



wwPDB EM Validation Summary Report ⓘ

Jul 20, 2026 – 08:26 PM EDT

PDB ID : 9Q6F / pdb_00009q6f
EMDB ID : EMD-72277
Title : Structure of Plasmodium falciparum 20S proteasome bound to an asparagine
-ethylenediamine based inhibitor TDI6245
Authors : Hsu, H.C.; Li, H.
Deposited on : 2025-08-22
Resolution : 2.86 Å(reported)
Based on initial model : 8G6E

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:

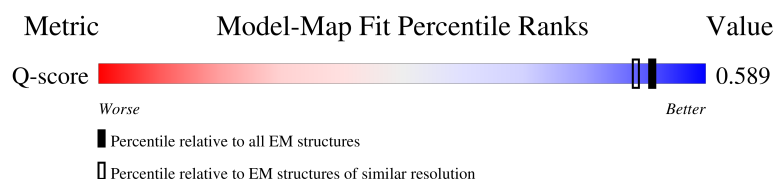
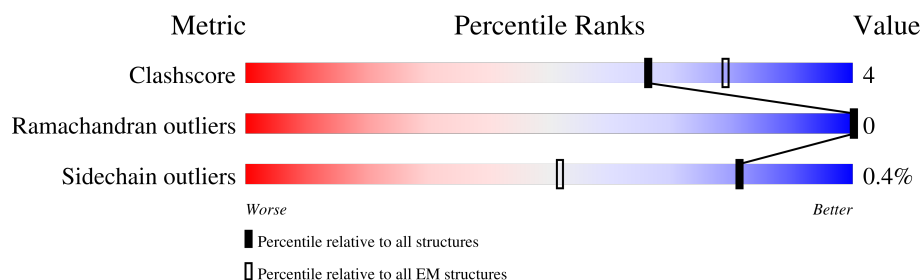
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.50

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 2.86 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.



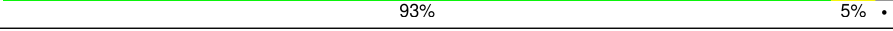
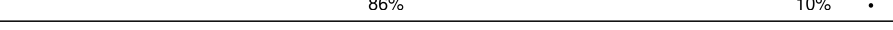
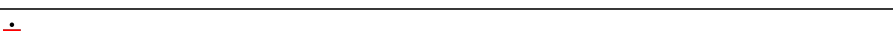
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	260	93% 5% .
1	O	260	90% 7% .
2	B	235	88% 10% .
2	P	235	86% 12% .

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Mol	Chain	Length	Quality of chain
3	C	246	 89% 9%
3	Q	246	 92% 7%
4	D	241	 91% 7%
4	R	241	 89% 9%
5	E	256	 80% 12% 9%
5	S	256	 79% 13% 9%
6	F	253	 85% 9% 6%
6	T	253	 87% 8% 6%
7	G	252	 92% 6%
7	U	252	 93% 5%
8	H	252	 76% 10% 13%
8	V	252	 74% 12% 13%
9	I	229	 87% 9%
9	W	229	 86% 10%
10	J	218	 85% 11%
10	X	218	 86% 10%
11	K	195	 91% 9%
11	Y	195	 90% 10%
12	L	211	 91% 9%
12	Z	211	 92% 8%
13	M	240	 74% 15% 10%
13	a	240	 74% 15% 10%
14	N	302	 69% 8% 23%
14	b	302	 69% 8% 23%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 50840 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
1	A	253	Total	C	N	O	S	0	0
			2006	1259	337	395	15		
1	O	253	Total	C	N	O	S	0	0
			2006	1259	337	395	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1830	1177	299	348	6		
2	P	230	Total	C	N	O	S	0	0
			1830	1177	299	348	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1938	1241	315	379	3		
3	Q	242	Total	C	N	O	S	0	0
			1938	1241	315	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1870	1192	318	352	8		
4	R	236	Total	C	N	O	S	0	0
			1870	1192	318	352	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1805	1136	300	358	11		
5	S	234	Total	C	N	O	S	0	0
			1805	1136	300	358	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	239	Total	C	N	O	S	0	0
			1897	1204	313	369	11		
6	T	239	Total	C	N	O	S	0	0
			1897	1204	313	369	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	247	Total	C	N	O	S	0	0
			2025	1289	338	385	13		
7	U	247	Total	C	N	O	S	0	0
			2025	1289	338	385	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	218	Total	C	N	O	S	0	0
			1750	1111	302	326	11		
8	V	218	Total	C	N	O	S	0	0
			1750	1111	302	326	11		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	1	0
			1703	1076	297	316	14		
9	W	221	Total	C	N	O	S	1	0
			1703	1076	297	316	14		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	210	Total	C	N	O	S	0	0
			1653	1055	269	315	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	210	Total	C	N	O	S	0	0
			1653	1055	269	315	14		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		
11	Y	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1663	1060	275	320	8		
12	Z	211	Total	C	N	O	S	0	0
			1663	1060	275	320	8		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	215	Total	C	N	O	S	0	0
			1711	1096	285	323	7		
13	a	215	Total	C	N	O	S	0	0
			1711	1096	285	323	7		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	233	Total	C	N	O	S	0	0
			1920	1223	327	363	7		
14	b	233	Total	C	N	O	S	0	0
			1920	1223	327	363	7		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	266	GLU	-	expression tag	UNP W7K6I2
N	267	ASN	-	expression tag	UNP W7K6I2
N	268	LEU	-	expression tag	UNP W7K6I2
N	269	TYR	-	expression tag	UNP W7K6I2

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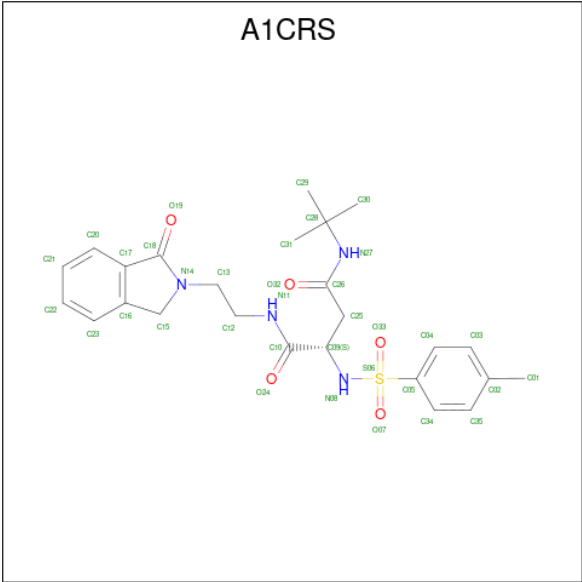
Chain	Residue	Modelled	Actual	Comment	Reference
N	270	PHE	-	expression tag	UNP W7K6I2
N	271	GLN	-	expression tag	UNP W7K6I2
N	272	SER	-	expression tag	UNP W7K6I2
N	273	SER	-	expression tag	UNP W7K6I2
N	274	ALA	-	expression tag	UNP W7K6I2
N	275	TRP	-	expression tag	UNP W7K6I2
N	276	SER	-	expression tag	UNP W7K6I2
N	277	HIS	-	expression tag	UNP W7K6I2
N	278	PRO	-	expression tag	UNP W7K6I2
N	279	GLN	-	expression tag	UNP W7K6I2
N	280	PHE	-	expression tag	UNP W7K6I2
N	281	GLU	-	expression tag	UNP W7K6I2
N	282	LYS	-	expression tag	UNP W7K6I2
N	283	GLY	-	expression tag	UNP W7K6I2
N	284	GLY	-	expression tag	UNP W7K6I2
N	285	GLY	-	expression tag	UNP W7K6I2
N	286	SER	-	expression tag	UNP W7K6I2
N	287	GLY	-	expression tag	UNP W7K6I2
N	288	GLY	-	expression tag	UNP W7K6I2
N	289	GLY	-	expression tag	UNP W7K6I2
N	290	SER	-	expression tag	UNP W7K6I2
N	291	GLY	-	expression tag	UNP W7K6I2
N	292	GLY	-	expression tag	UNP W7K6I2
N	293	SER	-	expression tag	UNP W7K6I2
N	294	ALA	-	expression tag	UNP W7K6I2
N	295	TRP	-	expression tag	UNP W7K6I2
N	296	SER	-	expression tag	UNP W7K6I2
N	297	HIS	-	expression tag	UNP W7K6I2
N	298	PRO	-	expression tag	UNP W7K6I2
N	299	GLN	-	expression tag	UNP W7K6I2
N	300	PHE	-	expression tag	UNP W7K6I2
N	301	GLU	-	expression tag	UNP W7K6I2
N	302	LYS	-	expression tag	UNP W7K6I2
b	266	GLU	-	expression tag	UNP W7K6I2
b	267	ASN	-	expression tag	UNP W7K6I2
b	268	LEU	-	expression tag	UNP W7K6I2
b	269	TYR	-	expression tag	UNP W7K6I2
b	270	PHE	-	expression tag	UNP W7K6I2
b	271	GLN	-	expression tag	UNP W7K6I2
b	272	SER	-	expression tag	UNP W7K6I2
b	273	SER	-	expression tag	UNP W7K6I2
b	274	ALA	-	expression tag	UNP W7K6I2

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Chain	Residue	Modelled	Actual	Comment	Reference
b	275	TRP	-	expression tag	UNP W7K6I2
b	276	SER	-	expression tag	UNP W7K6I2
b	277	HIS	-	expression tag	UNP W7K6I2
b	278	PRO	-	expression tag	UNP W7K6I2
b	279	GLN	-	expression tag	UNP W7K6I2
b	280	PHE	-	expression tag	UNP W7K6I2
b	281	GLU	-	expression tag	UNP W7K6I2
b	282	LYS	-	expression tag	UNP W7K6I2
b	283	GLY	-	expression tag	UNP W7K6I2
b	284	GLY	-	expression tag	UNP W7K6I2
b	285	GLY	-	expression tag	UNP W7K6I2
b	286	SER	-	expression tag	UNP W7K6I2
b	287	GLY	-	expression tag	UNP W7K6I2
b	288	GLY	-	expression tag	UNP W7K6I2
b	289	GLY	-	expression tag	UNP W7K6I2
b	290	SER	-	expression tag	UNP W7K6I2
b	291	GLY	-	expression tag	UNP W7K6I2
b	292	GLY	-	expression tag	UNP W7K6I2
b	293	SER	-	expression tag	UNP W7K6I2
b	294	ALA	-	expression tag	UNP W7K6I2
b	295	TRP	-	expression tag	UNP W7K6I2
b	296	SER	-	expression tag	UNP W7K6I2
b	297	HIS	-	expression tag	UNP W7K6I2
b	298	PRO	-	expression tag	UNP W7K6I2
b	299	GLN	-	expression tag	UNP W7K6I2
b	300	PHE	-	expression tag	UNP W7K6I2
b	301	GLU	-	expression tag	UNP W7K6I2
b	302	LYS	-	expression tag	UNP W7K6I2

- Molecule 15 is N 4 -tert-butyl-N 2 -(4-methylbenzene-1-sulfonyl)-N 1 -[2-(1-oxo-1,3-dihydro-2H-isoindol-2-yl)ethyl]-L-aspartamide (CCD ID: A1CRS) (formula: C₂₅H₃₂N₄O₅S) (labeled as "Ligand of Interest" by depositor).

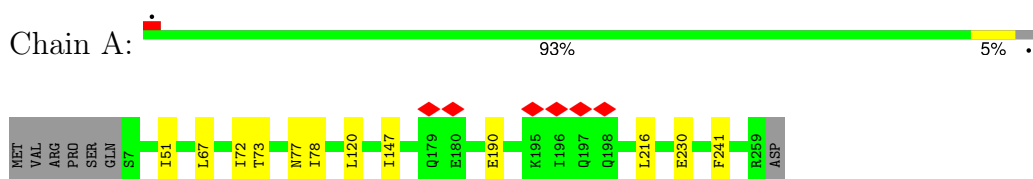


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	N	O	S	0
			35	25	4	5	1	
15	Z	1	Total	C	N	O	S	0
			35	25	4	5	1	

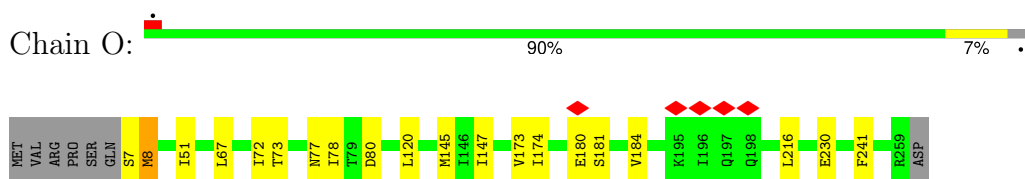
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

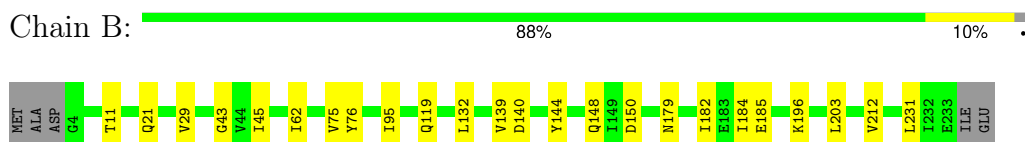
- Molecule 1: Proteasome subunit alpha type-6



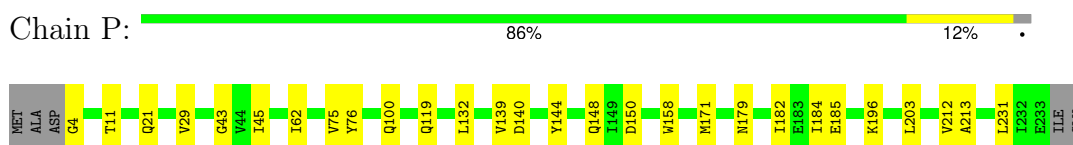
- Molecule 1: Proteasome subunit alpha type-6



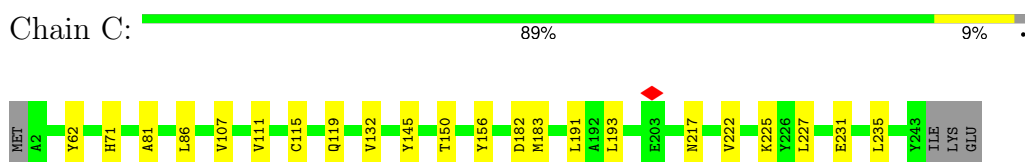
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-2



- Molecule 3: Proteasome subunit alpha type



- Molecule 3: Proteasome subunit alpha type

Chain Q:  92% 7%



- Molecule 4: Proteasome subunit alpha type

Chain D:  91% 7%



- Molecule 4: Proteasome subunit alpha type

Chain R:  89% 9%



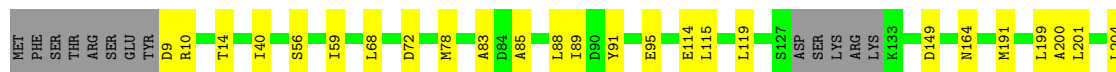
- Molecule 5: Proteasome subunit alpha type

Chain E:  80% 12% 9%



- Molecule 5: Proteasome subunit alpha type

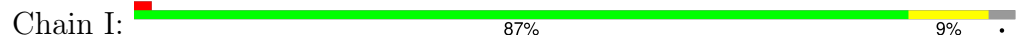
Chain S:  79% 13% 9%



- Molecule 6: Proteasome subunit alpha type-1

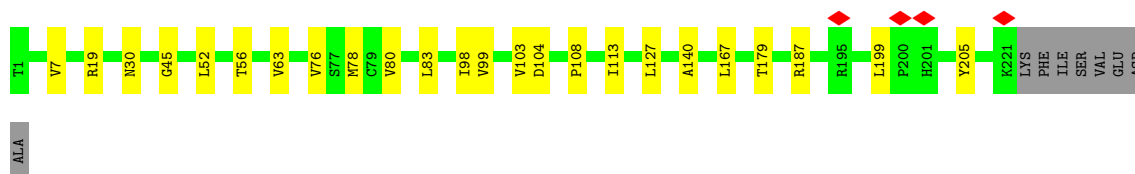
Chain F:  85% 9% 6%



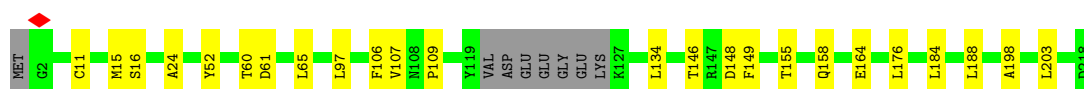
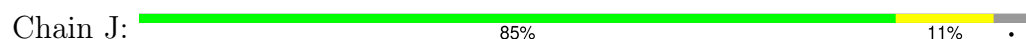




- Molecule 9: Proteasome subunit beta



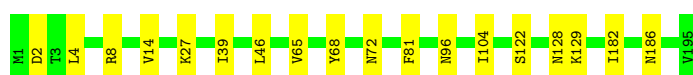
- Molecule 10: Proteasome subunit beta



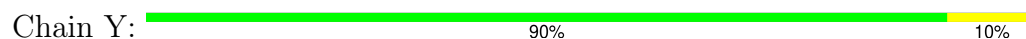
- Molecule 10: Proteasome subunit beta



- Molecule 11: Proteasome subunit beta



- Molecule 11: Proteasome subunit beta



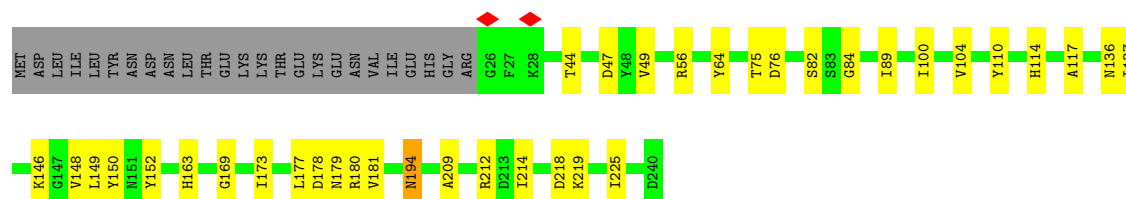
- Molecule 12: Proteasome subunit beta



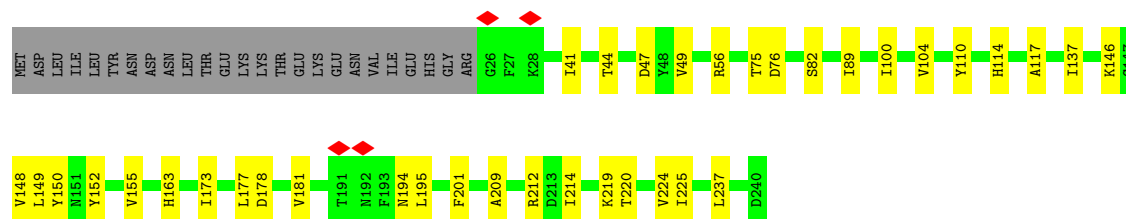
- Molecule 12: Proteasome subunit beta

T1
T2
T3
L4
I12
A20
S27
V31
A50
Y58
I62
S102
L139
Y143
I160
A163
V174
M211

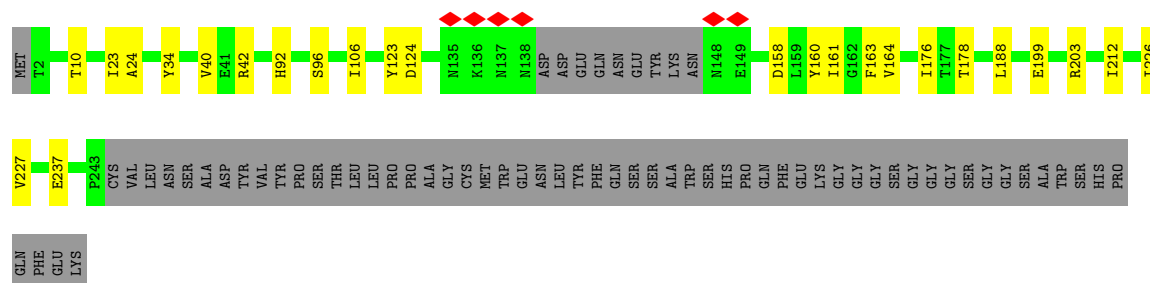
Chain M: 74% 15% 10%



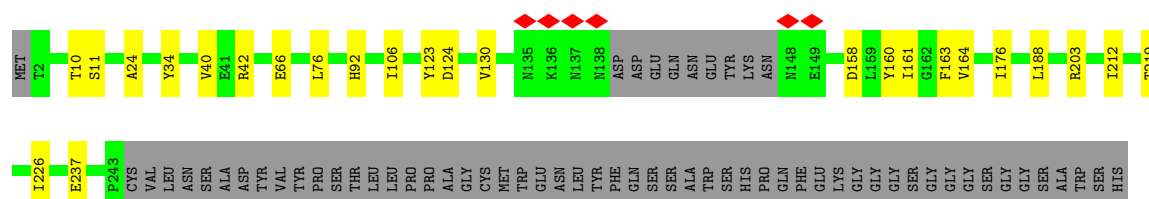
Chain a: 74% 15% 10%



Chain N: 69% 8% 23%



Chain b: 69% 8% 23%



PRO
GLN
PHE
GLU
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	124807	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.157	Depositor
Minimum map value	-1.246	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	317.952, 317.952, 317.952	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CRS

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	0.12	0/2033	0.24	0/2741
1	O	0.14	0/2033	0.26	0/2741
2	B	0.11	0/1864	0.25	0/2517
2	P	0.11	0/1864	0.24	0/2517
3	C	0.12	0/1974	0.25	0/2673
3	Q	0.12	0/1974	0.25	0/2673
4	D	0.11	0/1900	0.25	0/2563
4	R	0.11	0/1900	0.25	0/2563
5	E	0.11	0/1829	0.25	0/2470
5	S	0.11	0/1829	0.26	0/2470
6	F	0.11	0/1931	0.26	0/2600
6	T	0.11	0/1931	0.25	0/2600
7	G	0.11	0/2069	0.24	0/2796
7	U	0.13	0/2069	0.27	0/2796
8	H	0.14	0/1779	0.31	0/2387
8	V	0.14	0/1779	0.30	0/2387
9	I	0.13	0/1740	0.28	0/2365
9	W	0.13	0/1740	0.29	0/2365
10	J	0.13	0/1681	0.27	0/2268
10	X	0.12	0/1681	0.27	0/2268
11	K	0.14	0/1649	0.26	0/2223
11	Y	0.14	0/1649	0.26	0/2223
12	L	0.15	0/1697	0.25	0/2286
12	Z	0.15	0/1697	0.26	0/2286
13	M	0.13	0/1744	0.29	0/2360
13	a	0.14	0/1744	0.30	0/2360
14	N	0.11	0/1959	0.24	0/2644
14	b	0.11	0/1959	0.24	0/2644
All	All	0.12	0/51698	0.26	0/69786

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 ⓘ

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	2006	0	2003	7	0
1	O	2006	0	2003	12	0
2	B	1830	0	1847	20	0
2	P	1830	0	1847	21	0
3	C	1938	0	1932	12	0
3	Q	1938	0	1932	10	0
4	D	1870	0	1903	11	0
4	R	1870	0	1903	16	0
5	E	1805	0	1809	24	0
5	S	1805	0	1809	24	0
6	F	1897	0	1892	12	0
6	T	1897	0	1892	11	0
7	G	2025	0	1973	10	0
7	U	2025	0	1973	9	0
8	H	1750	0	1762	21	0
8	V	1750	0	1762	22	0
9	I	1703	0	1704	16	0
9	W	1703	0	1704	16	0
10	J	1653	0	1645	16	0
10	X	1653	0	1645	13	0
11	K	1614	0	1584	12	0
11	Y	1614	0	1584	11	0
12	L	1663	0	1618	11	0
12	Z	1663	0	1618	10	0
13	M	1711	0	1719	24	0
13	a	1711	0	1719	26	0
14	N	1920	0	1885	19	0
14	b	1920	0	1885	17	0
15	L	35	0	0	0	0
15	Z	35	0	0	0	0
All	All	50840	0	50552	399	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 4.

The worst 5 of 399 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)
1:A:78:ILE:HG21	1:A:120:LEU:HD21	1.72	0.71
4:D:83:LEU:HD22	4:D:129:ILE:HD11	1.76	0.68
10:X:65:LEU:HD22	10:X:107:VAL:HG11	1.75	0.68
7:G:80:TYR:OH	7:G:84:ASP:OD1	2.13	0.67
2:P:148:GLN:NE2	2:P:150:ASP:OD1	2.28	0.66

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	251/260 (96%)	247 (98%)	4 (2%)	0	100	100
1	O	251/260 (96%)	246 (98%)	5 (2%)	0	100	100
2	B	228/235 (97%)	223 (98%)	5 (2%)	0	100	100
2	P	228/235 (97%)	227 (100%)	1 (0%)	0	100	100
3	C	240/246 (98%)	238 (99%)	2 (1%)	0	100	100
3	Q	240/246 (98%)	237 (99%)	3 (1%)	0	100	100
4	D	234/241 (97%)	231 (99%)	3 (1%)	0	100	100
4	R	234/241 (97%)	229 (98%)	5 (2%)	0	100	100
5	E	230/256 (90%)	227 (99%)	3 (1%)	0	100	100
5	S	230/256 (90%)	228 (99%)	2 (1%)	0	100	100
6	F	237/253 (94%)	235 (99%)	2 (1%)	0	100	100
6	T	237/253 (94%)	234 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	245/252 (97%)	241 (98%)	4 (2%)	0	100	100
7	U	245/252 (97%)	241 (98%)	4 (2%)	0	100	100
8	H	214/252 (85%)	211 (99%)	3 (1%)	0	100	100
8	V	214/252 (85%)	210 (98%)	4 (2%)	0	100	100
9	I	220/229 (96%)	214 (97%)	6 (3%)	0	100	100
9	W	220/229 (96%)	215 (98%)	5 (2%)	0	100	100
10	J	206/218 (94%)	200 (97%)	6 (3%)	0	100	100
10	X	206/218 (94%)	198 (96%)	8 (4%)	0	100	100
11	K	193/195 (99%)	188 (97%)	5 (3%)	0	100	100
11	Y	193/195 (99%)	188 (97%)	5 (3%)	0	100	100
12	L	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
12	Z	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
13	M	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
13	a	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
14	N	229/302 (76%)	224 (98%)	5 (2%)	0	100	100
14	b	229/302 (76%)	224 (98%)	5 (2%)	0	100	100
All	All	6298/6780 (93%)	6179 (98%)	119 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	224/231 (97%)	222 (99%)	2 (1%)	70	84
1	O	224/231 (97%)	222 (99%)	2 (1%)	70	84
2	B	201/205 (98%)	201 (100%)	0	100	100
2	P	201/205 (98%)	200 (100%)	1 (0%)	81	90
3	C	209/213 (98%)	207 (99%)	2 (1%)	68	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	209/213 (98%)	207 (99%)	2 (1%)	68	83
4	D	202/207 (98%)	202 (100%)	0	100	100
4	R	202/207 (98%)	201 (100%)	1 (0%)	81	90
5	E	202/223 (91%)	202 (100%)	0	100	100
5	S	202/223 (91%)	201 (100%)	1 (0%)	81	90
6	F	213/226 (94%)	211 (99%)	2 (1%)	70	84
6	T	213/226 (94%)	213 (100%)	0	100	100
7	G	226/229 (99%)	226 (100%)	0	100	100
7	U	226/229 (99%)	226 (100%)	0	100	100
8	H	197/231 (85%)	196 (100%)	1 (0%)	81	90
8	V	197/231 (85%)	196 (100%)	1 (0%)	81	90
9	I	188/194 (97%)	187 (100%)	1 (0%)	81	90
9	W	188/194 (97%)	188 (100%)	0	100	100
10	J	184/191 (96%)	184 (100%)	0	100	100
10	X	184/191 (96%)	184 (100%)	0	100	100
11	K	174/174 (100%)	173 (99%)	1 (1%)	78	89
11	Y	174/174 (100%)	173 (99%)	1 (1%)	78	89
12	L	176/176 (100%)	175 (99%)	1 (1%)	78	89
12	Z	176/176 (100%)	175 (99%)	1 (1%)	78	89
13	M	192/216 (89%)	189 (98%)	3 (2%)	55	76
13	a	192/216 (89%)	192 (100%)	0	100	100
14	N	210/266 (79%)	210 (100%)	0	100	100
14	b	210/266 (79%)	209 (100%)	1 (0%)	81	90
All	All	5596/5964 (94%)	5572 (100%)	24 (0%)	81	92

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	77	ASN
3	Q	182	ASP
3	Q	121	TYR
4	R	52	LYS
8	H	190	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	67	GLN
6	T	100	ASN
2	P	145	HIS
4	R	68	HIS
7	U	64	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 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	A1CRS	Z	301	-	37,37,37	1.93	8 (21%)	54,54,54	2.21	13 (24%)
15	A1CRS	L	301	-	37,37,37	1.92	8 (21%)	54,54,54	2.20	13 (24%)

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	A1CRS	Z	301	-	-	3/30/42/42	0/3/3/3
15	A1CRS	L	301	-	-	2/30/42/42	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Z	301	A1CRS	C26-N27	6.23	1.44	1.34
15	L	301	A1CRS	C26-N27	6.11	1.44	1.34
15	Z	301	A1CRS	S06-N08	5.09	1.70	1.61
15	L	301	A1CRS	S06-N08	5.08	1.70	1.61
15	L	301	A1CRS	C18-N14	3.34	1.41	1.36

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	A1CRS	C34-C05-C04	-7.42	110.79	120.47
15	L	301	A1CRS	C34-C05-C04	-7.41	110.81	120.47
15	L	301	A1CRS	C03-C04-C05	6.07	125.34	119.44
15	Z	301	A1CRS	C03-C04-C05	6.01	125.29	119.44
15	Z	301	A1CRS	C35-C34-C05	5.78	125.07	119.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

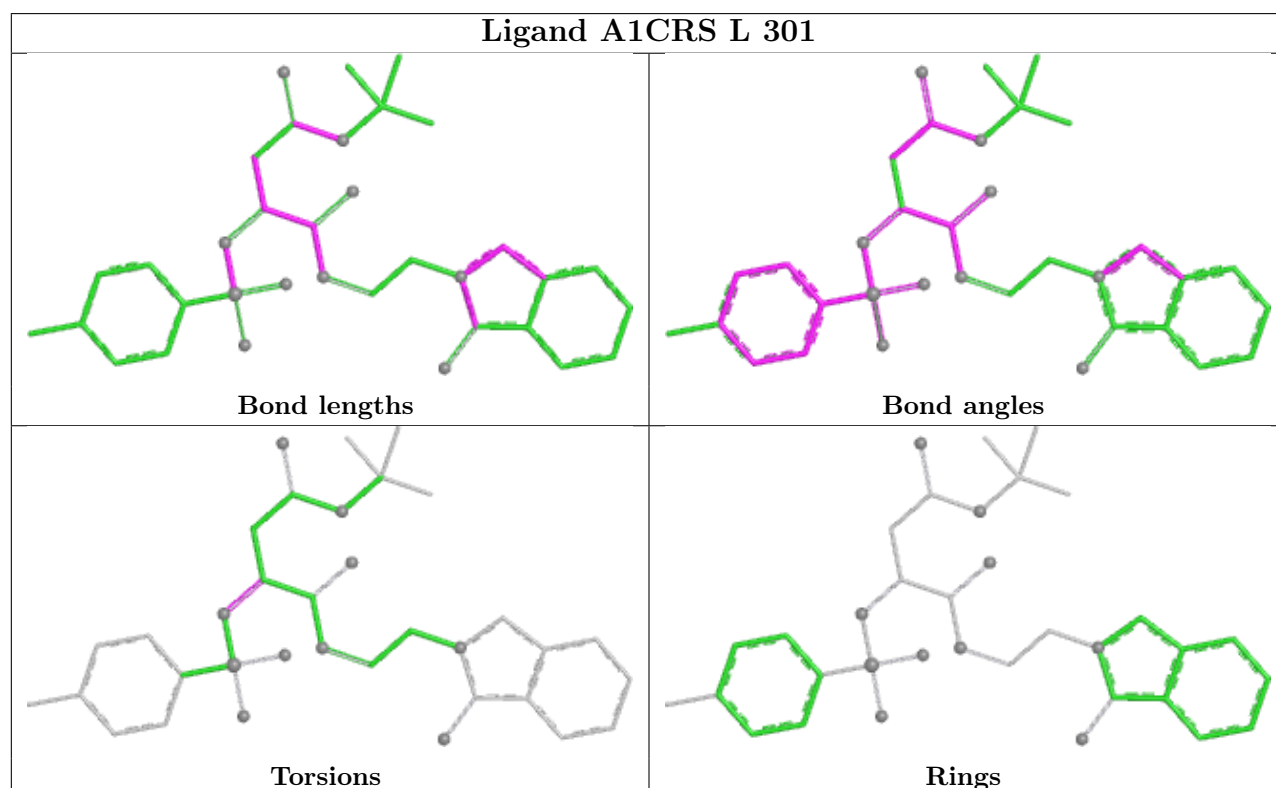
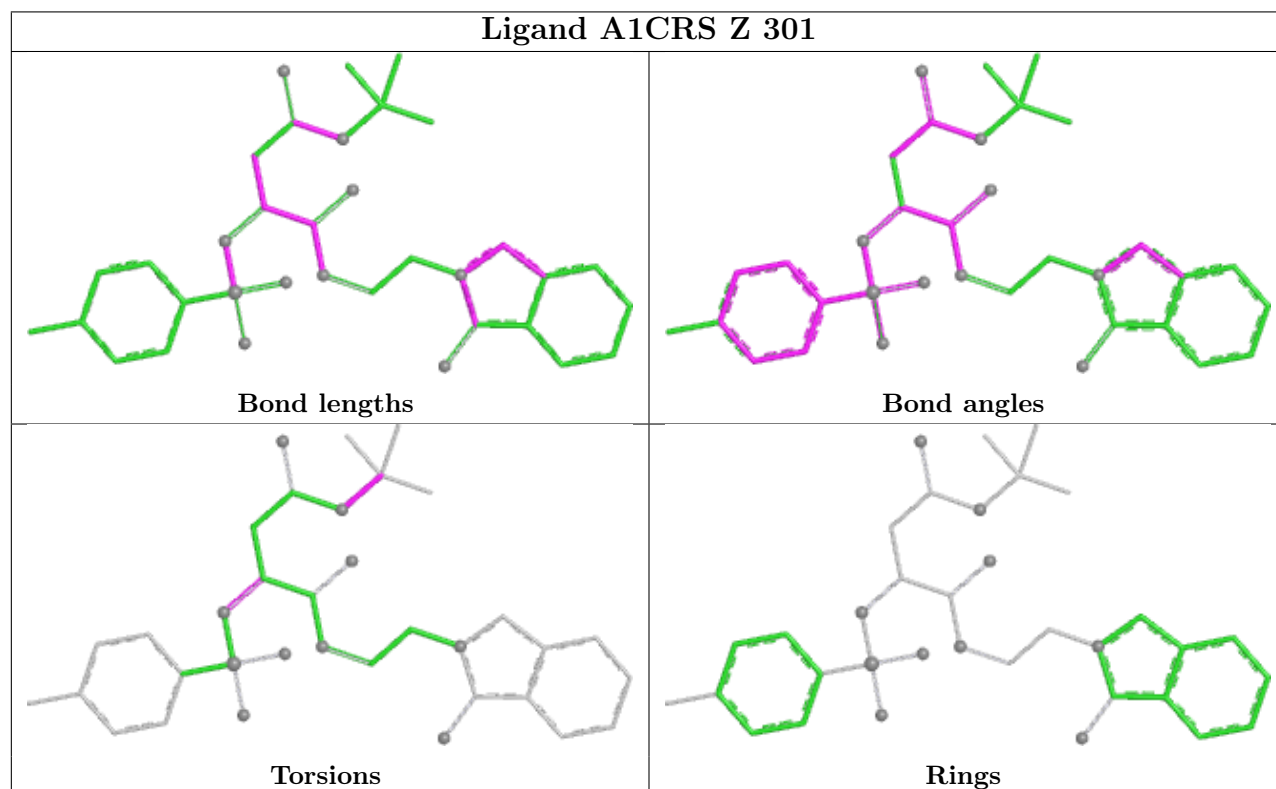
Mol	Chain	Res	Type	Atoms
15	L	301	A1CRS	C10-C09-N08-S06
15	Z	301	A1CRS	C10-C09-N08-S06
15	L	301	A1CRS	C25-C09-N08-S06
15	Z	301	A1CRS	C25-C09-N08-S06
15	Z	301	A1CRS	C31-C28-N27-C26

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.

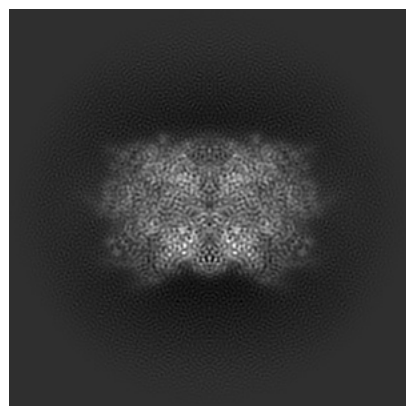
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72277. These allow visual inspection of the internal detail of the map and identification of artifacts.

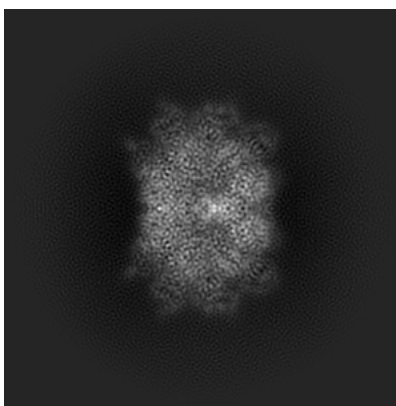
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

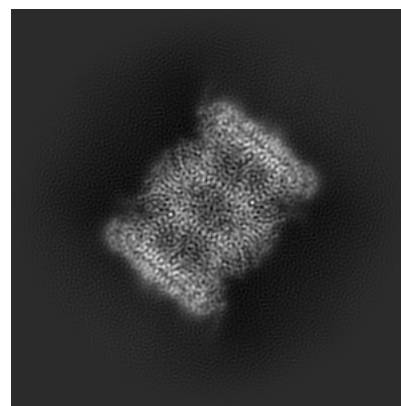
6.1.1 Primary map



X

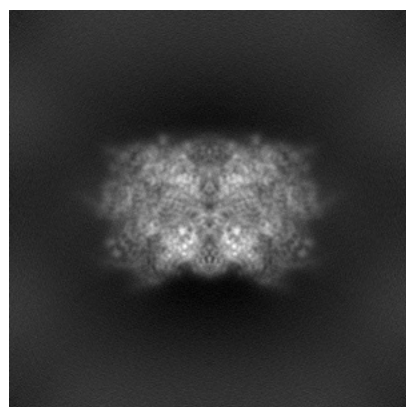


Y

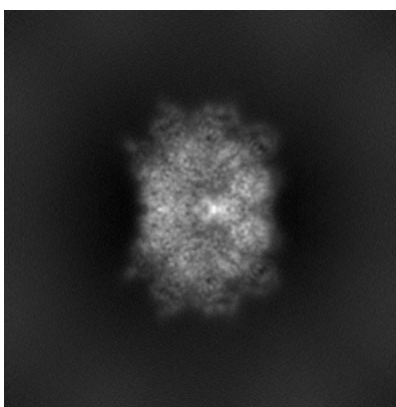


Z

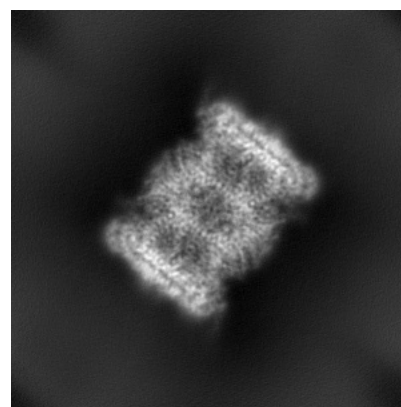
6.1.2 Raw map



X



Y

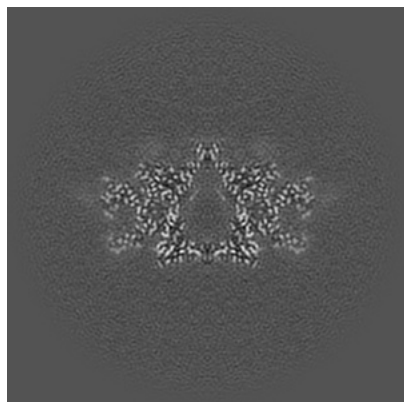


Z

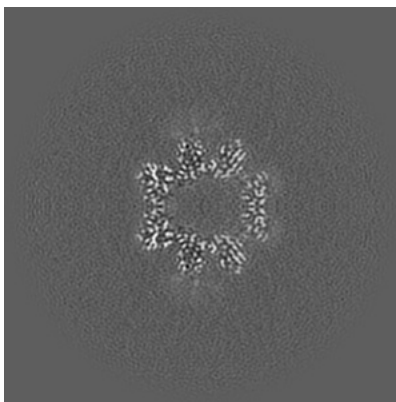
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

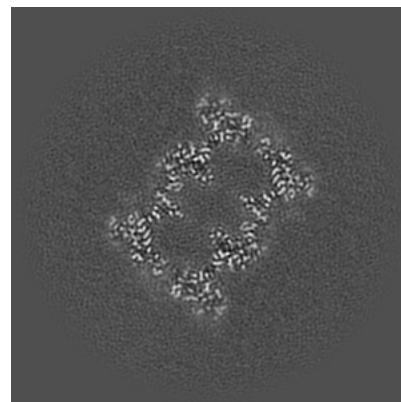
6.2.1 Primary map



X Index: 192

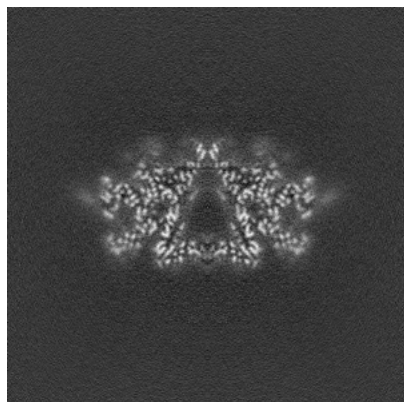


Y Index: 192

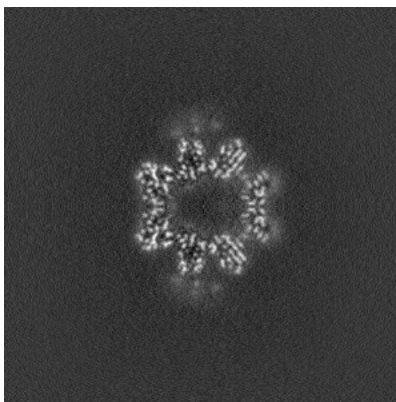


Z Index: 192

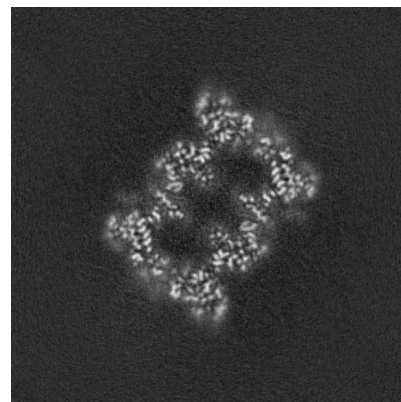
6.2.2 Raw map



X Index: 192



Y Index: 192

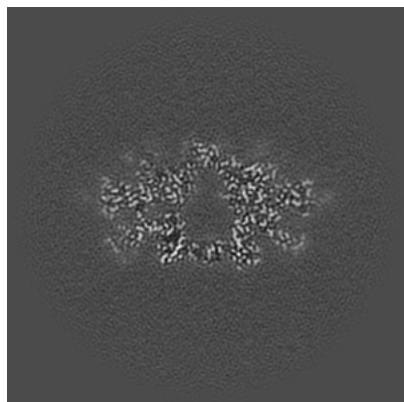


Z Index: 192

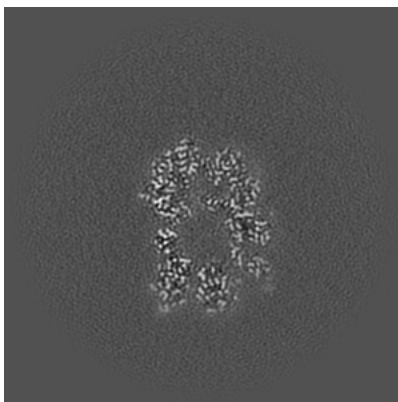
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

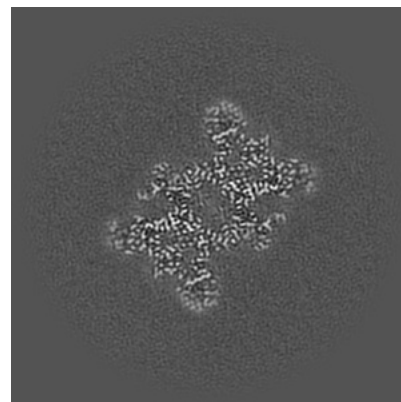
6.3.1 Primary map



X Index: 190

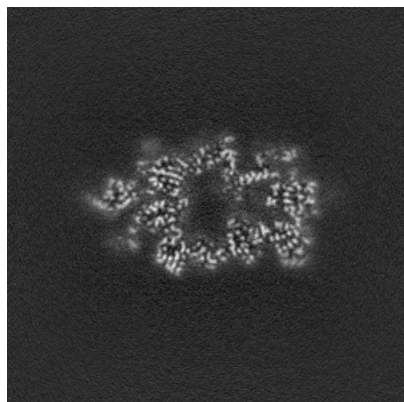


Y Index: 168

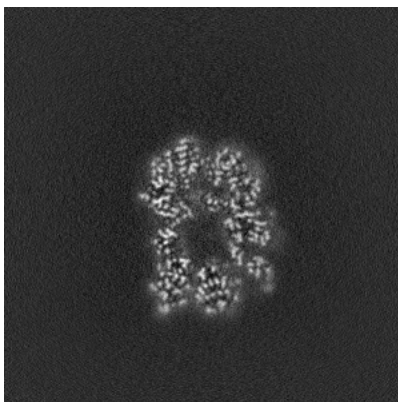


Z Index: 161

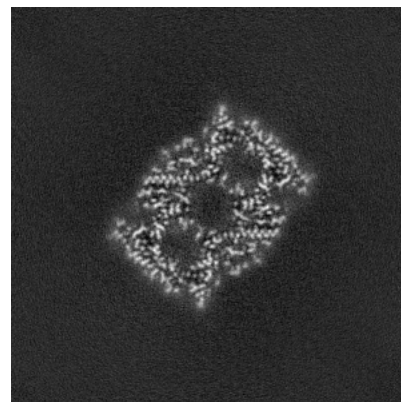
6.3.2 Raw map



X Index: 199



Y Index: 168

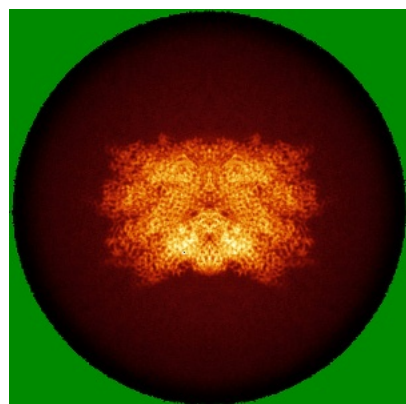


Z Index: 171

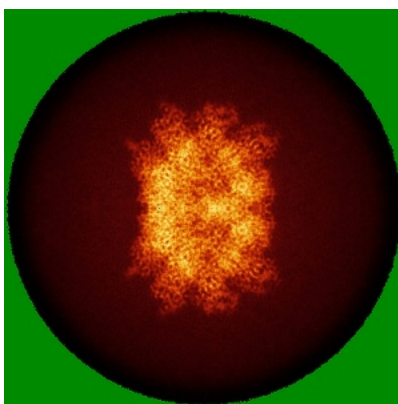
The images above show the largest variance slices of the map in three orthogonal directions.

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

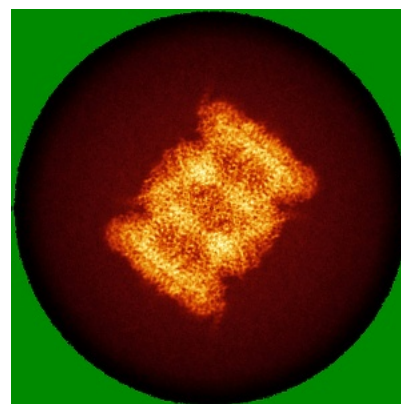
6.4.1 Primary map



X

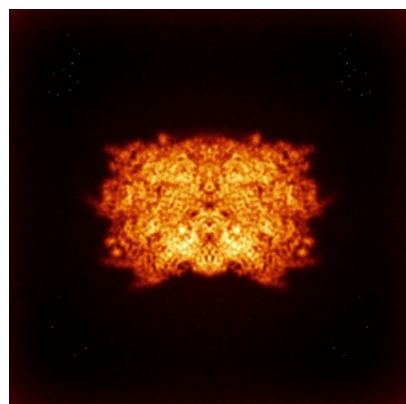


Y

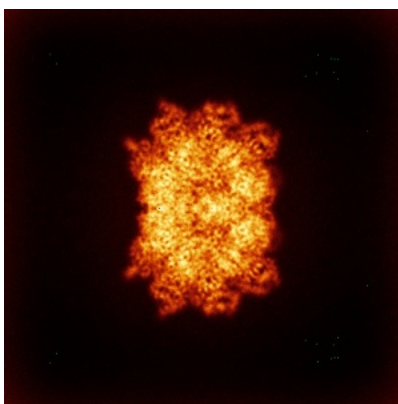


Z

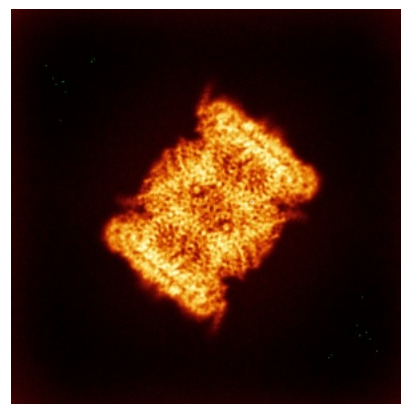
6.4.2 Raw map



X



Y

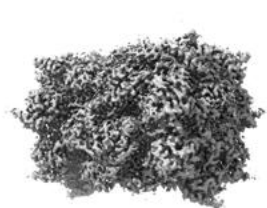


Z

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



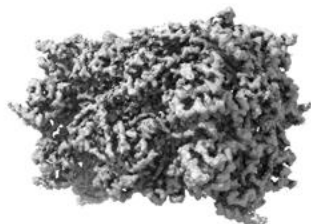
Y



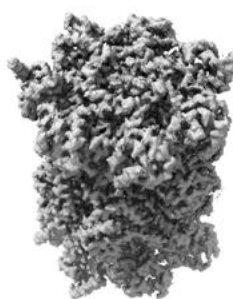
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

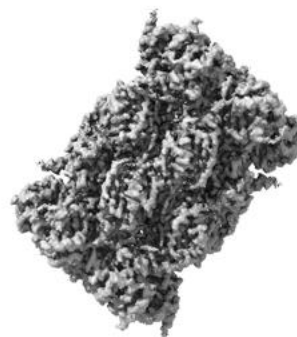
6.5.2 Raw map



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.

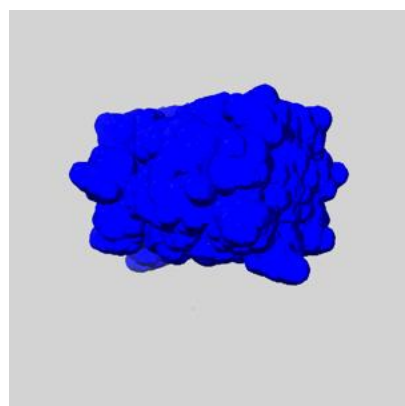
6.6 Mask visualisation [i](#)

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

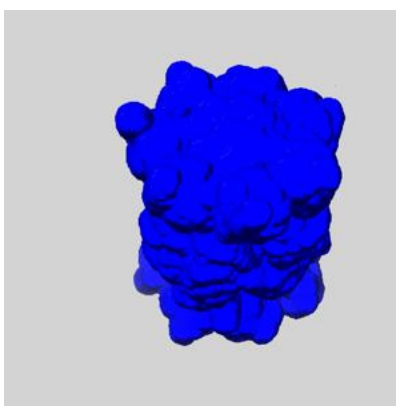
A mask typically either:

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

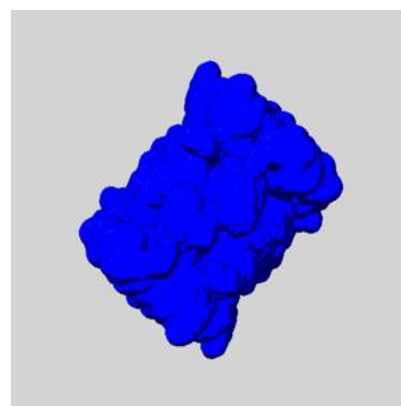
6.6.1 emd_72277_msk_1.map [i](#)



X



Y

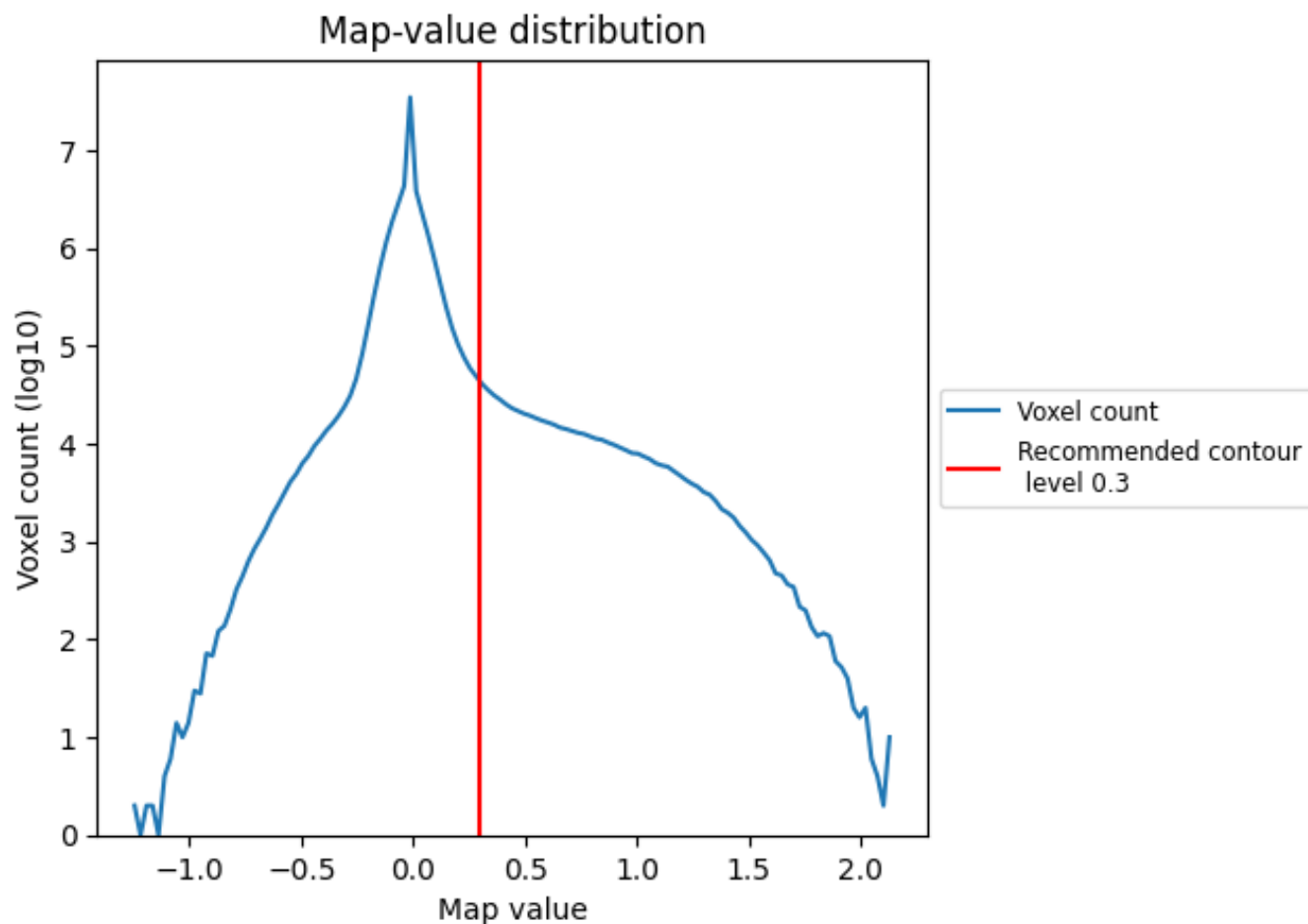


Z

7 Map analysis [i](#)

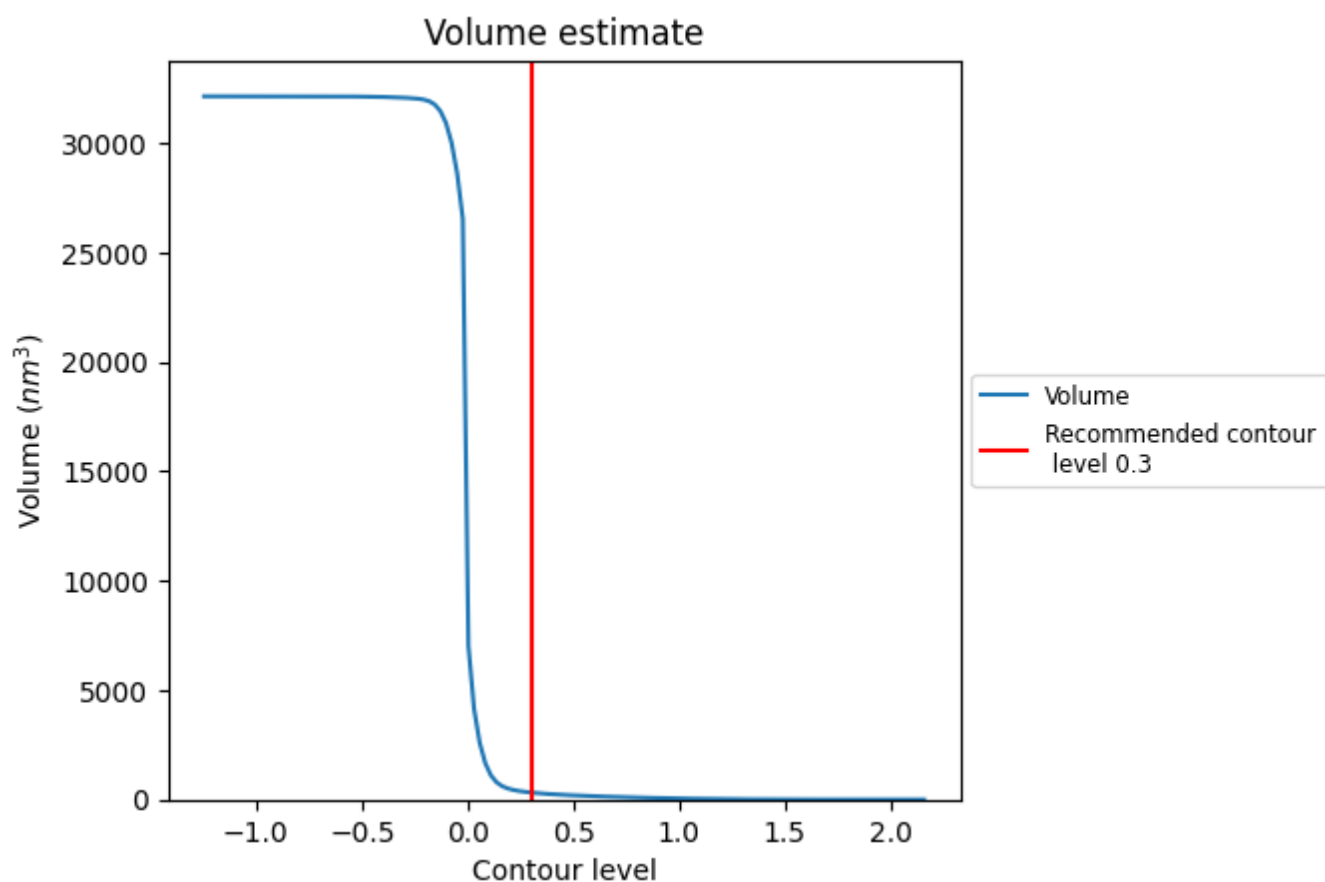
This section contains the results of statistical analysis of the map.

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.

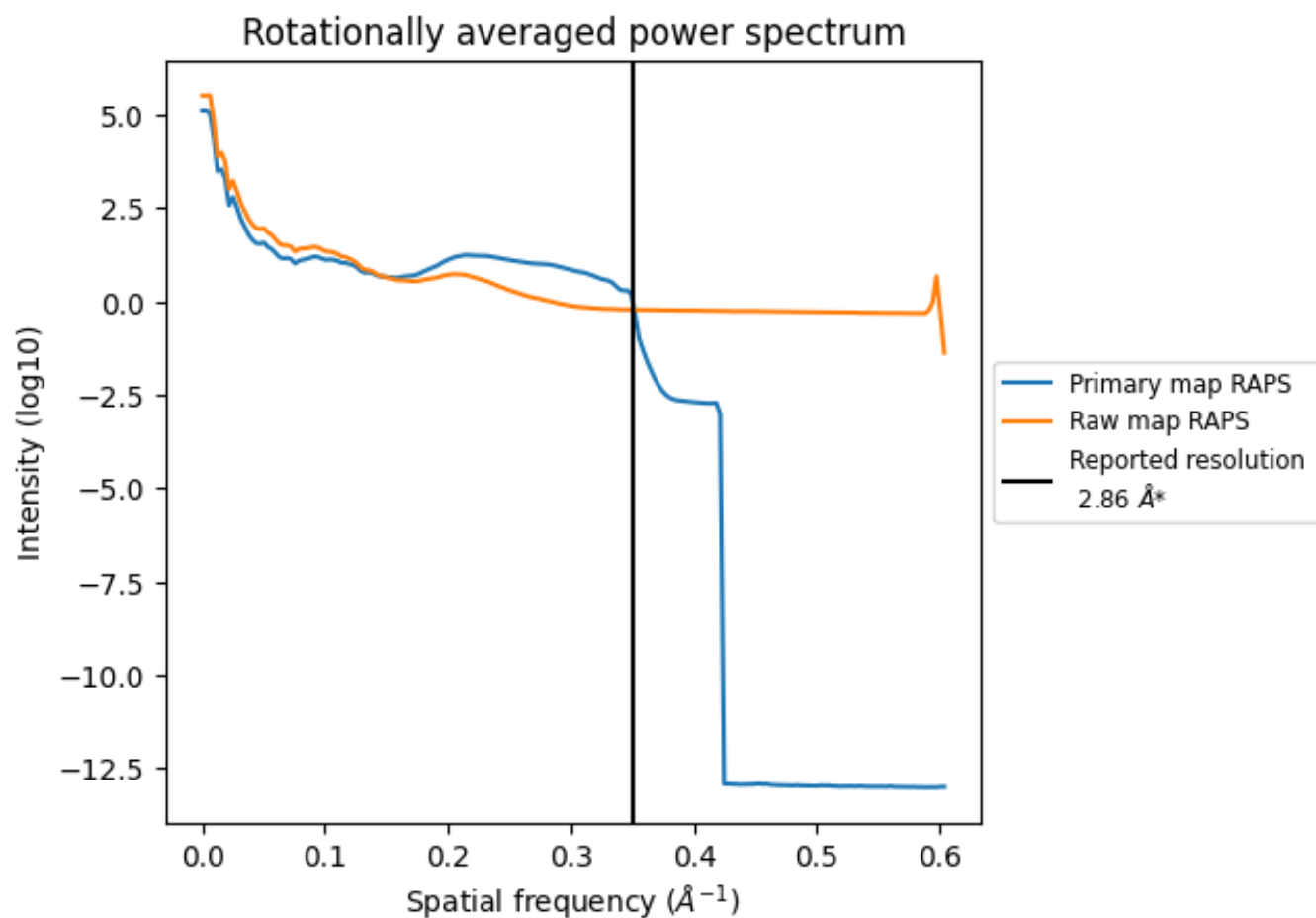
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 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 ⓘ

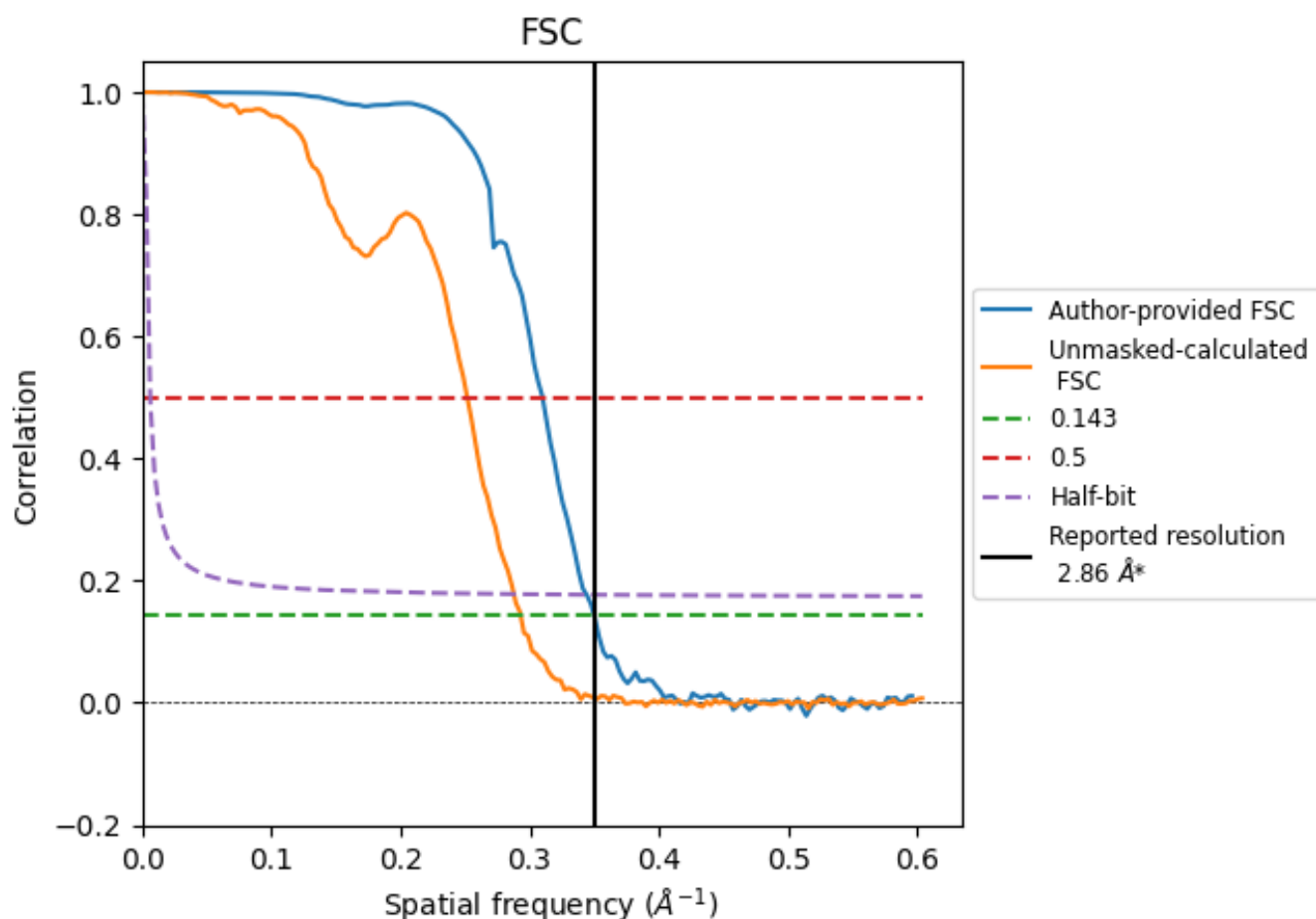


*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

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 0.350 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

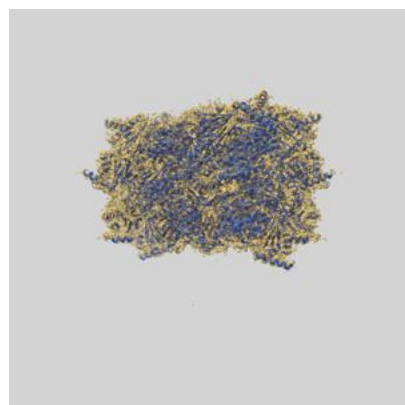
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.23	2.91
Unmasked-calculated*	3.41	3.97	3.47

*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 3.41 differs from the reported value 2.86 by more than 10 %

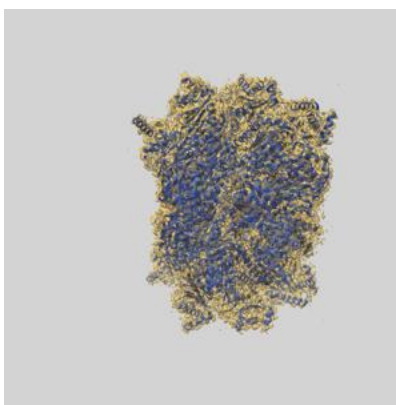
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72277 and PDB model 9Q6F. Per-residue inclusion information can be found in section [3](#) on page [10](#).

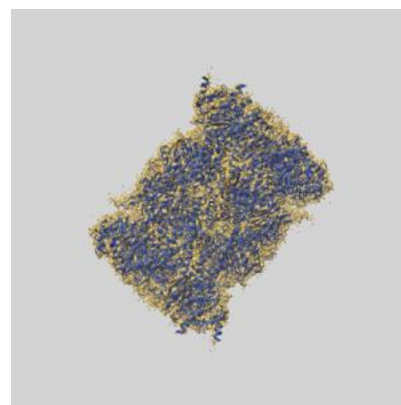
9.1 Map-model overlay [i](#)



X



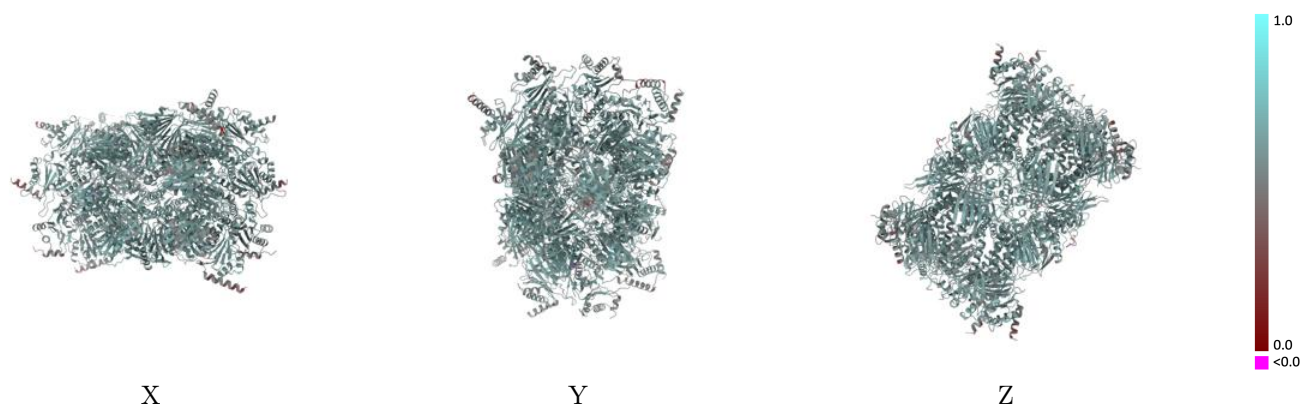
Y



Z

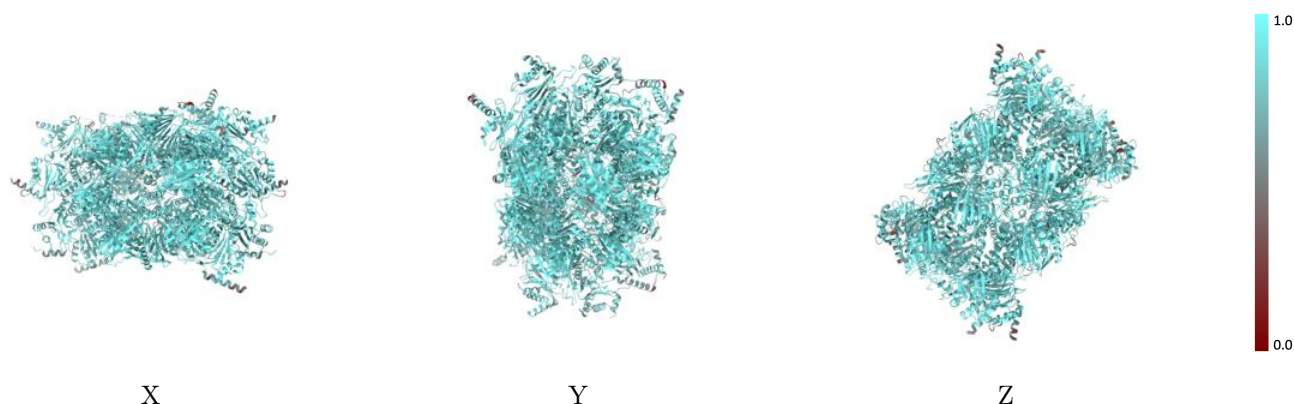
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



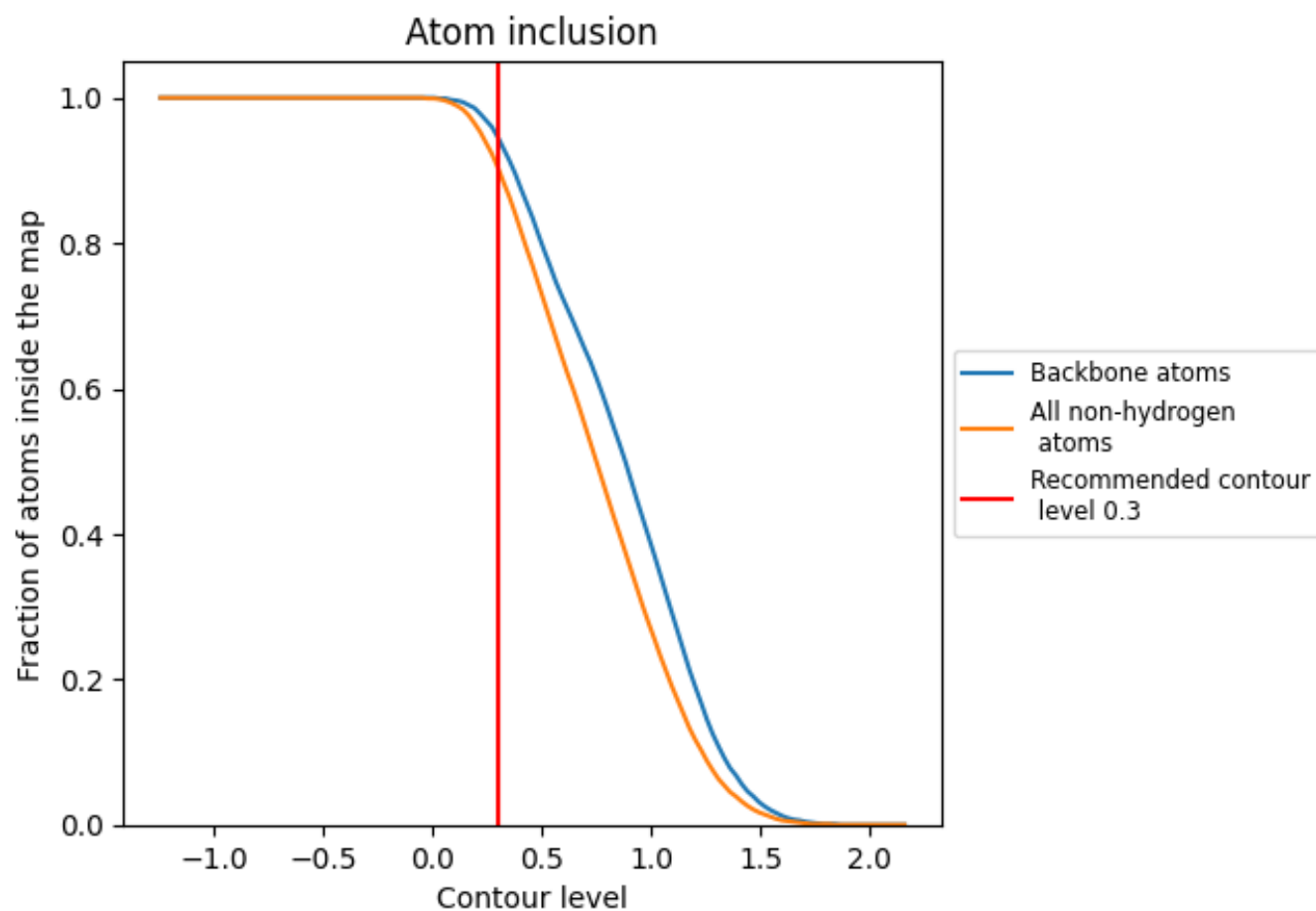
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.5890
A	 0.8690	 0.5670
B	 0.8770	 0.5670
C	 0.8900	 0.5770
D	 0.8690	 0.5670
E	 0.8600	 0.5610
F	 0.8790	 0.5760
G	 0.9060	 0.5920
H	 0.9020	 0.5990
I	 0.8970	 0.5850
J	 0.9490	 0.6150
K	 0.9520	 0.6200
L	 0.9480	 0.6210
M	 0.9210	 0.6040
N	 0.9140	 0.6080
O	 0.8640	 0.5590
P	 0.8870	 0.5760
Q	 0.8940	 0.5760
R	 0.8800	 0.5770
S	 0.8650	 0.5600
T	 0.8850	 0.5790
U	 0.9020	 0.5910
V	 0.9040	 0.6000
W	 0.8970	 0.5830
X	 0.9480	 0.6170
Y	 0.9520	 0.6200
Z	 0.9450	 0.6200
a	 0.9210	 0.6010
b	 0.9150	 0.6060

