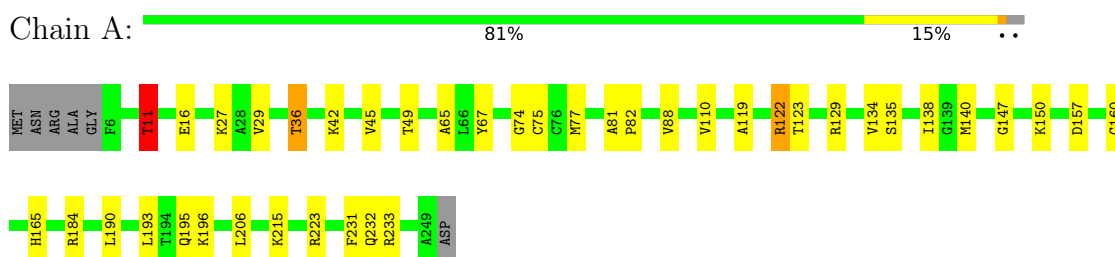
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Mol	Chain	Residues	Atoms		AltConf
16	K	9	Total 9	O 9	0
16	L	15	Total 15	O 15	0
16	M	13	Total 13	O 13	0
16	N	21	Total 21	O 21	0
16	O	11	Total 11	O 11	0
16	P	13	Total 13	O 13	0
16	Q	8	Total 8	O 8	0
16	R	9	Total 9	O 9	0
16	S	6	Total 6	O 6	0
16	T	8	Total 8	O 8	0
16	U	5	Total 5	O 5	0
16	V	19	Total 19	O 19	0
16	W	15	Total 15	O 15	0
16	X	23	Total 23	O 23	0
16	Y	8	Total 8	O 8	0
16	Z	17	Total 17	O 17	0
16	a	11	Total 11	O 11	0
16	b	20	Total 20	O 20	0

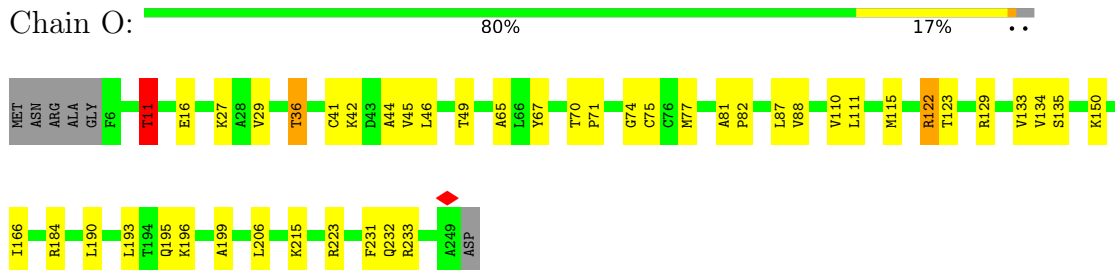
3 Residue-property plots [i](#)

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.

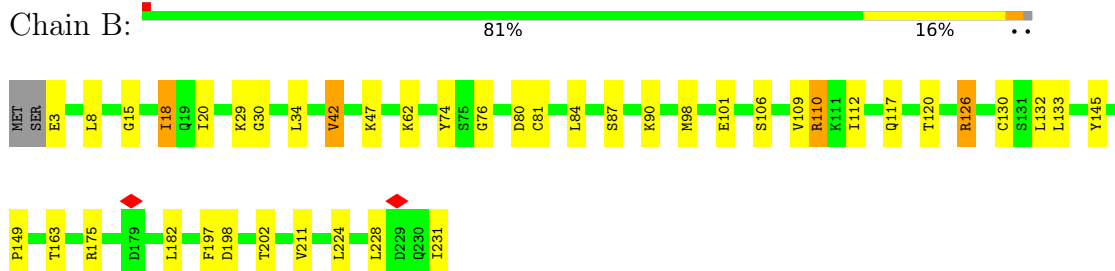
- Molecule 1: Proteasome alpha1 chain



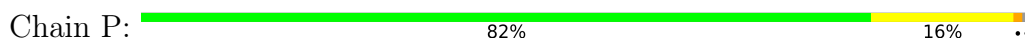
- Molecule 1: Proteasome alpha1 chain



- Molecule 2: Proteasome alpha2 chain

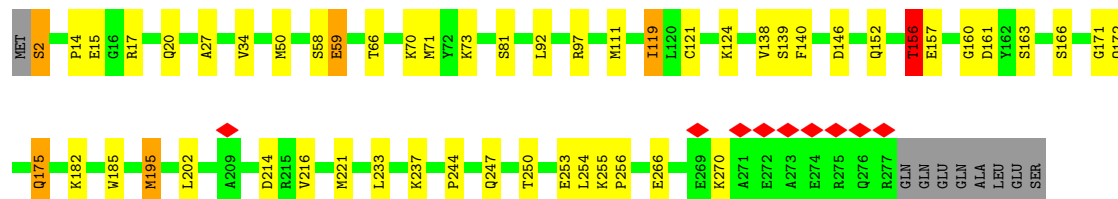
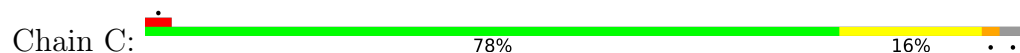


- Molecule 2: Proteasome alpha2 chain

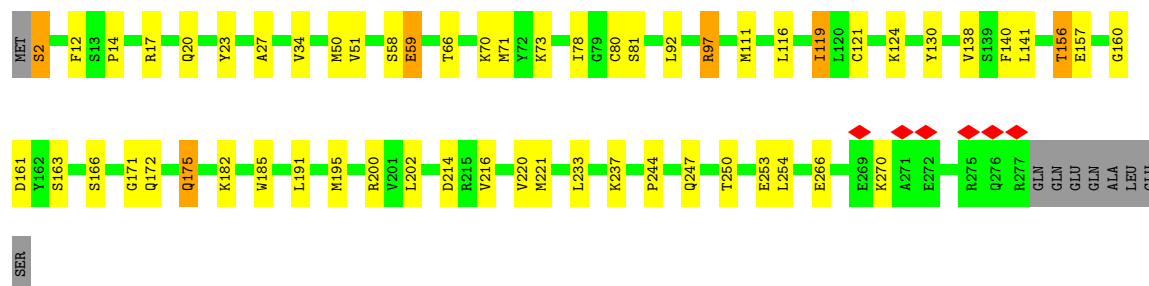
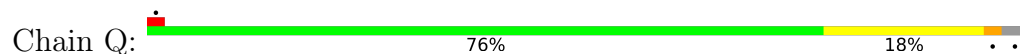




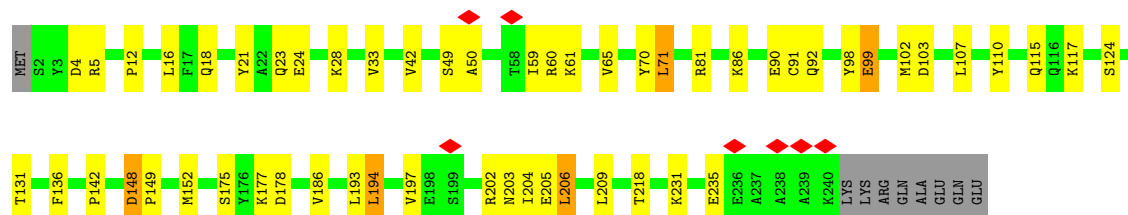
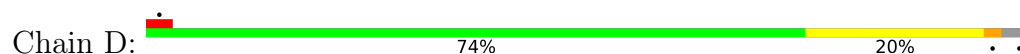
• Molecule 3: Proteasome alpha3 chain



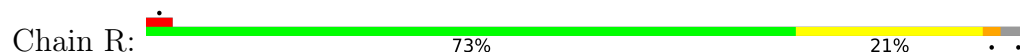
• Molecule 3: Proteasome alpha3 chain



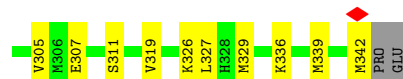
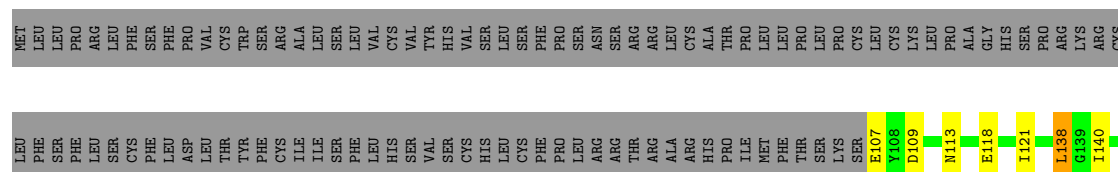
• Molecule 4: Proteasome alpha4 chain



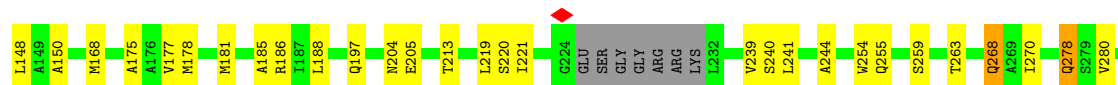
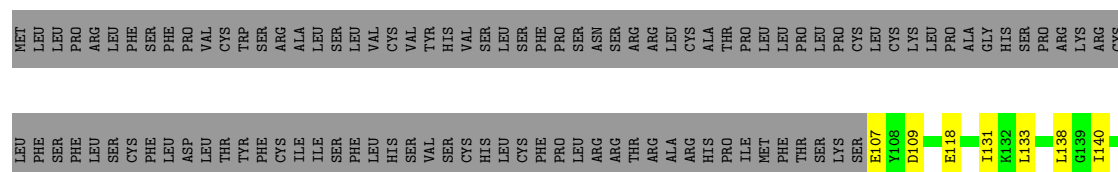
• Molecule 4: Proteasome alpha4 chain



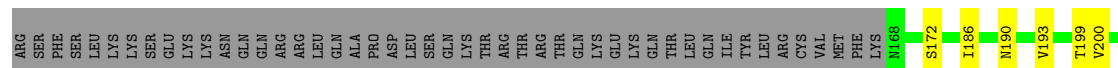
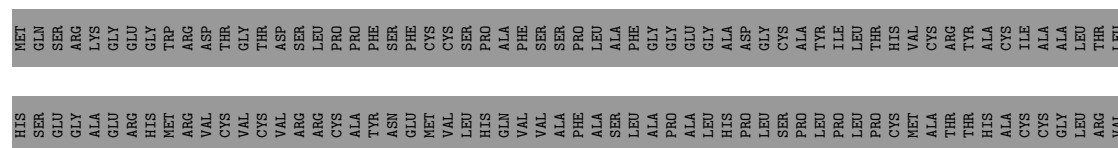
- Molecule 5: Proteasome alpha5 chain

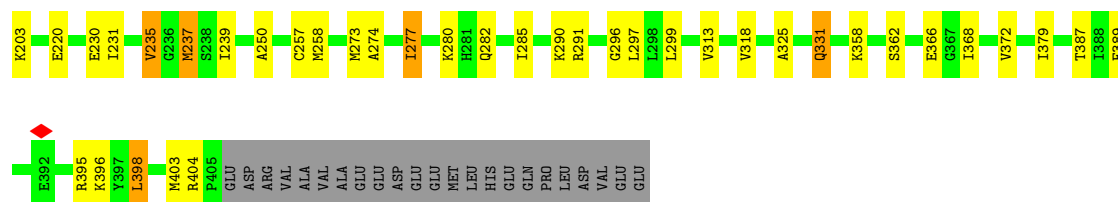


- Molecule 5: Proteasome alpha5 chain



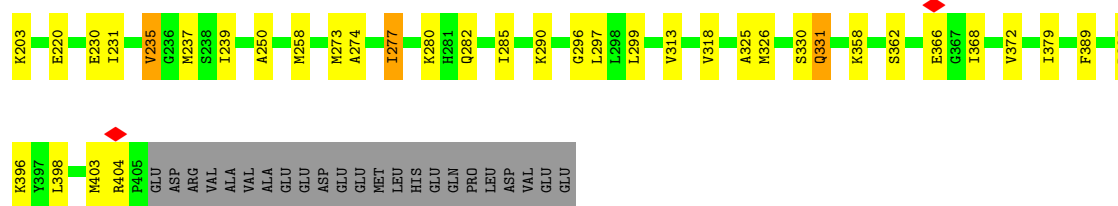
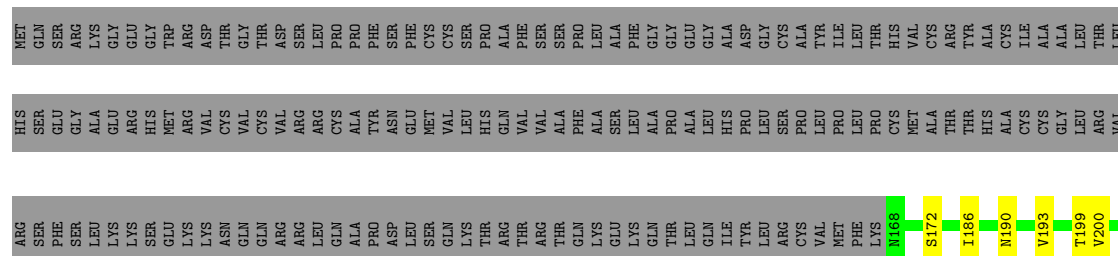
- Molecule 6: Proteasome alpha6 chain





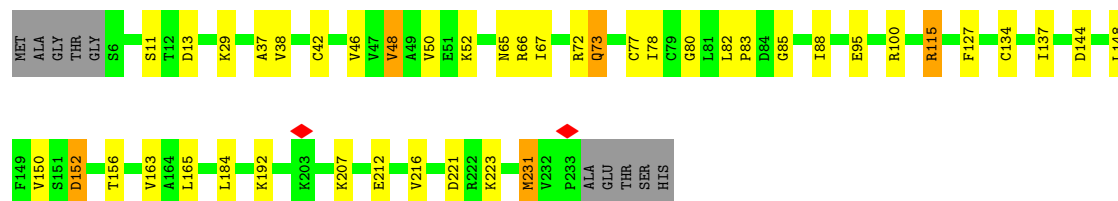
• Molecule 6: Proteasome alpha6 chain

Chain T: 46% 9% 44%



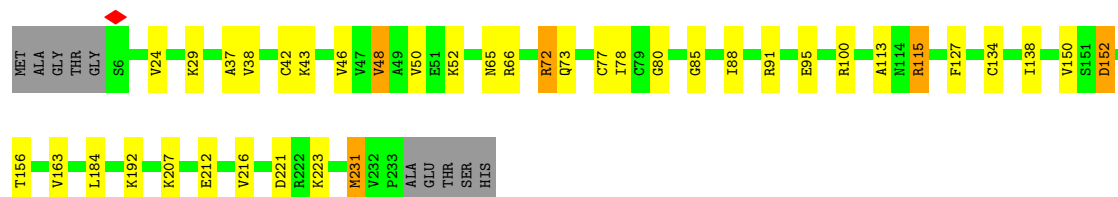
• Molecule 7: Proteasome alpha7 chain

Chain G: 78% 16% 6%



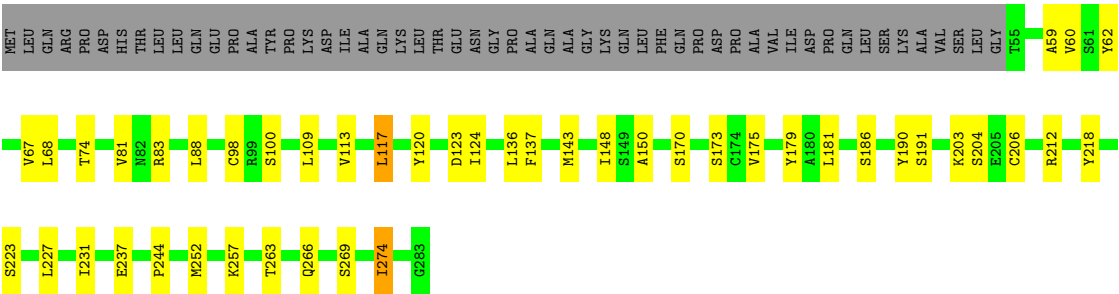
• Molecule 7: Proteasome alpha7 chain

Chain U: 79% 14% 7%



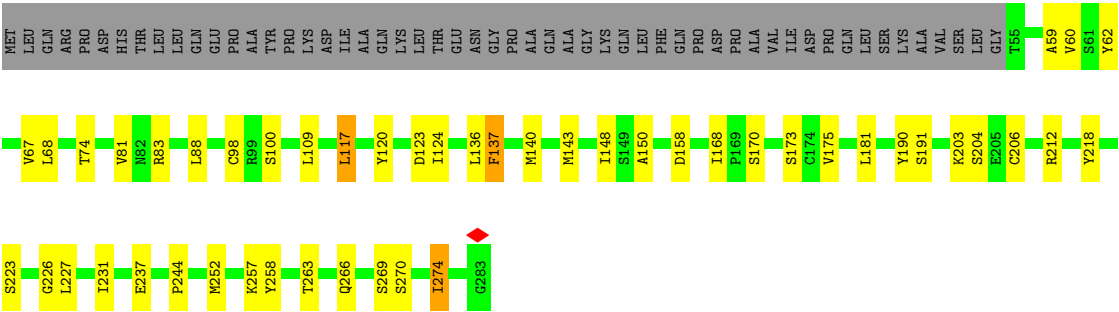
• Molecule 8: Proteasome beta1 chain

Chain H: 65% 16% 19%



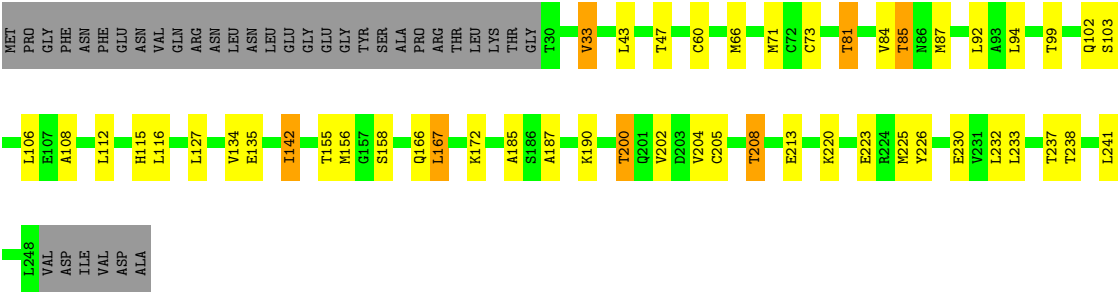
• Molecule 8: Proteasome beta1 chain

Chain V: 64% 16% 19%



• Molecule 9: Proteasome beta2 chain

Chain I: 67% 17% 14%



• Molecule 9: Proteasome beta2 chain

Chain W: 67% 17% 14%



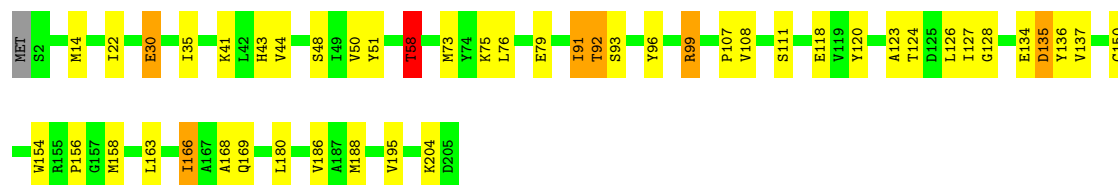
• Molecule 10: Proteasome beta3 chain

Chain J:  79% 17% .



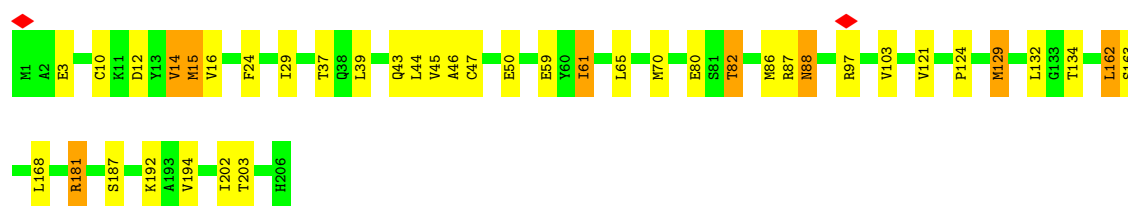
- Molecule 10: Proteasome beta3 chain

Chain X:  77% 20% .



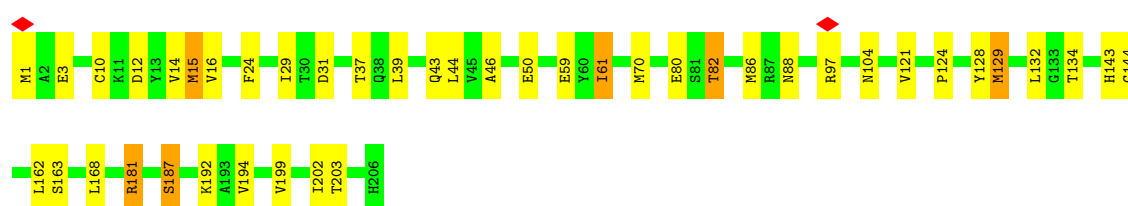
- Molecule 11: Proteasome beta4 chain

Chain K:  80% 16% .



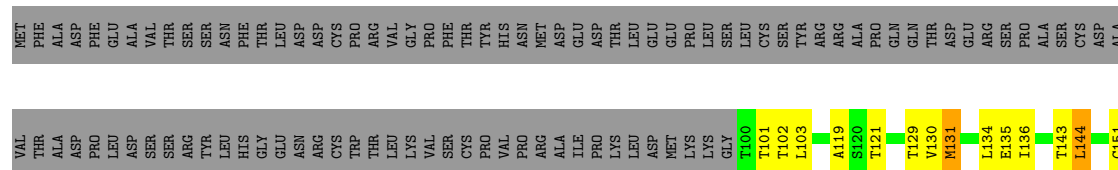
- Molecule 11: Proteasome beta4 chain

Chain Y:  79% 18% .



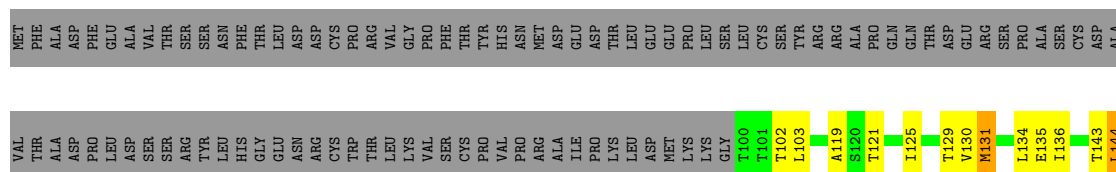
- Molecule 12: Proteasome beta5 chain

Chain L:  56% 10% 33%

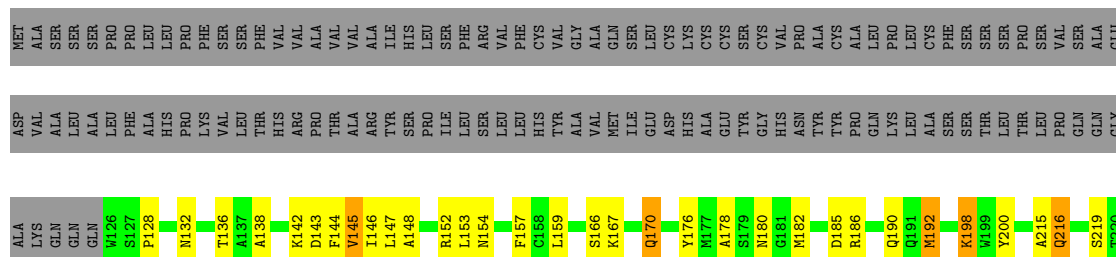




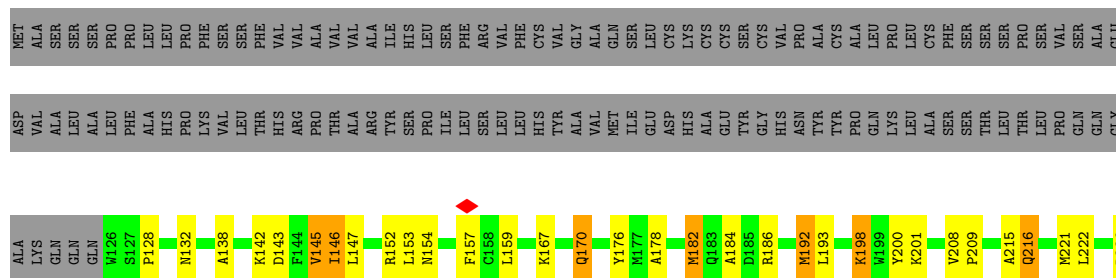
• Molecule 12: Proteasome beta5 chain



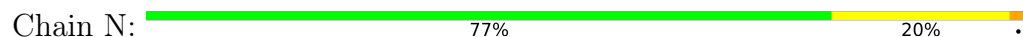
• Molecule 13: Proteasome beta6 chain

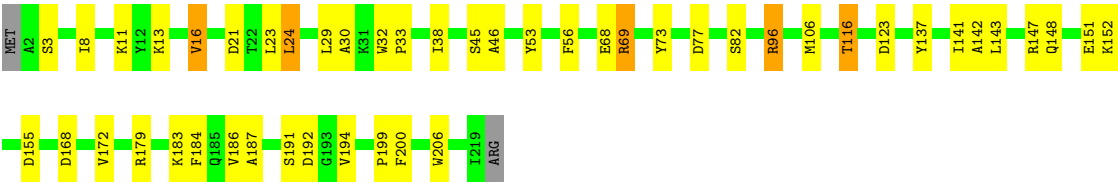


• Molecule 13: Proteasome beta6 chain

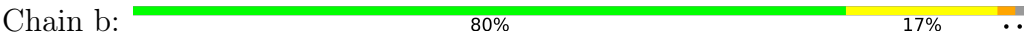


• Molecule 14: Proteasome beta7 chain





● Molecule 14: Proteasome beta7 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182775	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.622	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0667	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: J6E

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	0.94	0/1889	1.56	2/2562 (0.1%)
1	O	0.94	0/1889	1.54	2/2562 (0.1%)
2	B	0.92	0/1787	1.49	0/2421
2	P	0.91	0/1787	1.48	0/2421
3	C	0.94	0/2242	1.51	1/3034 (0.0%)
3	Q	0.94	0/2242	1.49	1/3034 (0.0%)
4	D	0.97	0/1902	1.57	2/2562 (0.1%)
4	R	0.94	0/1902	1.57	0/2562
5	E	0.97	0/1784	1.56	2/2414 (0.1%)
5	S	0.96	0/1784	1.57	4/2414 (0.2%)
6	F	0.94	0/1907	1.44	0/2575
6	T	0.94	0/1907	1.44	0/2575
7	G	0.94	0/1759	1.51	3/2379 (0.1%)
7	U	0.93	0/1759	1.49	2/2379 (0.1%)
8	H	0.90	0/1742	1.46	1/2359 (0.0%)
8	V	0.91	0/1742	1.46	2/2359 (0.1%)
9	I	0.91	0/1685	1.48	1/2284 (0.0%)
9	W	0.92	0/1685	1.47	2/2284 (0.1%)
10	J	0.90	0/1583	1.48	2/2135 (0.1%)
10	X	0.92	0/1583	1.47	3/2135 (0.1%)
11	K	0.91	0/1643	1.49	1/2222 (0.0%)
11	Y	0.91	0/1643	1.48	0/2222
12	L	0.88	0/1613	1.44	0/2183
12	Z	0.88	0/1613	1.45	2/2183 (0.1%)
13	M	0.90	0/1743	1.48	1/2354 (0.0%)
13	a	0.89	0/1743	1.49	3/2354 (0.1%)
14	N	0.89	0/1748	1.48	3/2363 (0.1%)
14	b	0.89	0/1748	1.49	4/2363 (0.2%)
All	All	0.92	0/50054	1.50	44/67694 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	C	0	2
3	Q	0	3
10	J	0	1
10	X	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	138	LEU	CA-C-N	7.55	126.78	121.65
5	E	138	LEU	C-N-CA	7.55	126.78	121.65
13	M	232	THR	CB-CA-C	7.03	120.17	110.34
5	S	138	LEU	CA-C-N	6.60	126.73	122.18
5	S	138	LEU	C-N-CA	6.60	126.73	122.18

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	140	PHE	Peptide
3	C	171	GLY	Peptide
10	J	204	LYS	Peptide
2	P	132	LEU	Peptide
3	Q	130	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1857	0	1871	17	0
1	O	1857	0	1871	18	0
2	B	1754	0	1741	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1754	0	1741	14	0
3	C	2195	0	2142	22	0
3	Q	2195	0	2142	25	0
4	D	1873	0	1868	17	0
4	R	1873	0	1868	22	0
5	E	1756	0	1736	21	0
5	S	1756	0	1736	24	0
6	F	1869	0	1823	22	0
6	T	1869	0	1823	19	0
7	G	1727	0	1691	23	0
7	U	1727	0	1691	18	0
8	H	1710	0	1665	20	0
8	V	1710	0	1665	19	0
9	I	1659	0	1684	23	0
9	W	1659	0	1684	22	0
10	J	1557	0	1552	26	0
10	X	1557	0	1552	29	0
11	K	1612	0	1571	18	0
11	Y	1612	0	1571	22	0
12	L	1579	0	1538	16	0
12	Z	1579	0	1538	16	0
13	M	1702	0	1638	30	0
13	a	1702	0	1638	26	0
14	N	1712	0	1668	28	0
14	b	1712	0	1668	22	0
15	L	30	0	0	0	0
15	Z	30	0	0	0	0
16	A	9	0	0	1	0
16	B	9	0	0	0	0
16	C	8	0	0	0	0
16	D	6	0	0	0	0
16	E	8	0	0	0	0
16	F	8	0	0	0	0
16	G	12	0	0	0	0
16	H	21	0	0	1	0
16	I	7	0	0	0	0
16	J	15	0	0	0	0
16	K	9	0	0	0	0
16	L	15	0	0	0	0
16	M	13	0	0	0	0
16	N	21	0	0	0	0
16	O	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	13	0	0	0	0
16	Q	8	0	0	0	0
16	R	9	0	0	0	0
16	S	6	0	0	0	0
16	T	8	0	0	0	0
16	U	5	0	0	0	0
16	V	19	0	0	0	0
16	W	15	0	0	1	0
16	X	23	0	0	0	0
16	Y	8	0	0	0	0
16	Z	17	0	0	0	0
16	a	11	0	0	0	0
16	b	20	0	0	1	0
All	All	49518	0	48376	525	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 5.

The worst 5 of 525 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:15:MET:HE1	11:Y:168:LEU:HD23	1.38	1.05
11:K:15:MET:HE1	11:K:168:LEU:HD23	1.36	1.02
4:D:91:CYS:SG	4:D:107:LEU:HD13	2.20	0.82
1:O:36:THR:HG22	1:O:49:THR:HG23	1.62	0.82
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.66	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/250 (97%)	233 (96%)	9 (4%)	0	100	100
1	O	242/250 (97%)	233 (96%)	9 (4%)	0	100	100
2	B	227/231 (98%)	216 (95%)	11 (5%)	0	100	100
2	P	227/231 (98%)	218 (96%)	9 (4%)	0	100	100
3	C	274/285 (96%)	266 (97%)	8 (3%)	0	100	100
3	Q	274/285 (96%)	265 (97%)	9 (3%)	0	100	100
4	D	237/248 (96%)	228 (96%)	7 (3%)	2 (1%)	16	44
4	R	237/248 (96%)	226 (95%)	9 (4%)	2 (1%)	16	44
5	E	225/344 (65%)	222 (99%)	3 (1%)	0	100	100
5	S	225/344 (65%)	221 (98%)	4 (2%)	0	100	100
6	F	236/428 (55%)	230 (98%)	5 (2%)	1 (0%)	30	60
6	T	236/428 (55%)	229 (97%)	6 (2%)	1 (0%)	30	60
7	G	226/238 (95%)	218 (96%)	8 (4%)	0	100	100
7	U	226/238 (95%)	219 (97%)	7 (3%)	0	100	100
8	H	227/283 (80%)	212 (93%)	14 (6%)	1 (0%)	30	60
8	V	227/283 (80%)	213 (94%)	13 (6%)	1 (0%)	30	60
9	I	217/254 (85%)	204 (94%)	10 (5%)	3 (1%)	9	30
9	W	217/254 (85%)	205 (94%)	9 (4%)	3 (1%)	9	30
10	J	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	24	55
10	X	202/205 (98%)	191 (95%)	10 (5%)	1 (0%)	24	55
11	K	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
11	Y	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
12	L	200/302 (66%)	188 (94%)	12 (6%)	0	100	100
12	Z	200/302 (66%)	188 (94%)	12 (6%)	0	100	100
13	M	212/339 (62%)	204 (96%)	5 (2%)	3 (1%)	9	30
13	a	212/339 (62%)	204 (96%)	5 (2%)	3 (1%)	9	30
14	N	216/220 (98%)	202 (94%)	14 (6%)	0	100	100
14	b	216/220 (98%)	204 (94%)	12 (6%)	0	100	100
All	All	6290/7666 (82%)	6020 (96%)	248 (4%)	22 (0%)	37	66

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	49	SER
4	R	49	SER
9	W	200	THR
9	I	200	THR
9	I	223	GLU

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	193/197 (98%)	174 (90%)	19 (10%)	7	25
1	O	193/197 (98%)	176 (91%)	17 (9%)	9	29
2	B	188/190 (99%)	163 (87%)	25 (13%)	4	14
2	P	188/190 (99%)	165 (88%)	23 (12%)	5	16
3	C	233/241 (97%)	204 (88%)	29 (12%)	4	16
3	Q	233/241 (97%)	203 (87%)	30 (13%)	4	14
4	D	200/208 (96%)	168 (84%)	32 (16%)	2	9
4	R	200/208 (96%)	169 (84%)	31 (16%)	2	9
5	E	193/301 (64%)	175 (91%)	18 (9%)	8	27
5	S	193/301 (64%)	175 (91%)	18 (9%)	8	27
6	F	200/363 (55%)	179 (90%)	21 (10%)	6	22
6	T	200/363 (55%)	181 (90%)	19 (10%)	8	26
7	G	184/190 (97%)	170 (92%)	14 (8%)	12	36
7	U	184/190 (97%)	167 (91%)	17 (9%)	8	27
8	H	184/229 (80%)	165 (90%)	19 (10%)	7	23
8	V	184/229 (80%)	163 (89%)	21 (11%)	5	19
9	I	180/209 (86%)	157 (87%)	23 (13%)	4	15
9	W	180/209 (86%)	157 (87%)	23 (13%)	4	15
10	J	167/168 (99%)	152 (91%)	15 (9%)	9	28
10	X	167/168 (99%)	151 (90%)	16 (10%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	172/172 (100%)	149 (87%)	23 (13%)	4	13
11	Y	172/172 (100%)	152 (88%)	20 (12%)	5	18
12	L	163/253 (64%)	151 (93%)	12 (7%)	13	37
12	Z	163/253 (64%)	150 (92%)	13 (8%)	11	34
13	M	181/288 (63%)	157 (87%)	24 (13%)	4	14
13	a	181/288 (63%)	156 (86%)	25 (14%)	3	12
14	N	181/183 (99%)	163 (90%)	18 (10%)	7	24
14	b	181/183 (99%)	163 (90%)	18 (10%)	7	24
All	All	5238/6384 (82%)	4655 (89%)	583 (11%)	8	20

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	218	TYR
14	b	82	SER
9	W	106	LEU
8	V	212	ARG
11	Y	163	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	236	ASN
14	b	75	ASN
4	R	23	GLN
14	b	44	HIS
12	Z	152	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	J6E	L	4000	-	34,34,34	0.39	0	44,48,48	0.79	2 (4%)
15	J6E	Z	4000	-	34,34,34	0.36	0	44,48,48	0.73	0

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	J6E	L	4000	-	-	3/14/31/31	0/5/5/5
15	J6E	Z	4000	-	-	4/14/31/31	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	4000	J6E	C15-N3-C16	2.32	106.16	104.91
15	L	4000	J6E	C17-N5-C14	-2.09	110.27	116.95

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	4000	J6E	C-C10-C11-C12
15	Z	4000	J6E	C-C10-C11-C12

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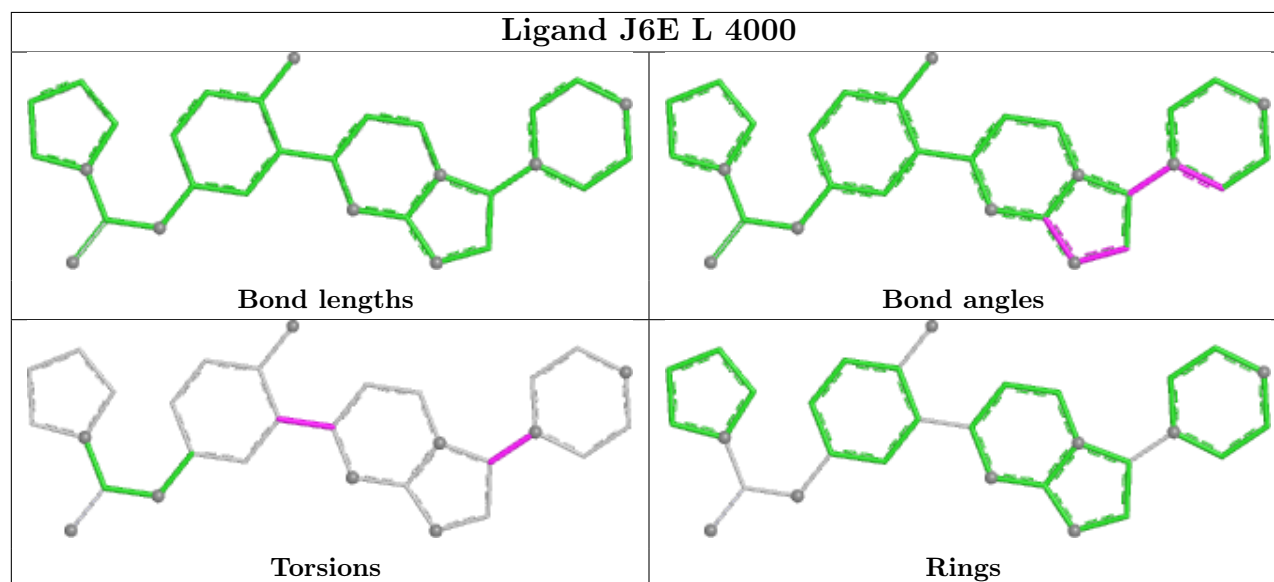
Continued from previous page...

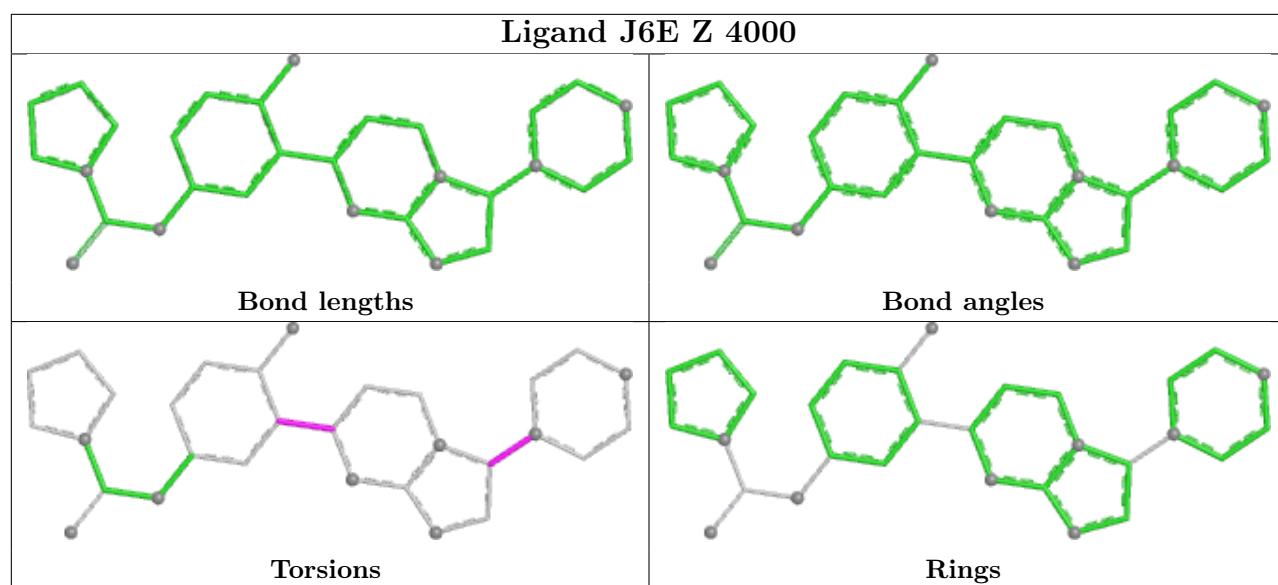
Mol	Chain	Res	Type	Atoms
15	Z	4000	J6E	N2-C14-N5-C20
15	L	4000	J6E	N2-C14-N5-C20
15	Z	4000	J6E	N2-C14-N5-C17

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.

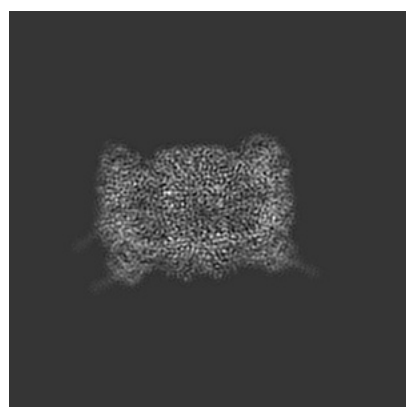
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4590. These allow visual inspection of the internal detail of the map and identification of artifacts.

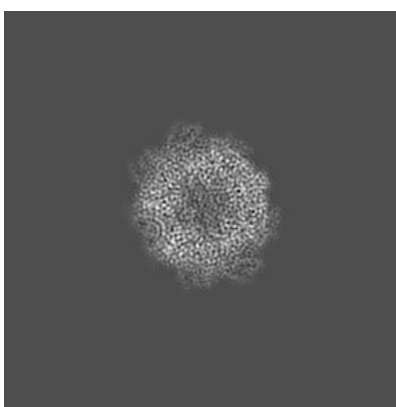
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

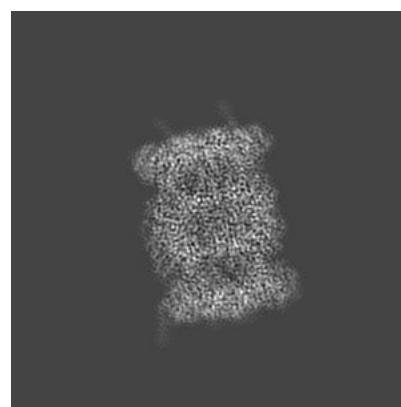
6.1.1 Primary map



X



Y



Z

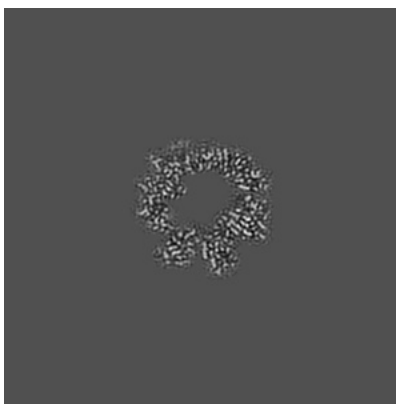
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

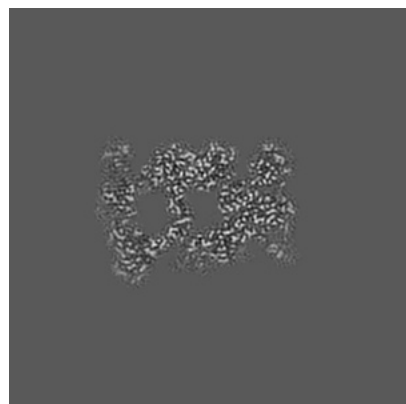


Z Index: 150

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: 174



Y Index: 121

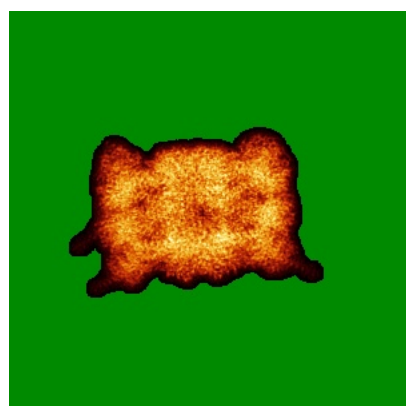


Z Index: 127

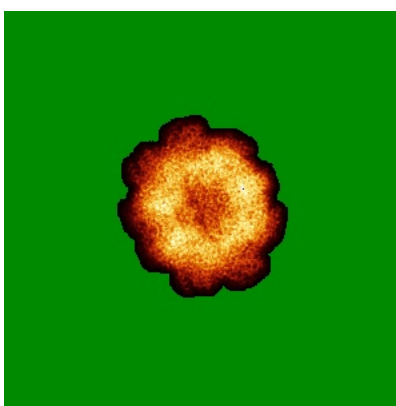
The images above show the largest variance slices of the map in three orthogonal directions.

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

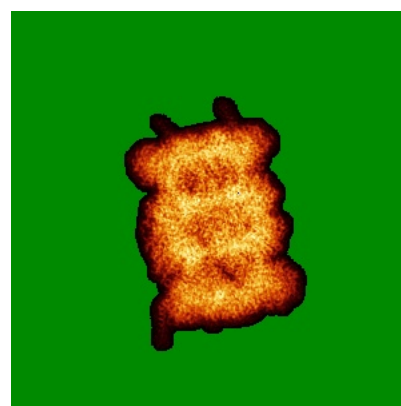
6.4.1 Primary map



X



Y

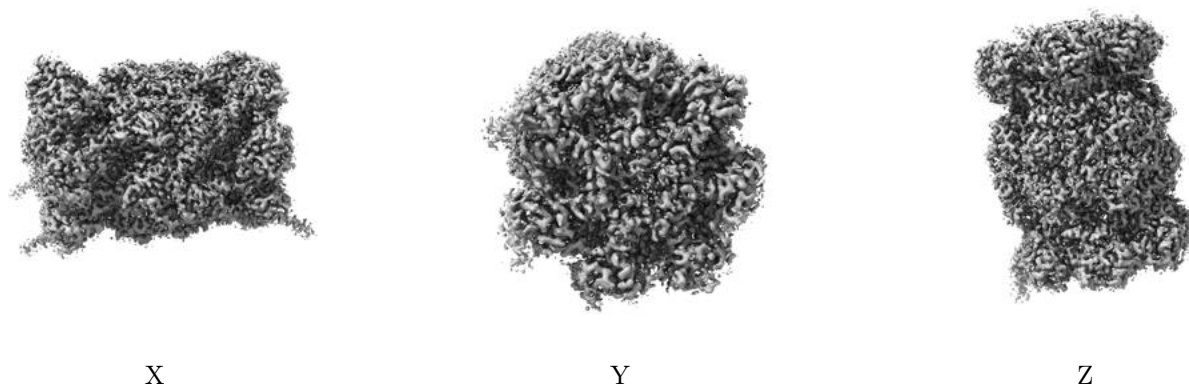


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0667. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

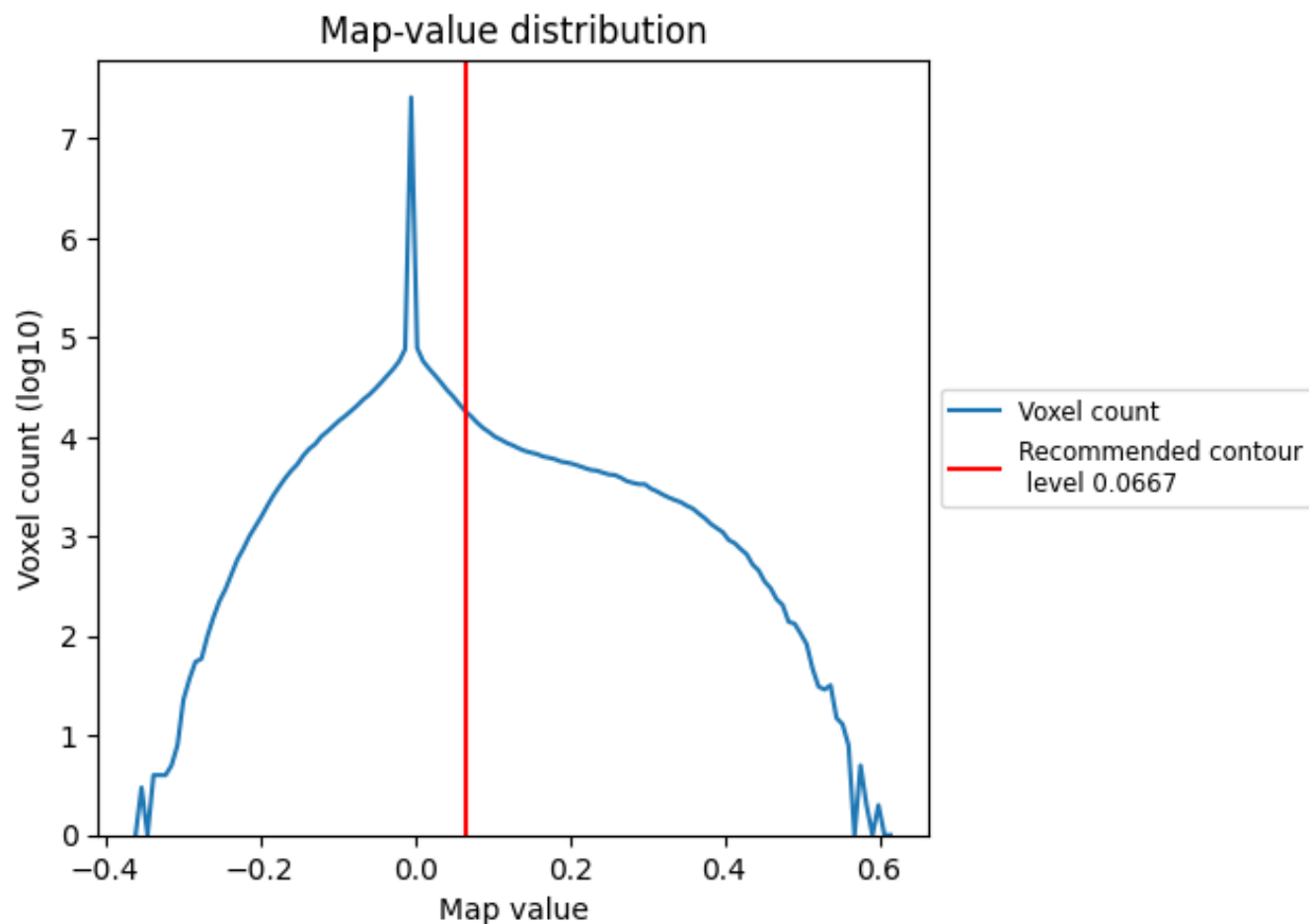
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

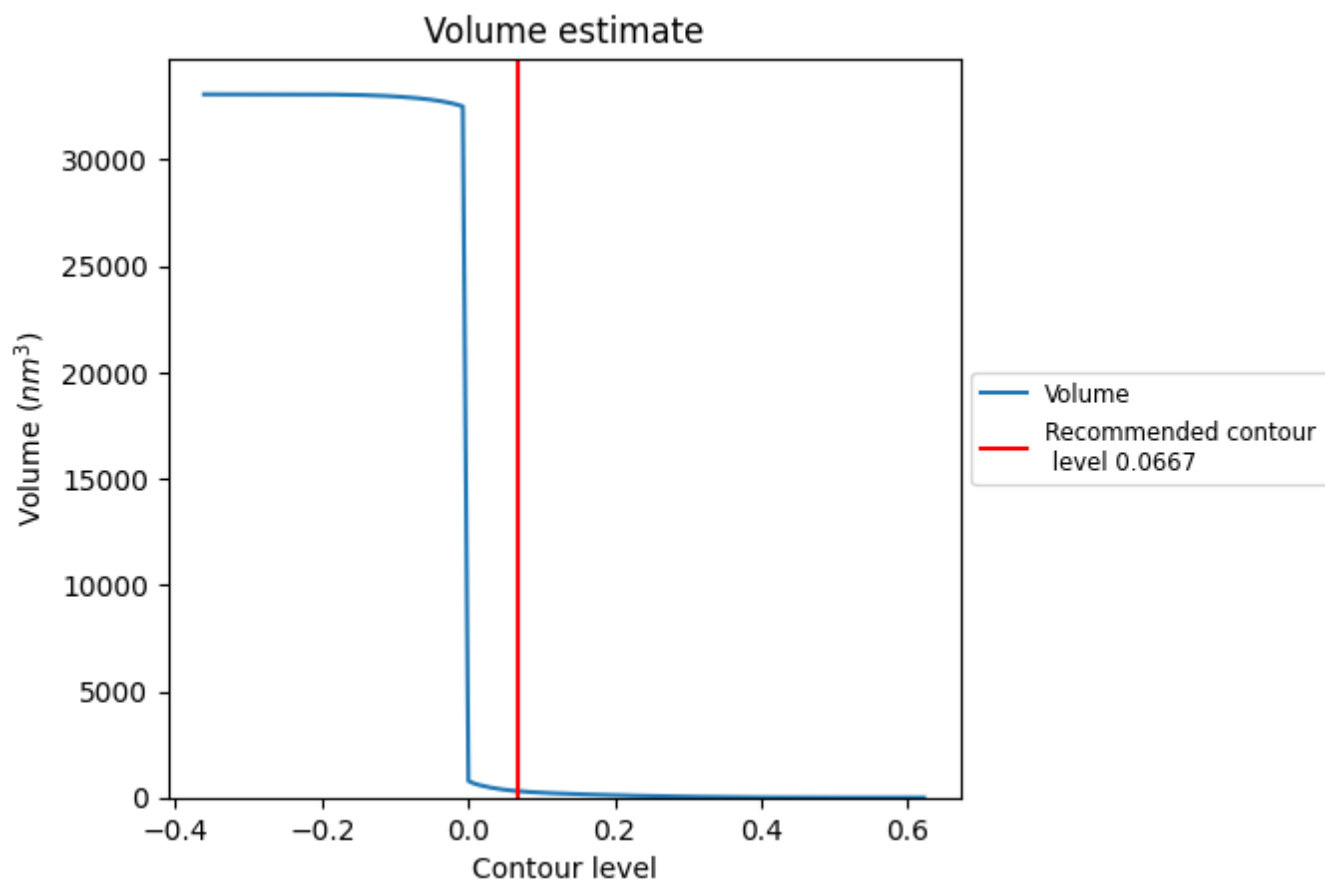
This section contains the results of statistical analysis of the map.

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.

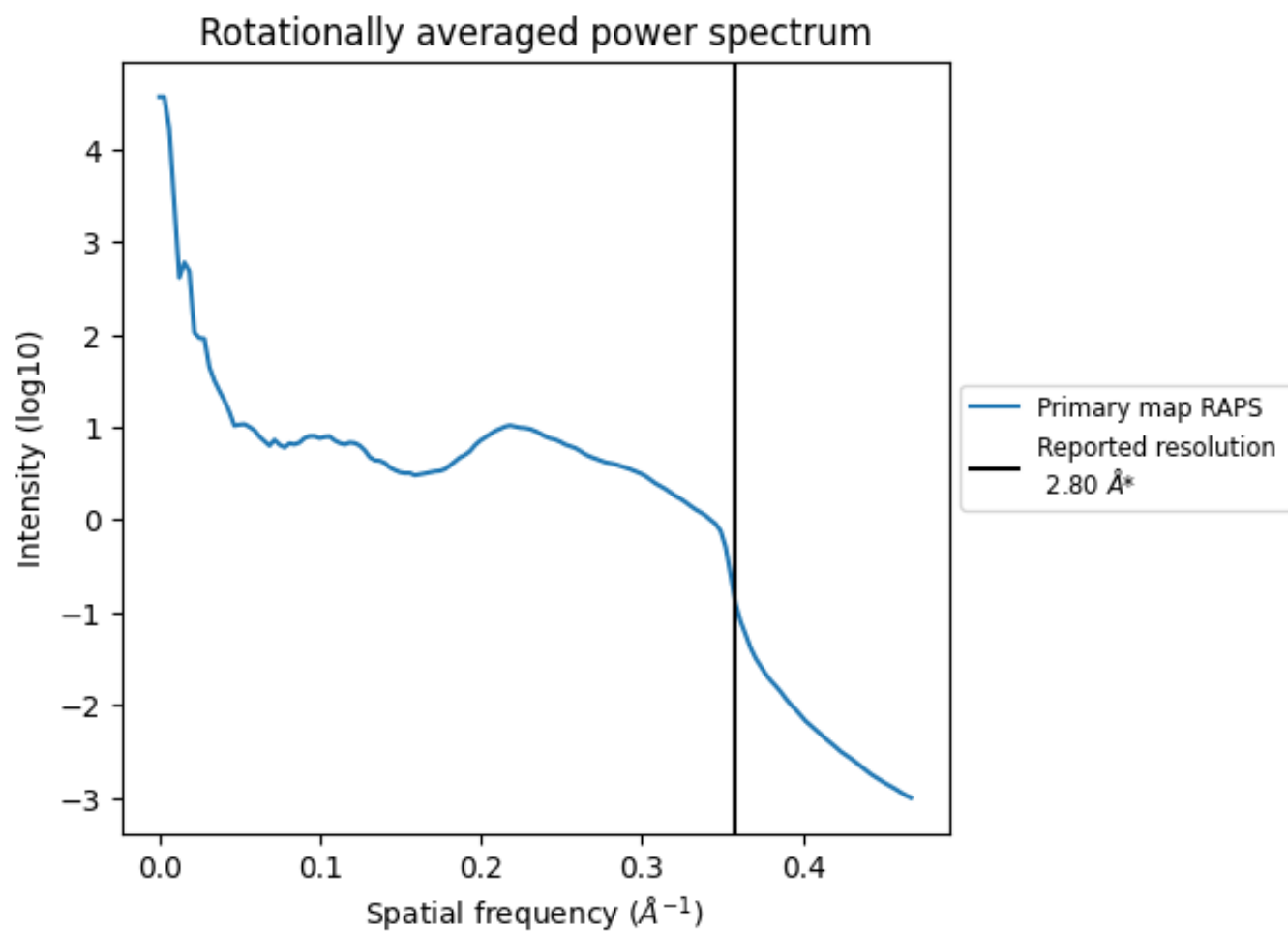
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 276 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 0.357 Å⁻¹

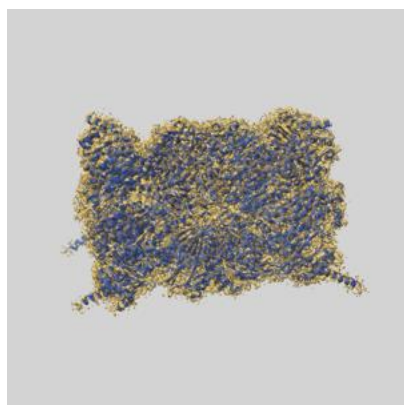
8 Fourier-Shell correlation

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

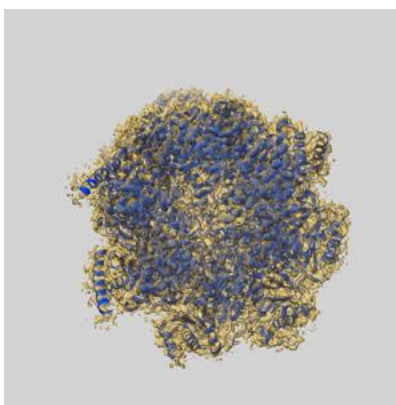
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4590 and PDB model 6QM7. Per-residue inclusion information can be found in section [3](#) on page [9](#).

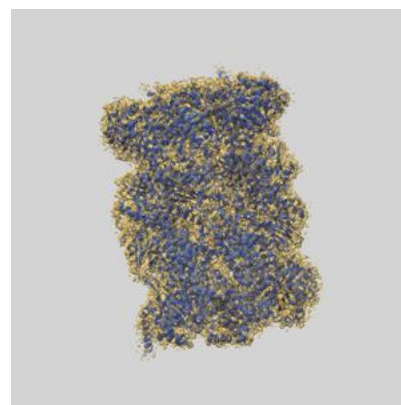
9.1 Map-model overlay [i](#)



X



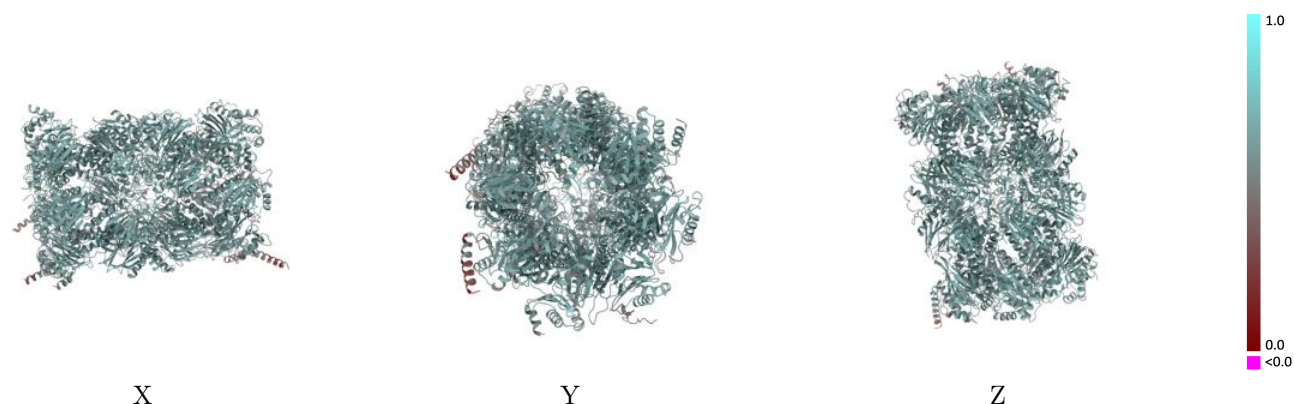
Y



Z

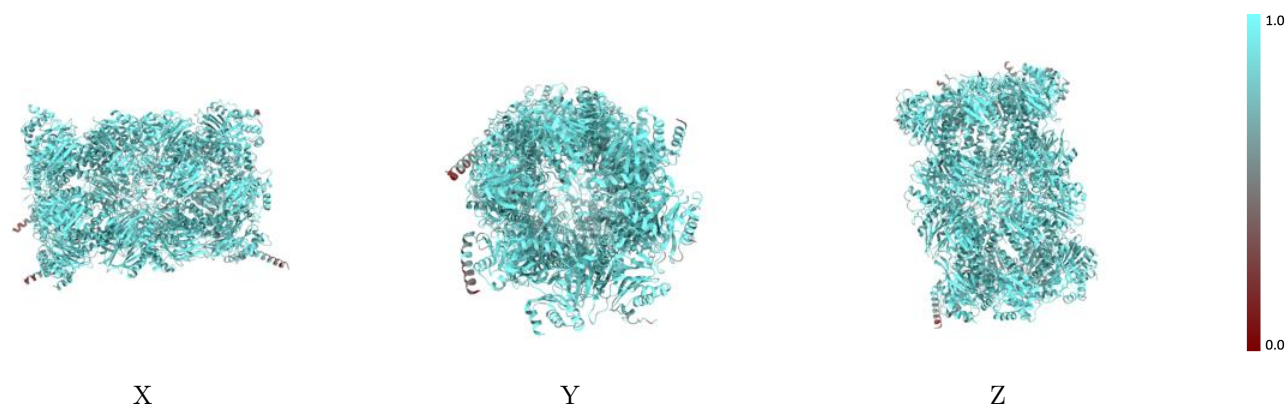
The images above show the 3D surface view of the map at the recommended contour level 0.0667 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



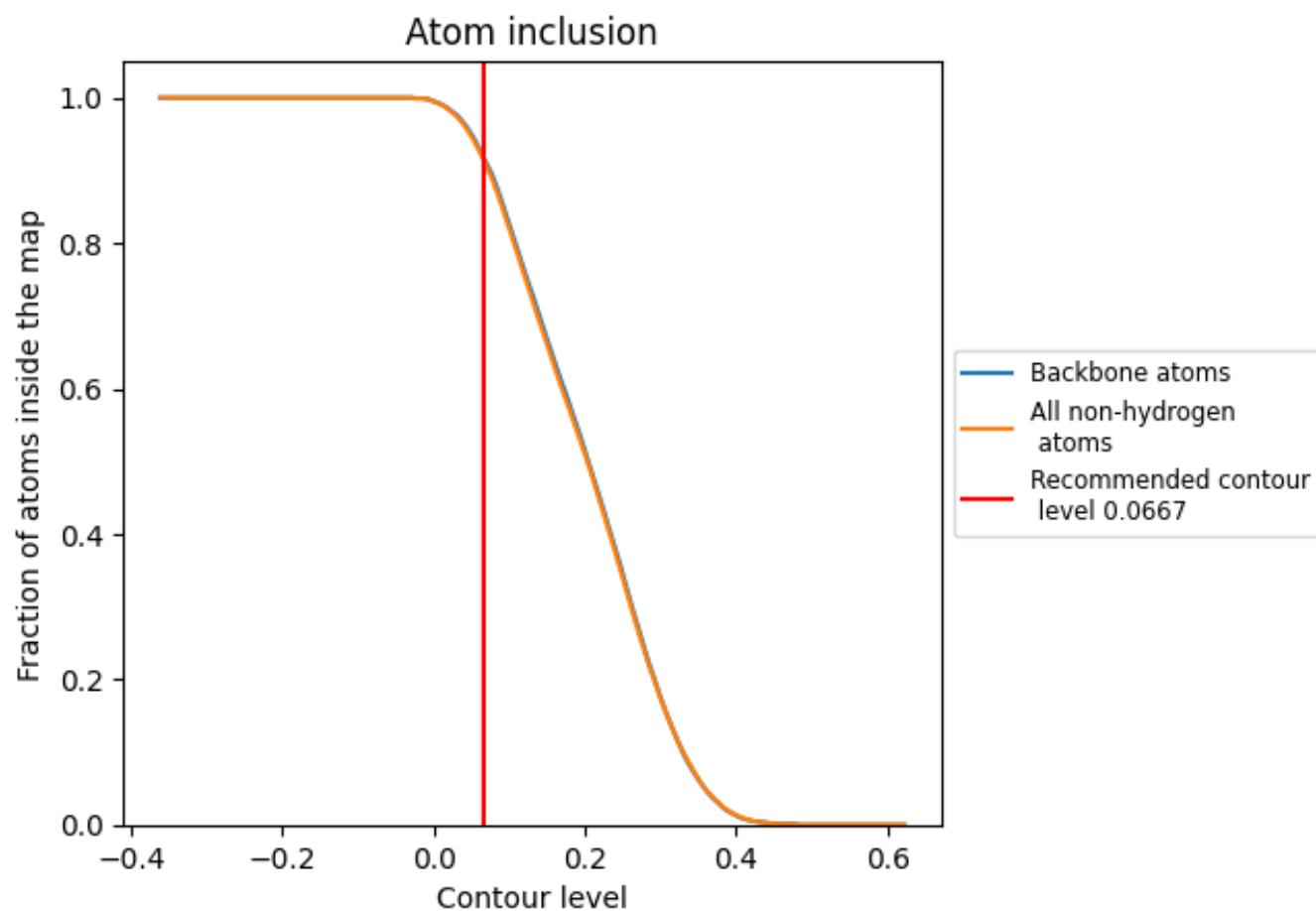
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0667).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0667) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.6070
A	 0.9100	 0.6080
B	 0.9070	 0.6070
C	 0.8770	 0.5890
D	 0.8670	 0.5780
E	 0.8930	 0.5980
F	 0.9040	 0.6040
G	 0.9150	 0.6100
H	 0.9610	 0.6310
I	 0.9270	 0.6180
J	 0.9430	 0.6280
K	 0.9350	 0.6140
L	 0.9500	 0.6310
M	 0.9440	 0.6180
N	 0.9400	 0.6280
O	 0.9150	 0.6040
P	 0.9120	 0.6030
Q	 0.8860	 0.5750
R	 0.8670	 0.5680
S	 0.9060	 0.5930
T	 0.9040	 0.5980
U	 0.9140	 0.6050
V	 0.9500	 0.6270
W	 0.9270	 0.6080
X	 0.9290	 0.6200
Y	 0.9380	 0.6110
Z	 0.9410	 0.6250
a	 0.9320	 0.6110
b	 0.9300	 0.6220

