



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:59 PM UTC

PDB ID : 8YSX / pdb_00008ysx
EMDB ID : EMD-39565
Title : canine immunoproteasome 20S subunit in complex with compound 2
Authors : Kashima, A.; Arai, Y.
Deposited on : 2024-03-24
Resolution : 2.20 Å(reported)

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 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) : 2.49

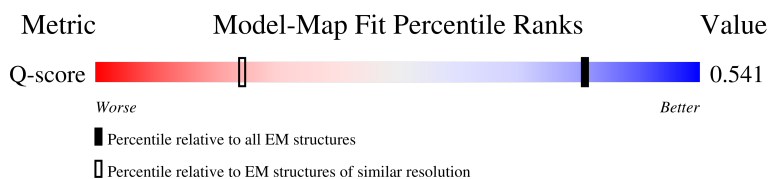
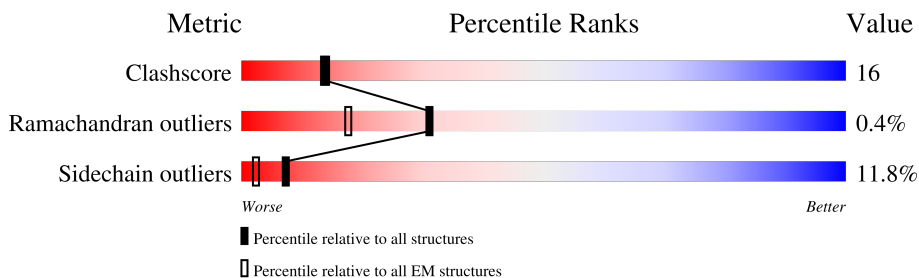
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	
1	F	199	
2	G	263	
2	L	263	

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Mol	Chain	Length	Quality of chain
3	H	241	
3	M	241	
4	I	248	
4	N	248	
5	O	261	
5	Z	261	
6	K	246	
6	R	246	
7	T	201	
7	V	201	
8	U	205	
8	Y	205	
9	W	264	
9	a	264	
10	C	204	
10	D	204	
11	P	234	
11	b	234	
12	S	241	
12	X	241	
13	J	255	
13	Q	255	
14	B	234	
14	E	234	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 47878 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	199	Total	C	N	O	S	0	0
			1488	934	254	290	10		
1	A	199	Total	C	N	O	S	0	0
			1488	934	254	290	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		
2	G	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		
3	H	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		
4	I	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		
5	Z	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	232	Total	C	N	O	S	0	0
			1783	1129	297	344	13		
6	K	232	Total	C	N	O	S	0	0
			1783	1129	297	344	13		

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		
7	V	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		
8	Y	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		
9	W	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		

- Molecule 10 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	201	Total	C	N	O	S	0	0
			1568	980	269	306	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	201	Total	C	N	O	S	0	0
			1568	980	269	306	13		

- Molecule 11 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		
11	P	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		
12	S	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		

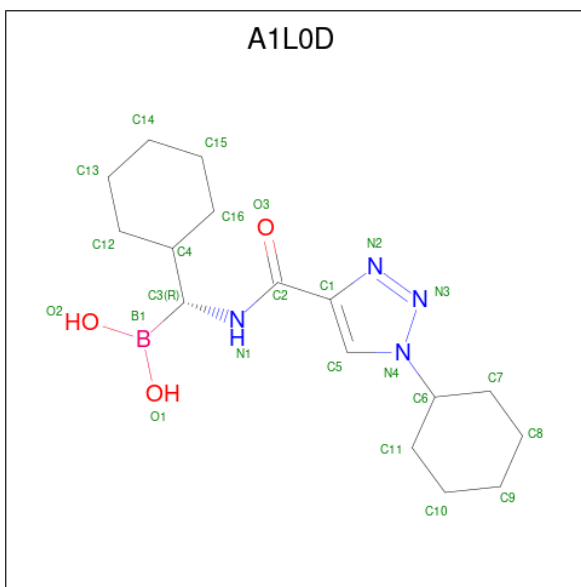
- Molecule 13 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		
13	Q	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		
14	B	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		

- Molecule 15 is [(R)-cyclohexyl-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]methyl]boronic acid (CCD ID: A1L0D) (formula: C₁₆H₂₇BN₄O₃).



Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	C	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	A	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	D	1	Total	B	C	N	O	0
			23	1	16	4	2	

- Molecule 16 is water.

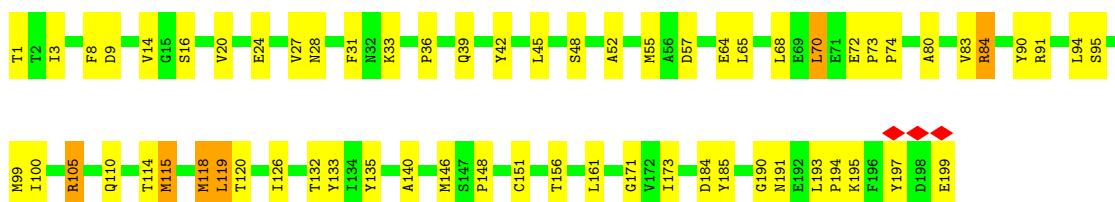
Mol	Chain	Residues	Atoms		AltConf
16	F	3	Total	O	0
			3	3	
16	C	2	Total	O	0
			2	2	
16	X	1	Total	O	0
			1	1	
16	E	2	Total	O	0
			2	2	
16	B	2	Total	O	0
			2	2	
16	A	3	Total	O	0
			3	3	
16	D	2	Total	O	0
			2	2	
16	S	1	Total	O	0
			1	1	

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.

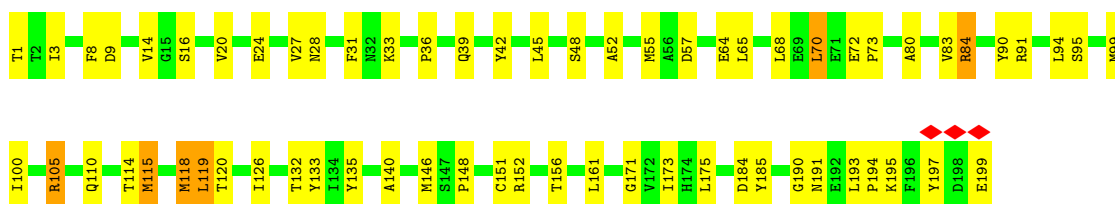
- Molecule 1: Proteasome subunit beta

Chain F: 



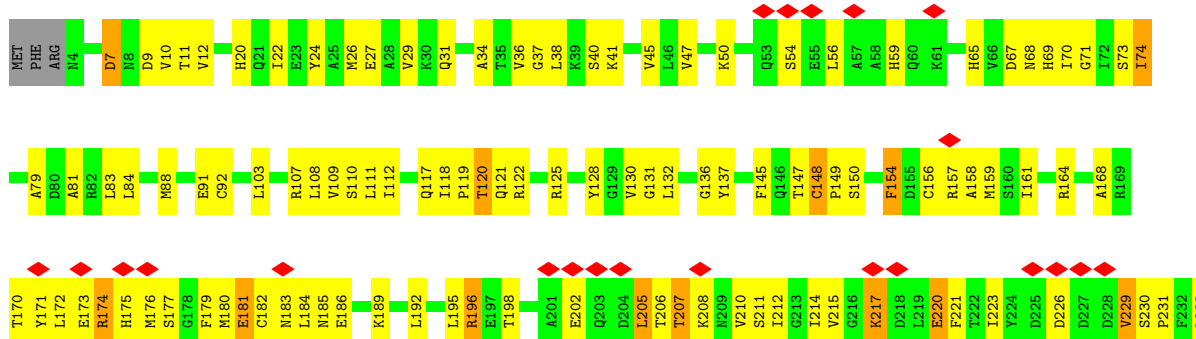
- Molecule 1: Proteasome subunit beta

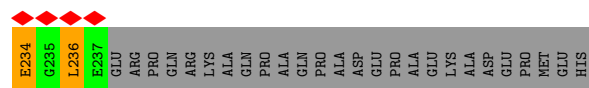
Chain A: 



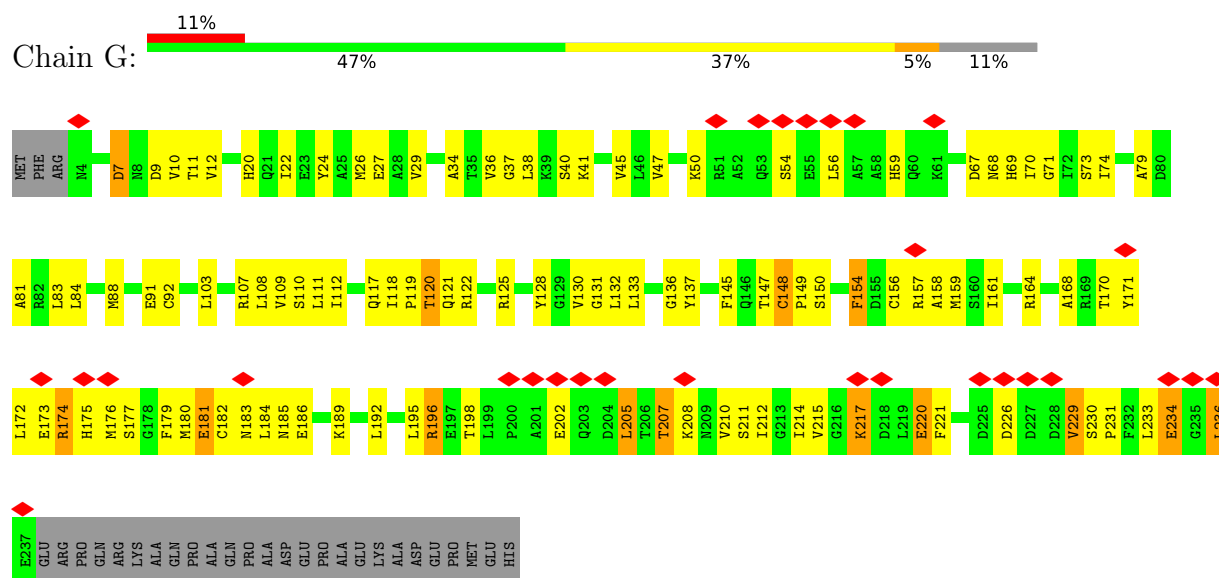
- Molecule 2: Proteasome subunit alpha type

Chain L: 

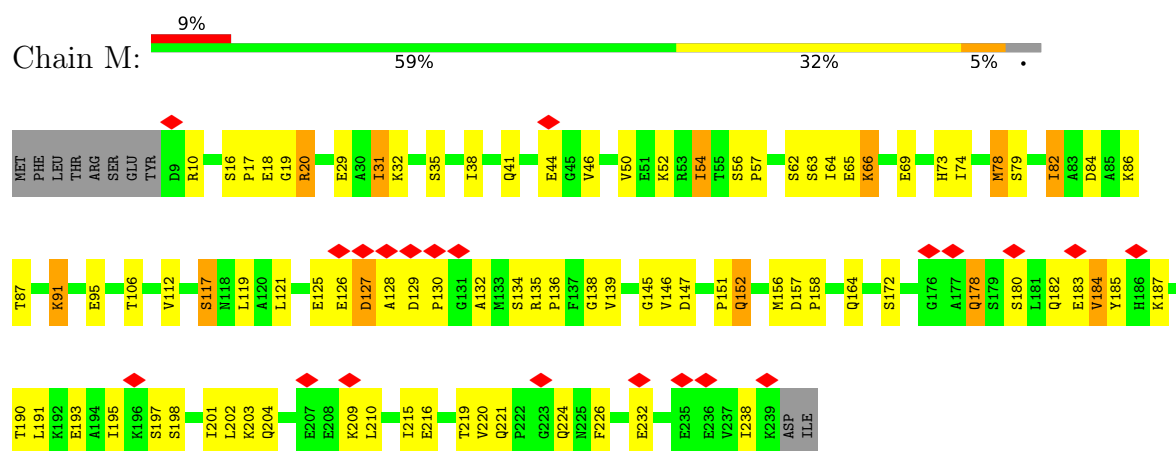




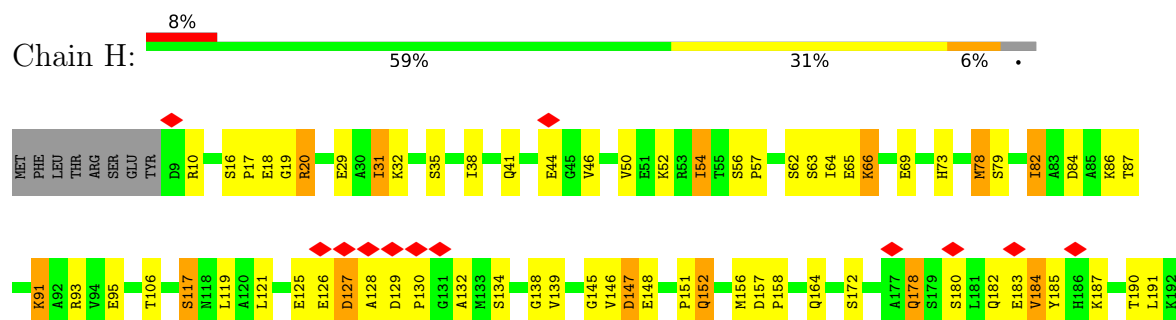
• Molecule 2: Proteasome subunit alpha type

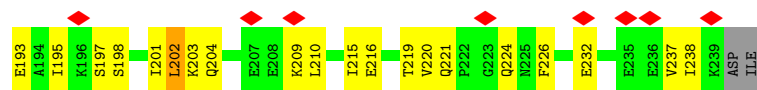


• Molecule 3: Proteasome subunit alpha type

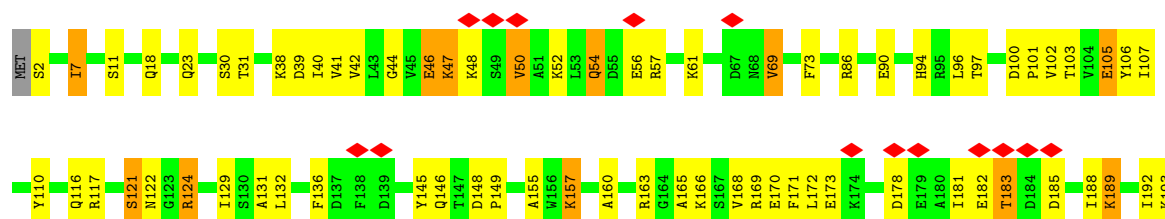


• Molecule 3: Proteasome subunit alpha type

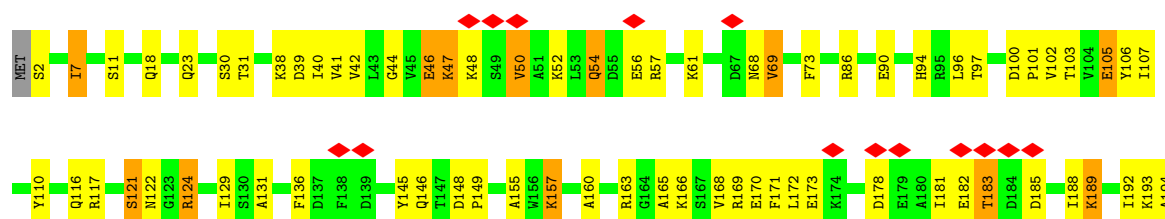




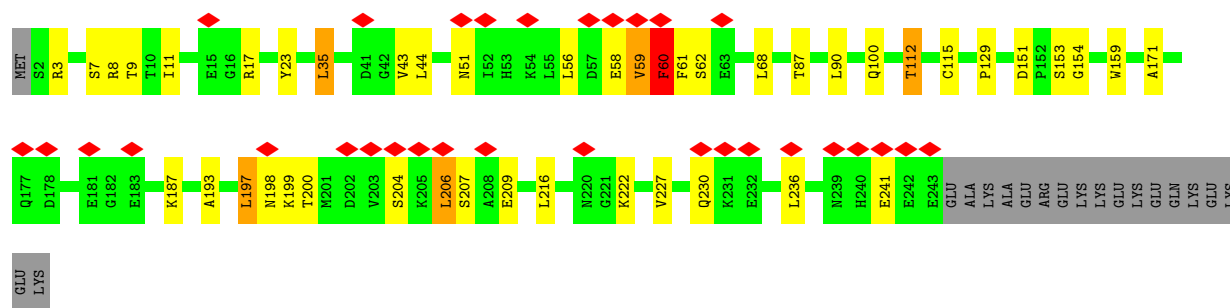
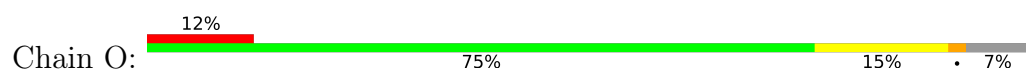
• Molecule 4: Proteasome subunit alpha type



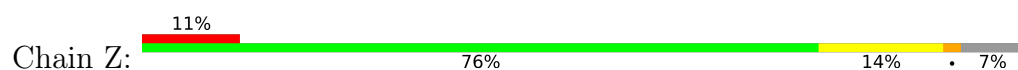
• Molecule 4: Proteasome subunit alpha type

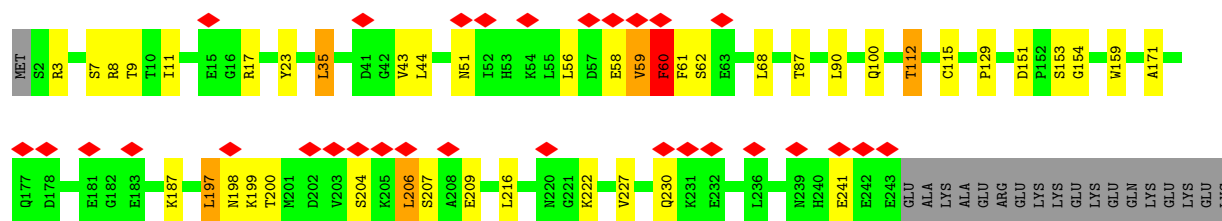


• Molecule 5: Proteasome subunit alpha type

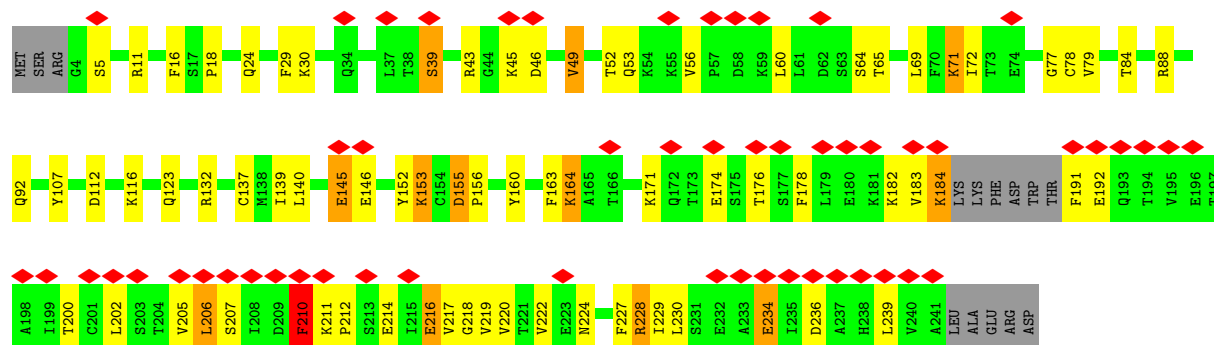


• Molecule 5: Proteasome subunit alpha type

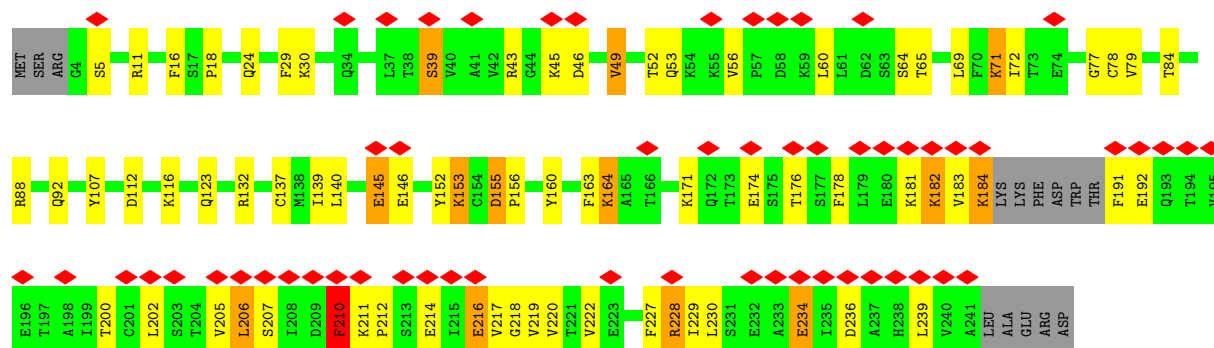




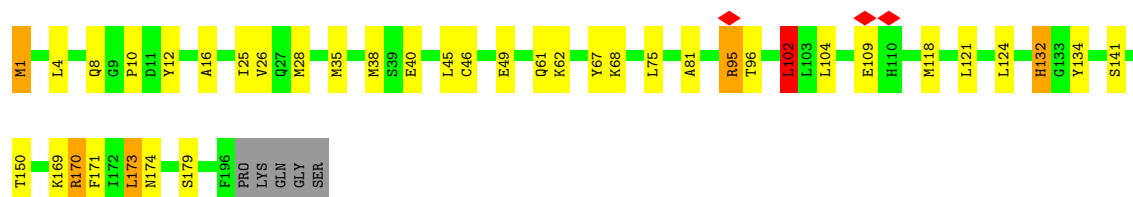
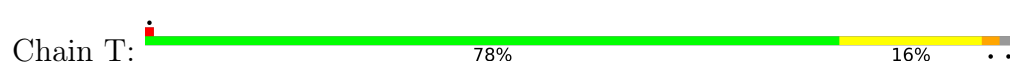
• Molecule 6: Proteasome subunit alpha type



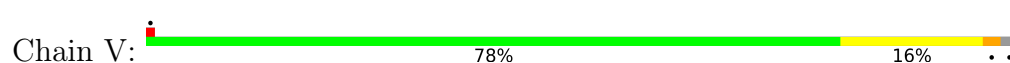
• Molecule 6: Proteasome subunit alpha type

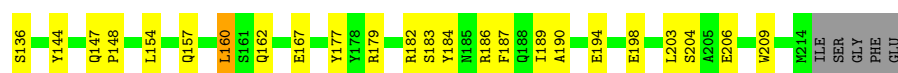


• Molecule 7: Proteasome subunit beta

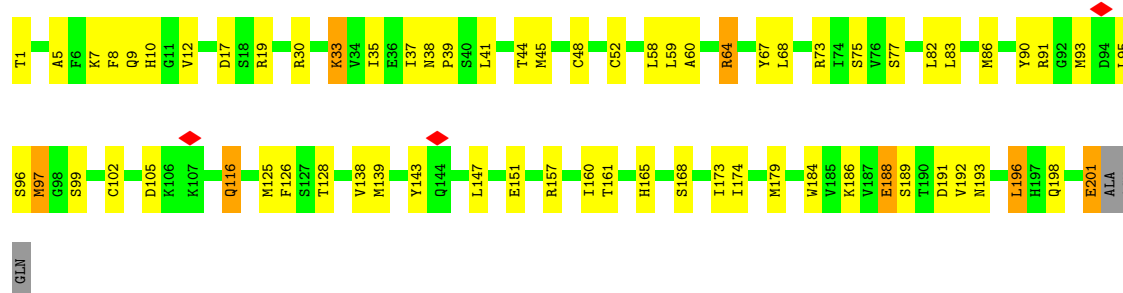


• Molecule 7: Proteasome subunit beta

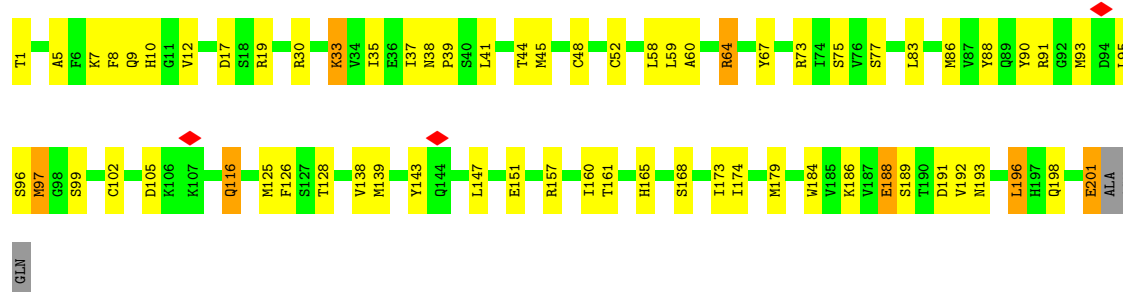




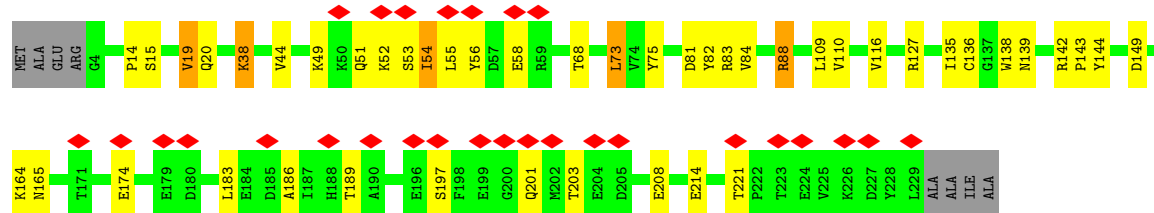
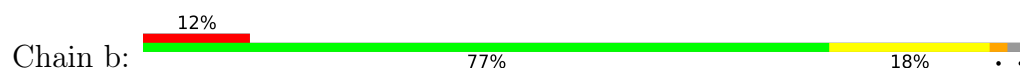
• Molecule 10: Proteasome subunit beta type-8



• Molecule 10: Proteasome subunit beta type-8

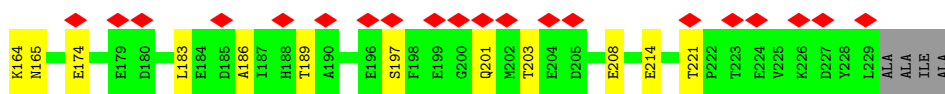


• Molecule 11: Proteasome subunit alpha type

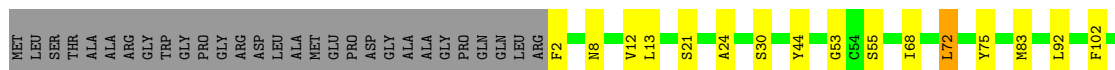


• Molecule 11: Proteasome subunit alpha type





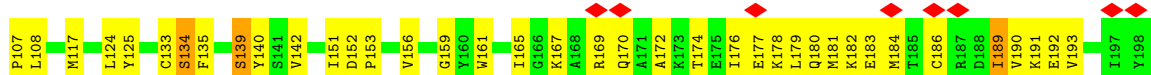
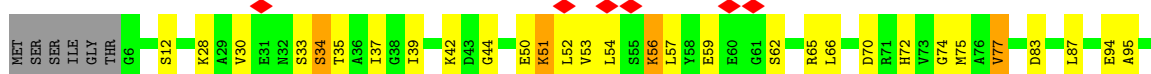
• Molecule 12: Proteasome subunit beta



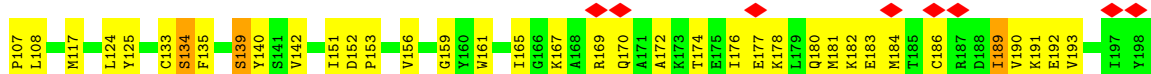
• Molecule 12: Proteasome subunit beta



• Molecule 13: Proteasome subunit alpha type

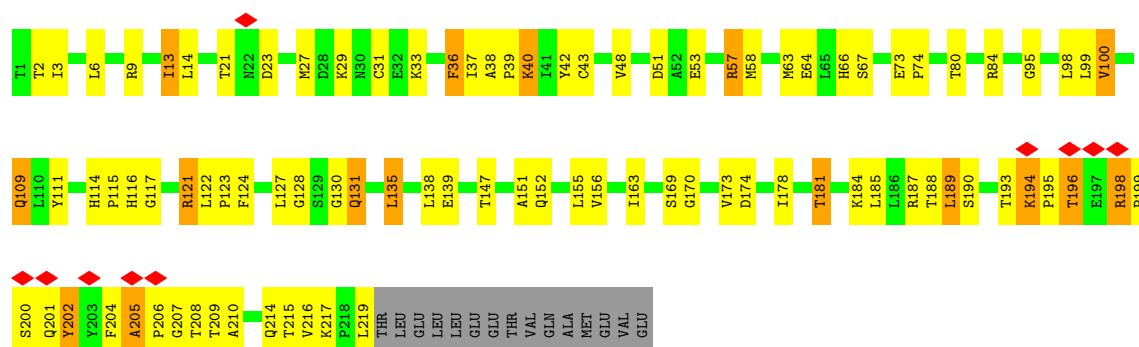


• Molecule 13: Proteasome subunit alpha type

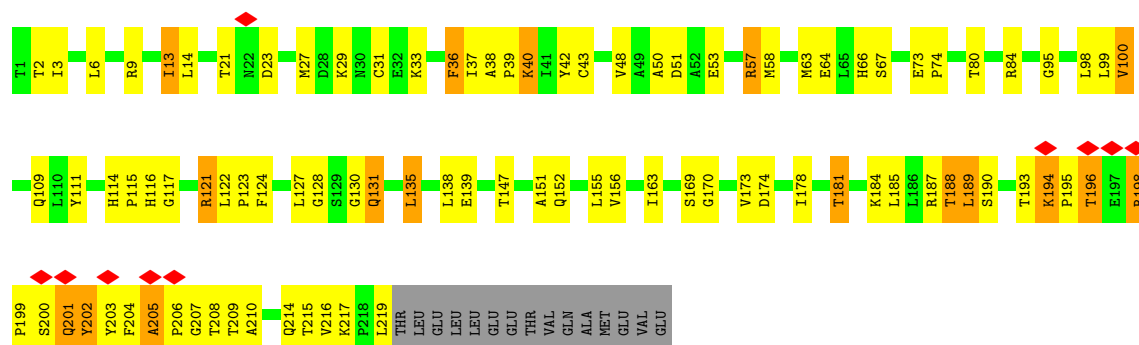




• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	304965	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size ($\text{\AA}$)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	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: A1L0D

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	0.38	0/1517	0.76	1/2058 (0.0%)
1	F	0.38	0/1517	0.76	1/2058 (0.0%)
2	G	0.33	0/1866	0.81	2/2522 (0.1%)
2	L	0.33	0/1866	0.81	2/2522 (0.1%)
3	H	0.34	0/1788	0.75	1/2415 (0.0%)
3	M	0.34	0/1788	0.75	1/2415 (0.0%)
4	I	0.32	0/1842	0.80	1/2489 (0.0%)
4	N	0.32	0/1842	0.80	1/2489 (0.0%)
5	O	0.75	0/1934	1.34	8/2608 (0.3%)
5	Z	0.75	0/1934	1.34	8/2608 (0.3%)
6	K	0.34	0/1813	0.79	4/2452 (0.2%)
6	R	0.34	0/1813	0.79	6/2452 (0.2%)
7	T	0.36	0/1599	0.77	1/2163 (0.0%)
7	V	0.36	0/1599	0.77	1/2163 (0.0%)
8	U	0.38	0/1622	0.82	3/2186 (0.1%)
8	Y	0.38	0/1622	0.82	3/2186 (0.1%)
9	W	0.36	0/1706	0.81	3/2308 (0.1%)
9	a	0.36	0/1706	0.81	4/2308 (0.2%)
10	C	0.81	0/1600	0.98	1/2160 (0.0%)
10	D	0.81	0/1600	0.98	1/2160 (0.0%)
11	P	0.78	0/1808	1.38	5/2449 (0.2%)
11	b	0.78	0/1808	1.38	5/2449 (0.2%)
12	S	0.81	0/1675	1.03	4/2258 (0.2%)
12	X	0.81	0/1675	1.03	4/2258 (0.2%)
13	J	0.33	0/1901	0.78	2/2559 (0.1%)
13	Q	0.33	0/1901	0.78	2/2559 (0.1%)
14	B	0.38	0/1650	0.82	1/2242 (0.0%)
14	E	0.38	0/1650	0.82	1/2242 (0.0%)
All	All	0.52	0/48642	0.93	77/65738 (0.1%)

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	54	ILE	N-CA-C	-6.96	106.02	112.43
11	P	54	ILE	N-CA-C	-6.96	106.03	112.43
2	G	148	CYS	CA-C-N	6.78	126.41	119.56
2	G	148	CYS	C-N-CA	6.78	126.41	119.56
2	L	148	CYS	CA-C-N	6.77	126.39	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1488	0	1444	58	0
1	F	1488	0	1444	57	0
2	G	1832	0	1823	98	0
2	L	1832	0	1823	104	0
3	H	1761	0	1749	66	0
3	M	1761	0	1749	63	0
4	I	1815	0	1845	77	0
4	N	1815	0	1845	76	0
5	O	1904	0	1918	21	0
5	Z	1904	0	1918	19	0
6	K	1783	0	1775	78	0
6	R	1783	0	1775	73	0
7	T	1567	0	1567	33	0
7	V	1567	0	1567	33	0
8	U	1593	0	1614	55	0
8	Y	1593	0	1614	53	0
9	W	1673	0	1650	60	0
9	a	1673	0	1650	63	0
10	C	1568	0	1513	61	0
10	D	1568	0	1513	60	0
11	P	1769	0	1761	29	0
11	b	1769	0	1761	29	0
12	S	1644	0	1638	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	1644	0	1638	36	0
13	J	1866	0	1855	71	0
13	Q	1866	0	1855	70	0
14	B	1622	0	1634	118	0
14	E	1622	0	1634	113	0
15	A	23	0	0	1	0
15	C	23	0	0	0	0
15	D	23	0	0	0	0
15	F	23	0	0	1	0
16	A	3	0	0	0	0
16	B	2	0	0	1	0
16	C	2	0	0	0	0
16	D	2	0	0	0	0
16	E	2	0	0	1	0
16	F	3	0	0	0	0
16	S	1	0	0	0	0
16	X	1	0	0	0	0
All	All	47878	0	47572	1497	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 16.

The worst 5 of 1497 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)
13:Q:37:ILE:HD11	13:Q:193:VAL:HG13	1.23	1.20
2:G:196:ARG:CB	2:G:205:LEU:HD11	1.70	1.19
4:I:48:LYS:HE2	4:I:163:ARG:NH1	1.57	1.19
2:L:196:ARG:CB	2:L:205:LEU:HD11	1.70	1.19
4:N:48:LYS:HE2	4:N:163:ARG:NH1	1.57	1.16

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	197/199 (99%)	192 (98%)	4 (2%)	1 (0%)	24	27
1	F	197/199 (99%)	192 (98%)	4 (2%)	1 (0%)	24	27
2	G	232/263 (88%)	223 (96%)	9 (4%)	0	100	100
2	L	232/263 (88%)	223 (96%)	9 (4%)	0	100	100
3	H	229/241 (95%)	219 (96%)	9 (4%)	1 (0%)	30	34
3	M	229/241 (95%)	219 (96%)	9 (4%)	1 (0%)	30	34
4	I	229/248 (92%)	221 (96%)	8 (4%)	0	100	100
4	N	229/248 (92%)	221 (96%)	8 (4%)	0	100	100
5	O	240/261 (92%)	229 (95%)	7 (3%)	4 (2%)	7	5
5	Z	240/261 (92%)	229 (95%)	7 (3%)	4 (2%)	7	5
6	K	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
6	R	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
7	T	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
7	V	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
8	U	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
8	Y	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
9	a	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
10	C	199/204 (98%)	190 (96%)	9 (4%)	0	100	100
10	D	199/204 (98%)	190 (96%)	9 (4%)	0	100	100
11	P	224/234 (96%)	212 (95%)	12 (5%)	0	100	100
11	b	224/234 (96%)	212 (95%)	12 (5%)	0	100	100
12	S	210/241 (87%)	206 (98%)	4 (2%)	0	100	100
12	X	210/241 (87%)	206 (98%)	4 (2%)	0	100	100
13	J	236/255 (92%)	224 (95%)	11 (5%)	1 (0%)	30	34
13	Q	236/255 (92%)	224 (95%)	11 (5%)	1 (0%)	30	34
14	B	217/234 (93%)	204 (94%)	7 (3%)	6 (3%)	4	2
14	E	217/234 (93%)	204 (94%)	7 (3%)	6 (3%)	4	2
All	All	6098/6592 (92%)	5852 (96%)	220 (4%)	26 (0%)	31	34

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	O	59	VAL
5	Z	59	VAL
5	O	204	SER
5	Z	204	SER
5	O	60	PHE

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	152/152 (100%)	134 (88%)	18 (12%)	5	5
1	F	152/152 (100%)	134 (88%)	18 (12%)	5	5
2	G	199/223 (89%)	169 (85%)	30 (15%)	3	2
2	L	199/223 (89%)	169 (85%)	30 (15%)	3	2
3	H	193/203 (95%)	160 (83%)	33 (17%)	2	2
3	M	193/203 (95%)	160 (83%)	33 (17%)	2	2
4	I	195/211 (92%)	159 (82%)	36 (18%)	1	1
4	N	195/211 (92%)	159 (82%)	36 (18%)	1	1
5	O	204/221 (92%)	189 (93%)	15 (7%)	13	14
5	Z	204/221 (92%)	189 (93%)	15 (7%)	13	14
6	K	194/210 (92%)	170 (88%)	24 (12%)	4	4
6	R	194/210 (92%)	170 (88%)	24 (12%)	4	4
7	T	167/171 (98%)	152 (91%)	15 (9%)	9	9
7	V	167/171 (98%)	152 (91%)	15 (9%)	9	9
8	U	174/175 (99%)	162 (93%)	12 (7%)	14	16
8	Y	174/175 (99%)	162 (93%)	12 (7%)	14	16
9	W	176/215 (82%)	157 (89%)	19 (11%)	6	6
9	a	176/215 (82%)	158 (90%)	18 (10%)	7	7
10	C	168/170 (99%)	152 (90%)	16 (10%)	8	8
10	D	168/170 (99%)	152 (90%)	16 (10%)	8	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	187/191 (98%)	172 (92%)	15 (8%)	11	13
11	b	187/191 (98%)	171 (91%)	16 (9%)	10	10
12	S	178/197 (90%)	169 (95%)	9 (5%)	21	27
12	X	178/197 (90%)	169 (95%)	9 (5%)	21	27
13	J	196/212 (92%)	167 (85%)	29 (15%)	3	2
13	Q	196/212 (92%)	167 (85%)	29 (15%)	3	2
14	B	174/188 (93%)	144 (83%)	30 (17%)	2	2
14	E	174/188 (93%)	144 (83%)	30 (17%)	2	2
All	All	5114/5478 (93%)	4512 (88%)	602 (12%)	7	5

5 of 602 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	B	29	LYS
10	D	189	SER
14	B	152	GLN
14	B	21	THR
1	A	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
7	V	82	ASN
14	B	30	ASN
12	S	157	ASN
8	Y	156	ASN
2	G	203	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](#)

4 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	A1L0D	F	301	1	22,25,26	0.40	0	29,33,35	0.83	2 (6%)
15	A1L0D	C	401	10	22,25,26	0.75	0	29,33,35	1.12	2 (6%)
15	A1L0D	A	301	1	22,25,26	0.41	0	29,33,35	0.83	2 (6%)
15	A1L0D	D	401	10	22,25,26	0.75	0	29,33,35	1.12	2 (6%)

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	A1L0D	F	301	1	-	0/13/34/36	0/3/3/3
15	A1L0D	C	401	10	-	0/13/34/36	0/3/3/3
15	A1L0D	A	301	1	-	0/13/34/36	0/3/3/3
15	A1L0D	D	401	10	-	0/13/34/36	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	301	A1L0D	C12-C4-C3	-2.76	109.44	112.16
15	F	301	A1L0D	C16-C4-C3	-2.75	109.45	112.16
15	C	401	A1L0D	C1-N2-N3	2.52	110.98	108.84
15	D	401	A1L0D	C1-N2-N3	2.52	110.98	108.84
15	C	401	A1L0D	C16-C4-C3	-2.46	109.74	112.16

There are no chirality outliers.

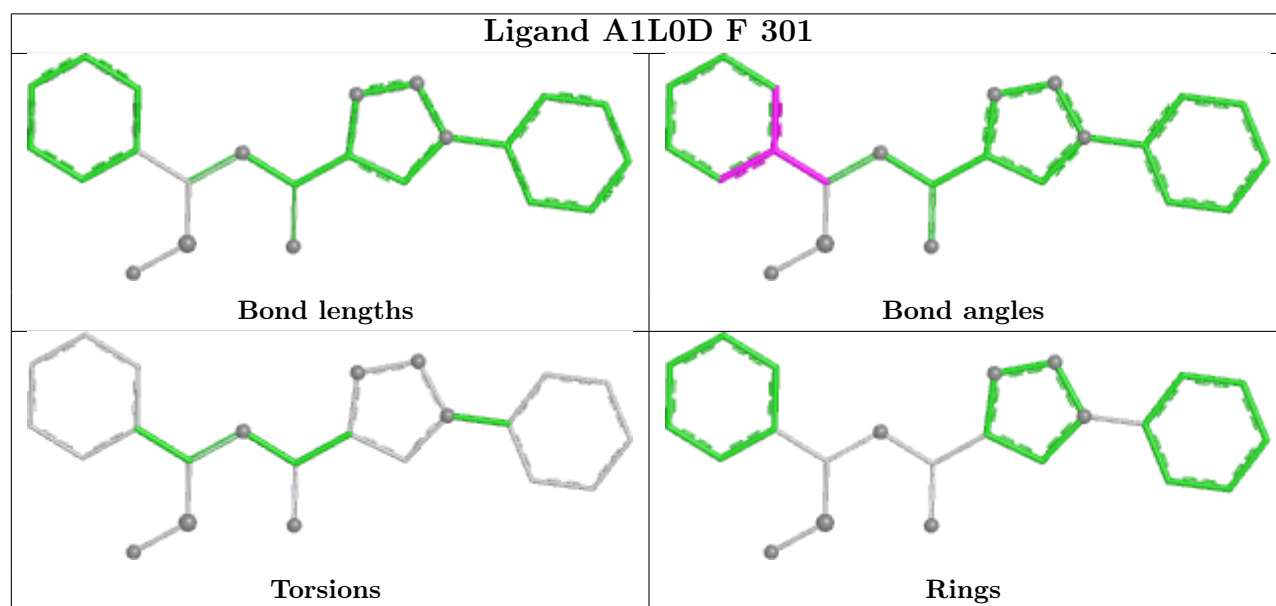
There are no torsion outliers.

There are no ring outliers.

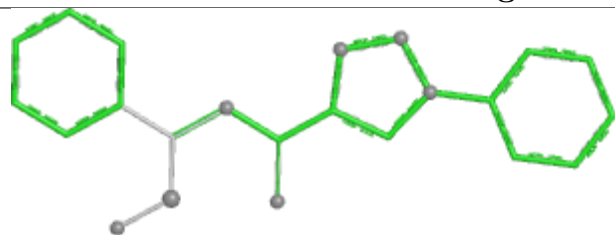
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	301	A1L0D	1	0
15	A	301	A1L0D	1	0

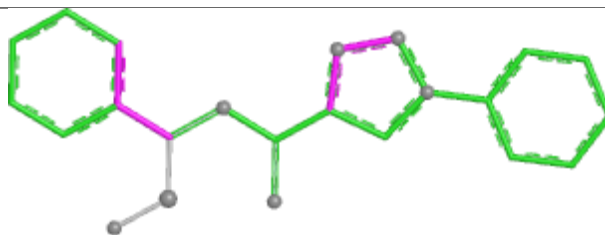
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



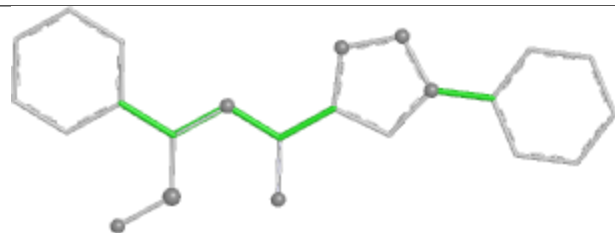
Ligand A1L0D C 401



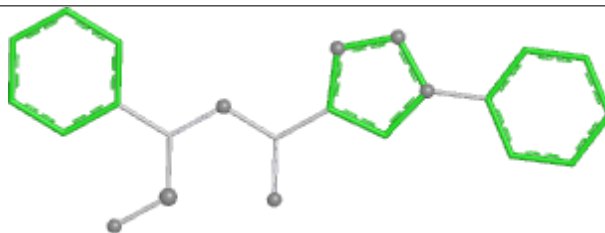
Bond lengths



Bond angles

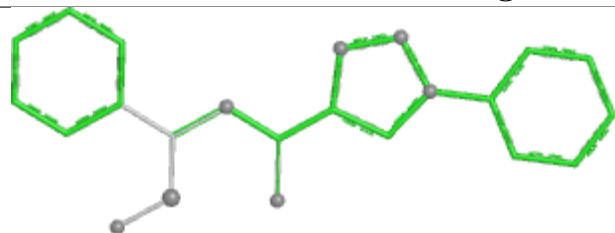


Torsions

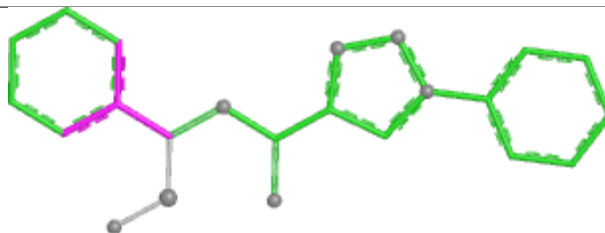


Rings

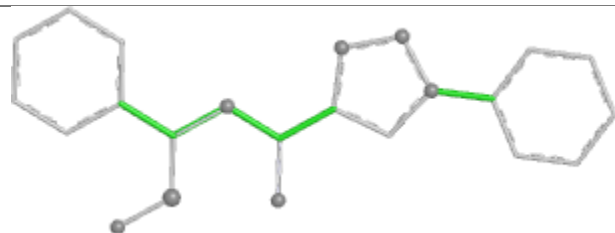
Ligand A1L0D A 301



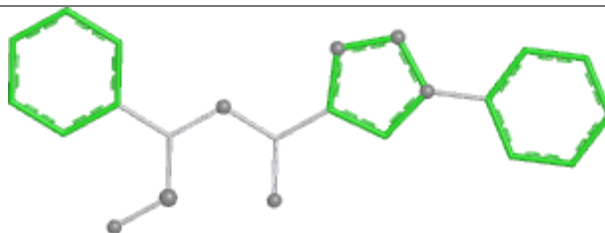
Bond lengths



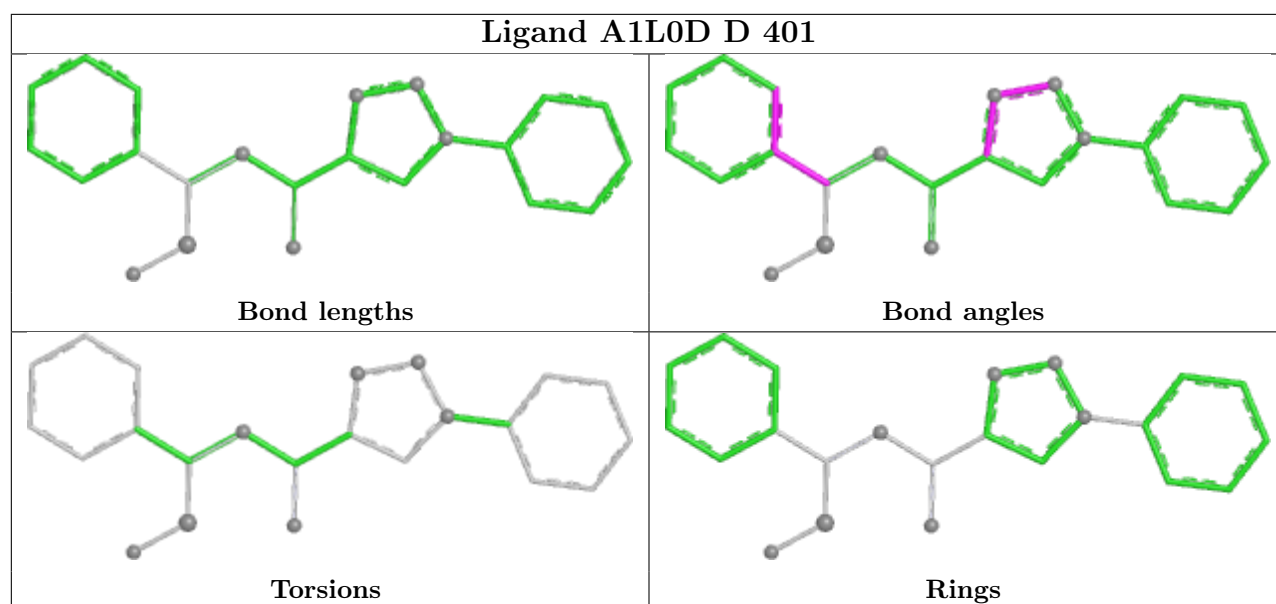
Bond angles



Torsions



Rings



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.

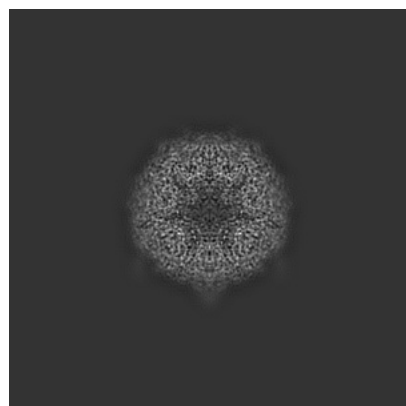
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39565. These allow visual inspection of the internal detail of the map and identification of artifacts.

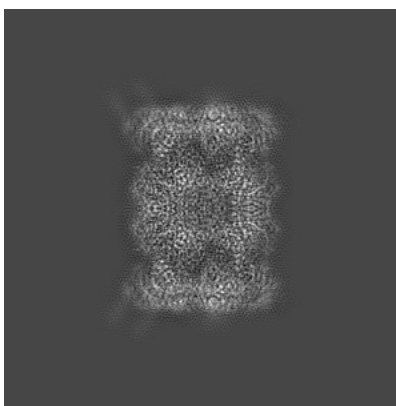
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

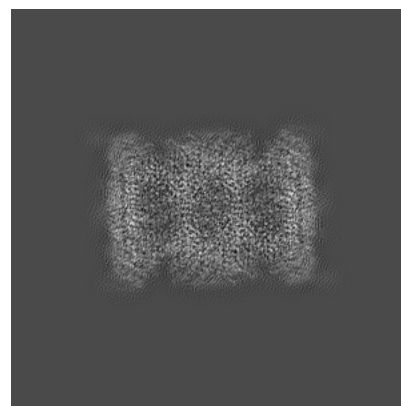
6.1.1 Primary map



X

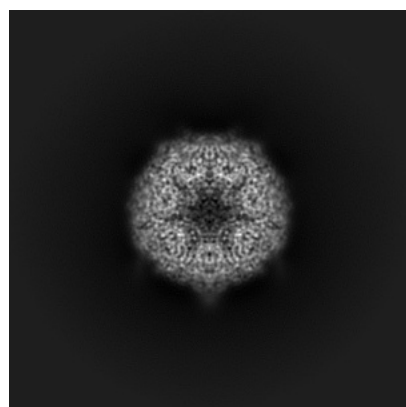


Y

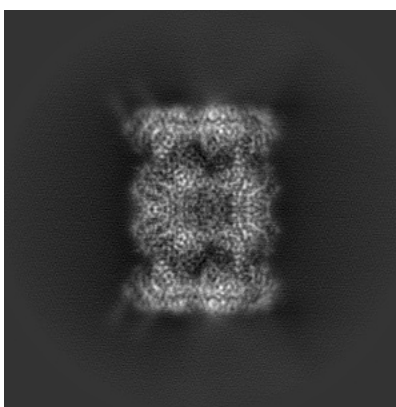


Z

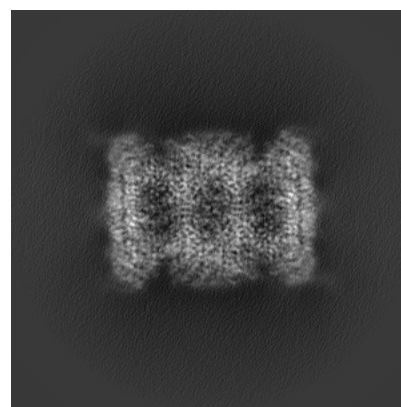
6.1.2 Raw map



X



Y

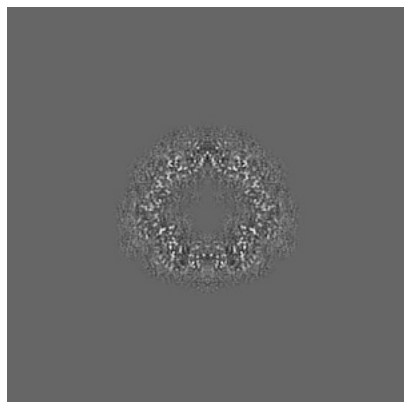


Z

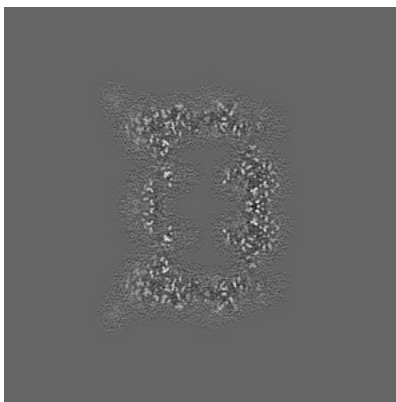
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

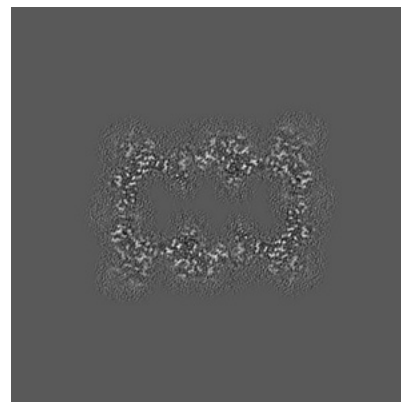
6.2.1 Primary map



X Index: 176

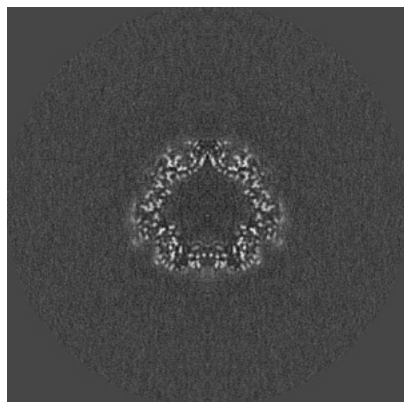


Y Index: 176

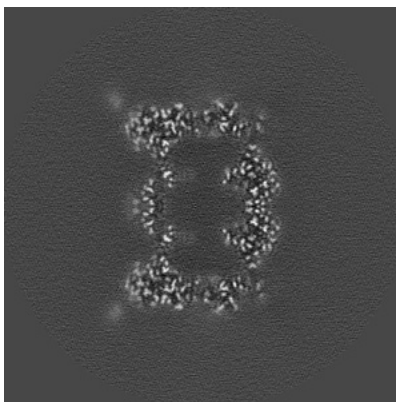


Z Index: 176

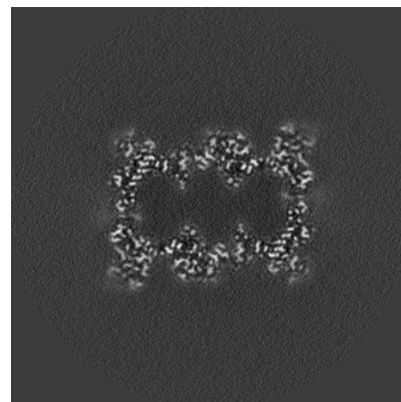
6.2.2 Raw map



X Index: 176



Y Index: 176

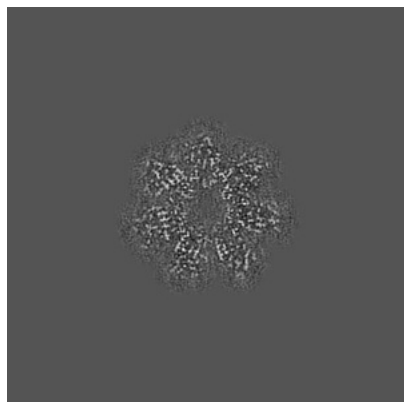


Z Index: 176

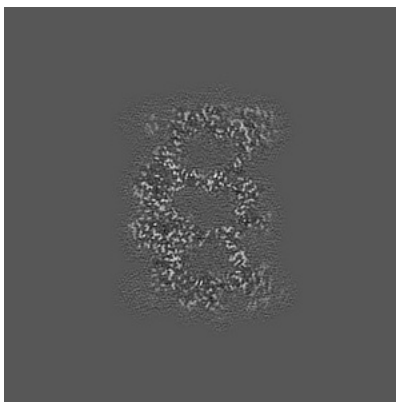
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

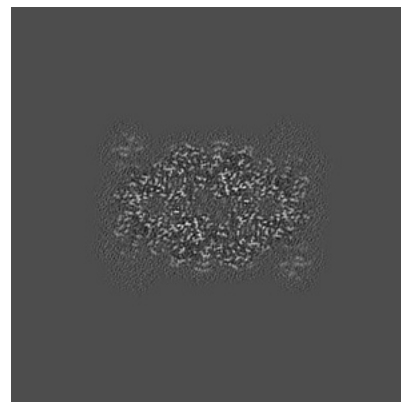
6.3.1 Primary map



X Index: 199

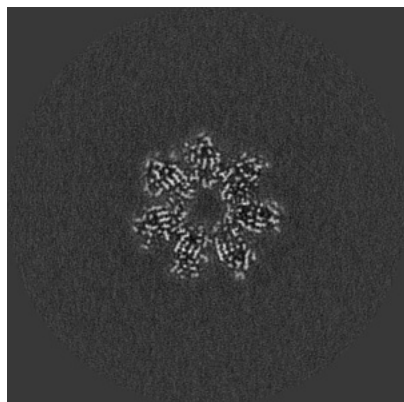


Y Index: 199

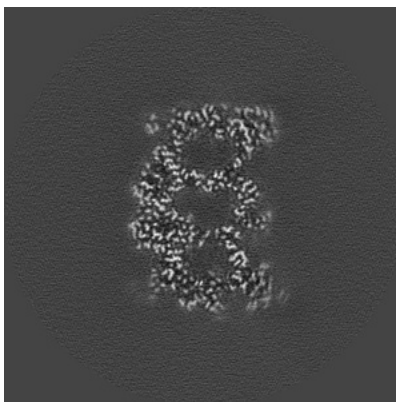


Z Index: 206

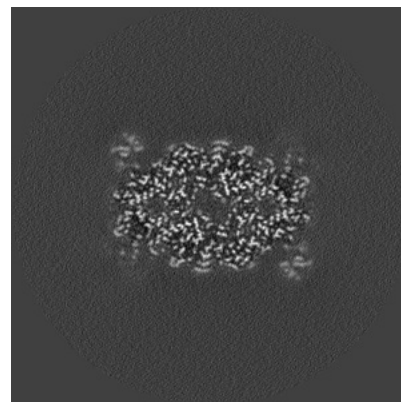
6.3.2 Raw map



X Index: 199



Y Index: 199

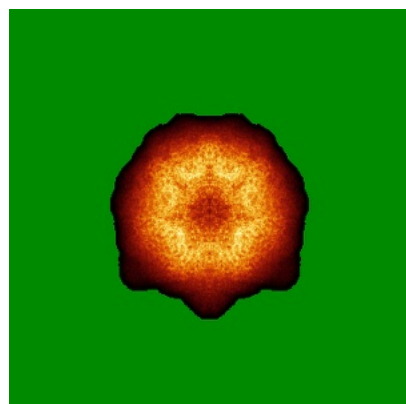


Z Index: 206

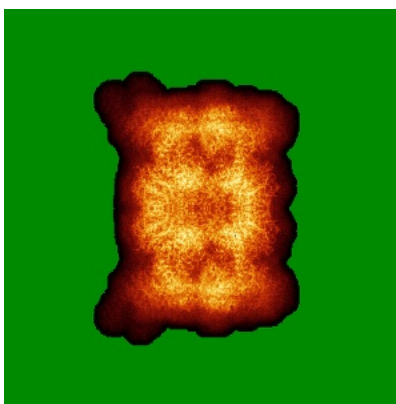
The images above show the largest variance slices of the map in three orthogonal directions.

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

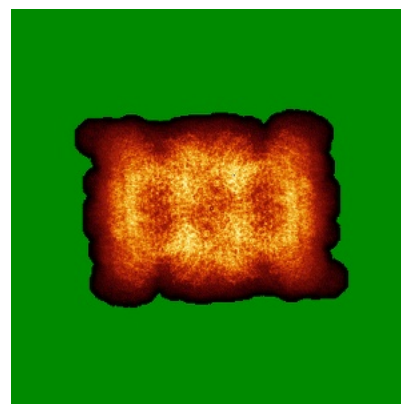
6.4.1 Primary map



X

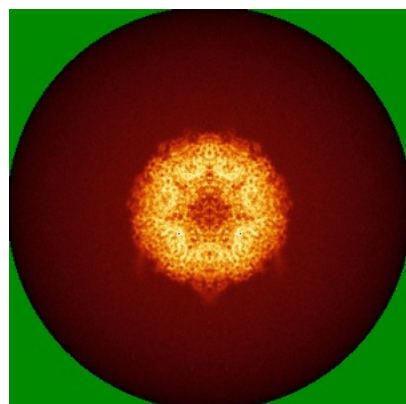


Y

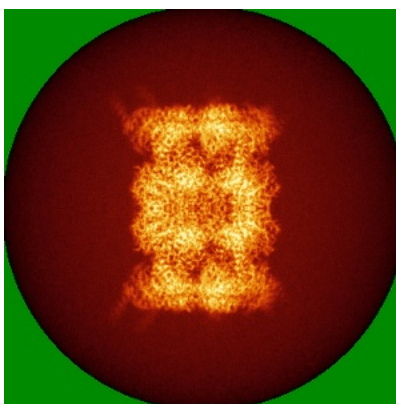


Z

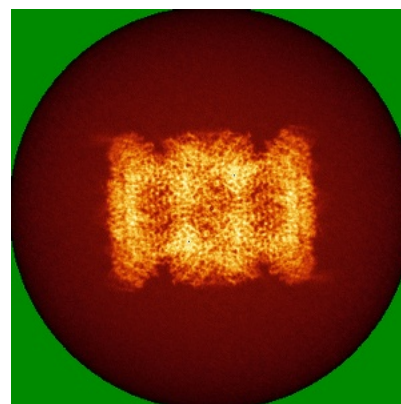
6.4.2 Raw map



X



Y

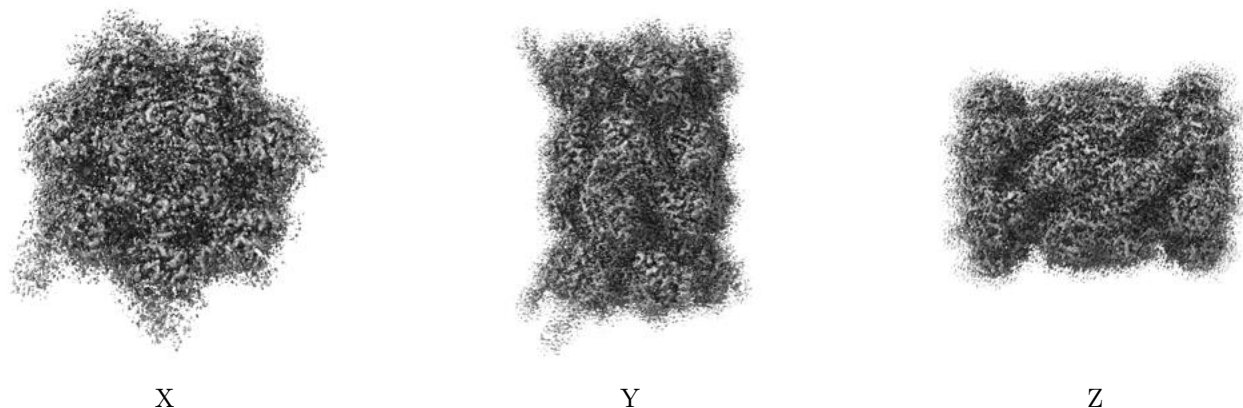


Z

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.

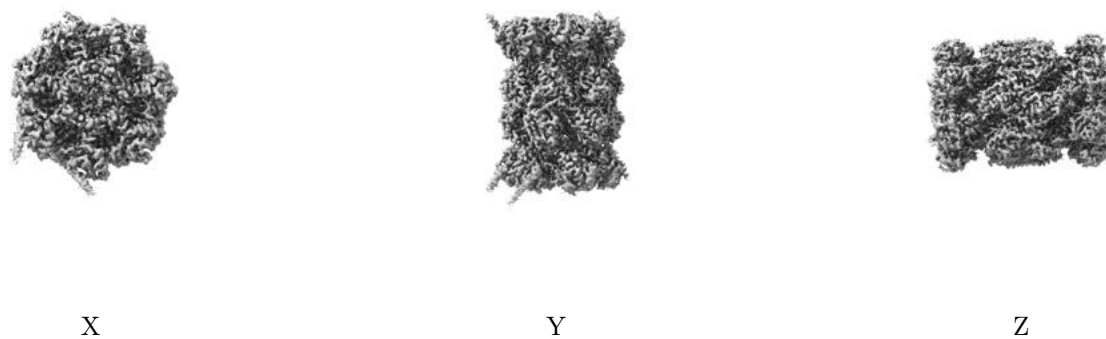
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. 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



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.

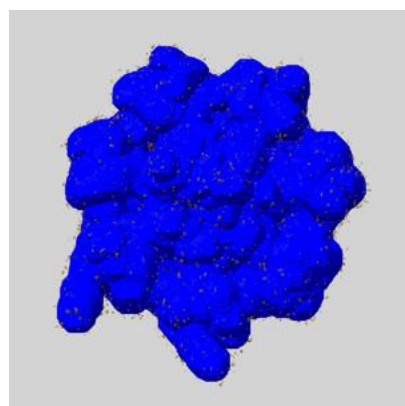
6.6 Mask visualisation [i](#)

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

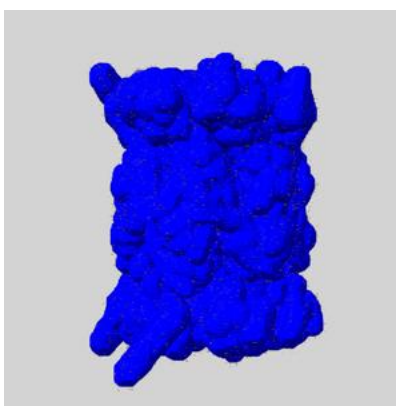
A mask typically either:

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

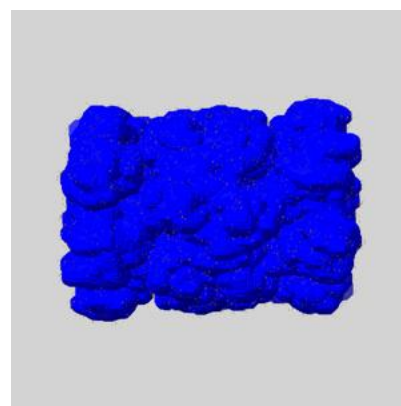
6.6.1 emd_39565_msk_1.map [i](#)



X



Y

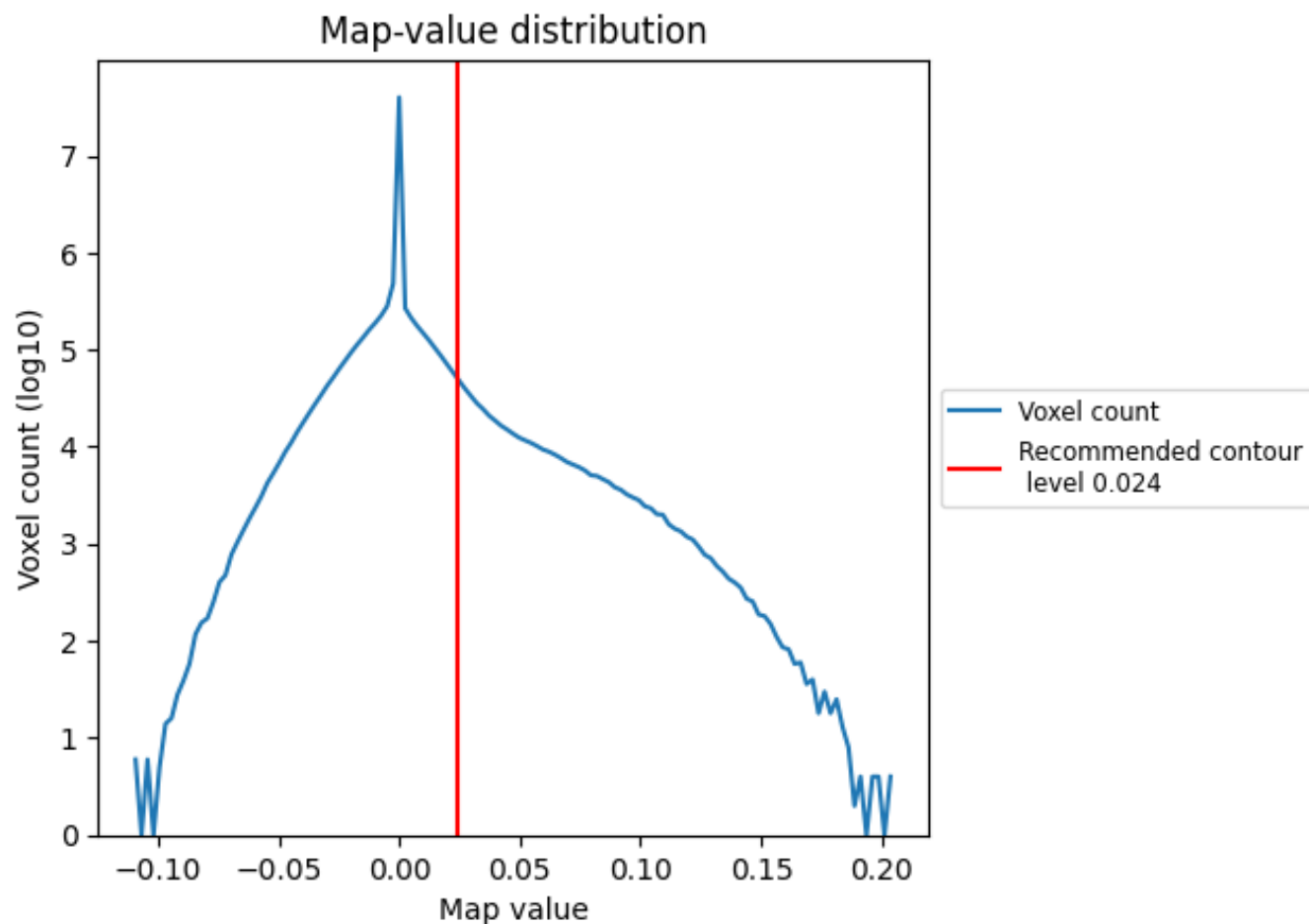


Z

7 Map analysis [i](#)

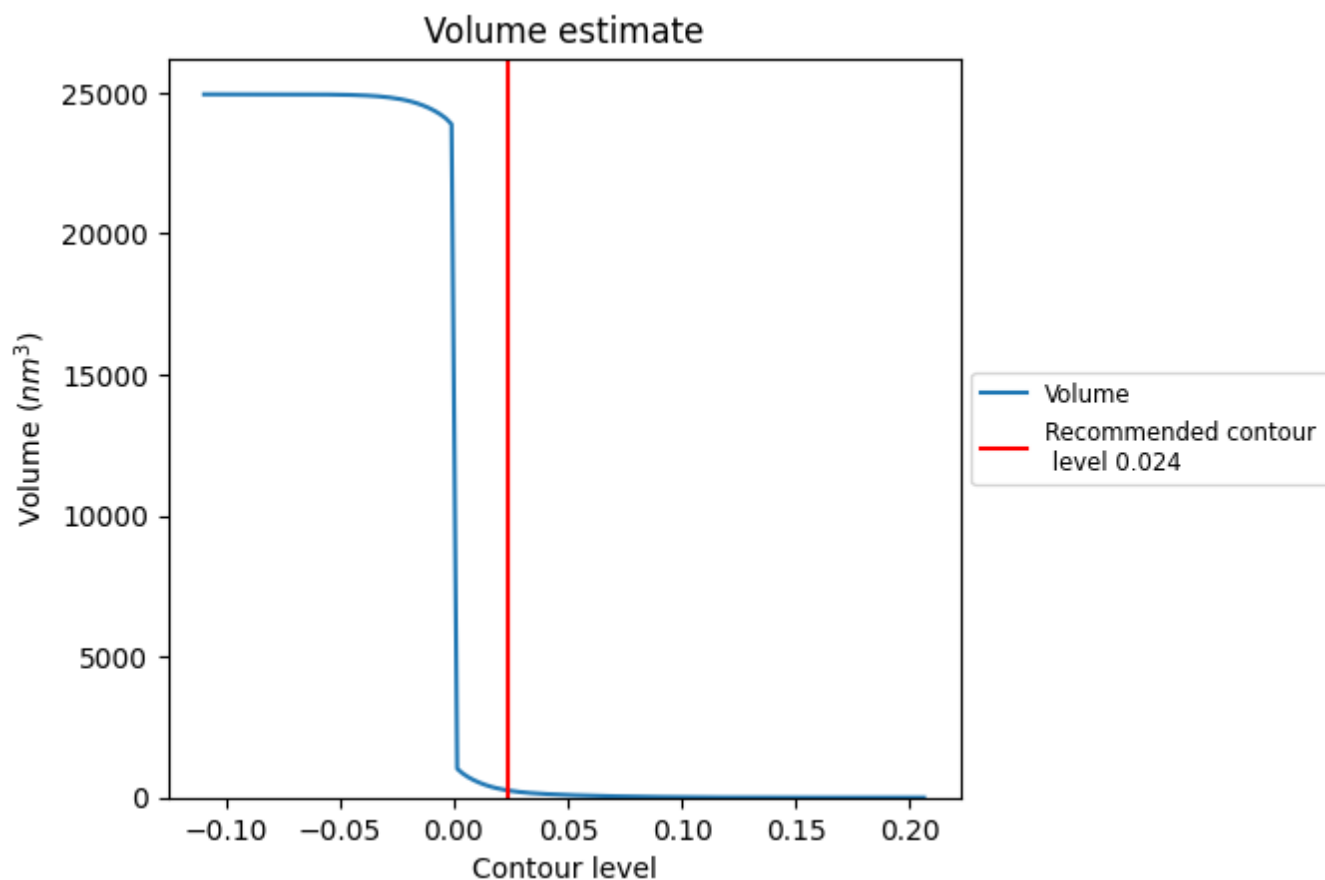
This section contains the results of statistical analysis of the map.

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.

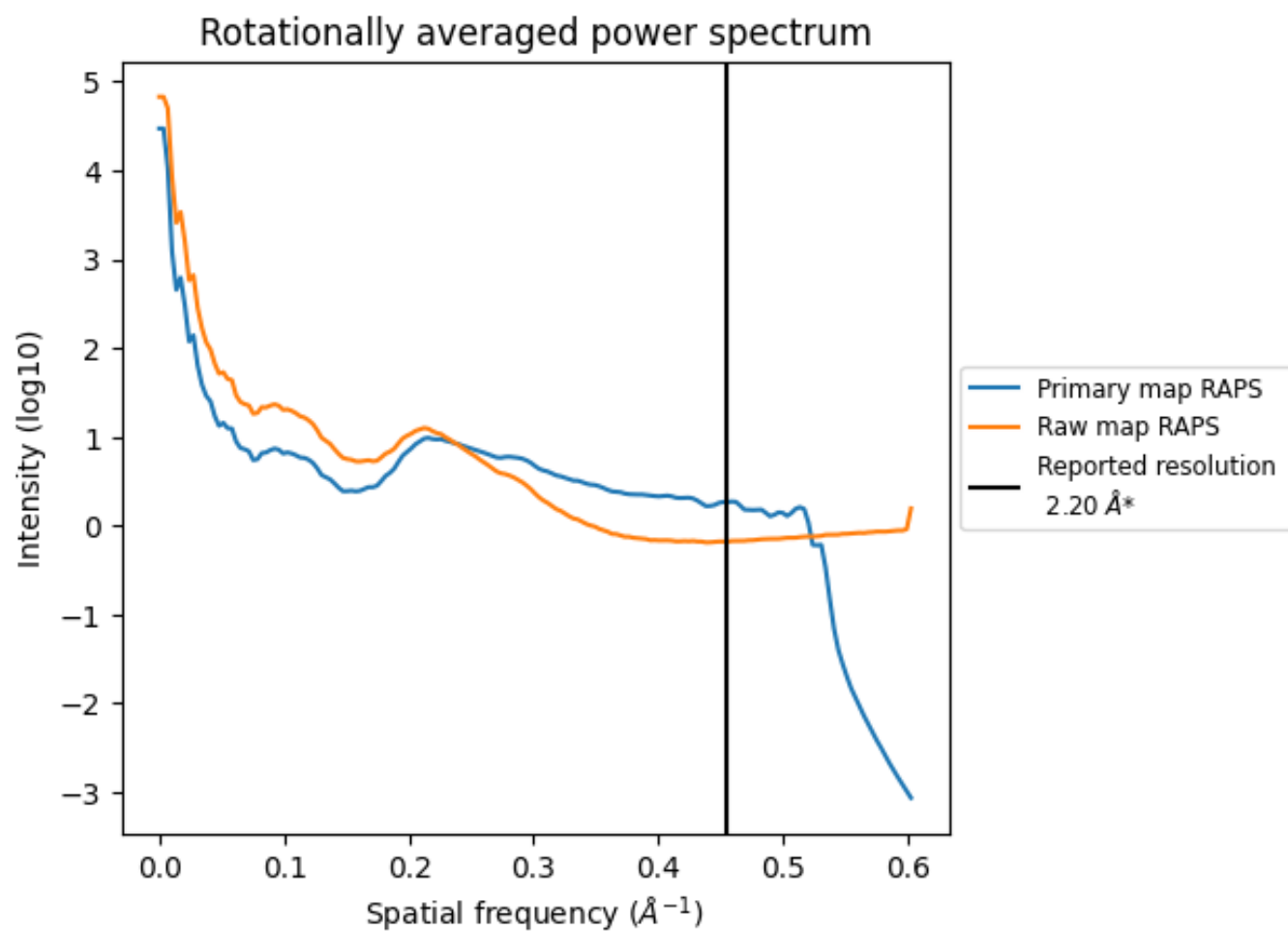
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 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 ⓘ

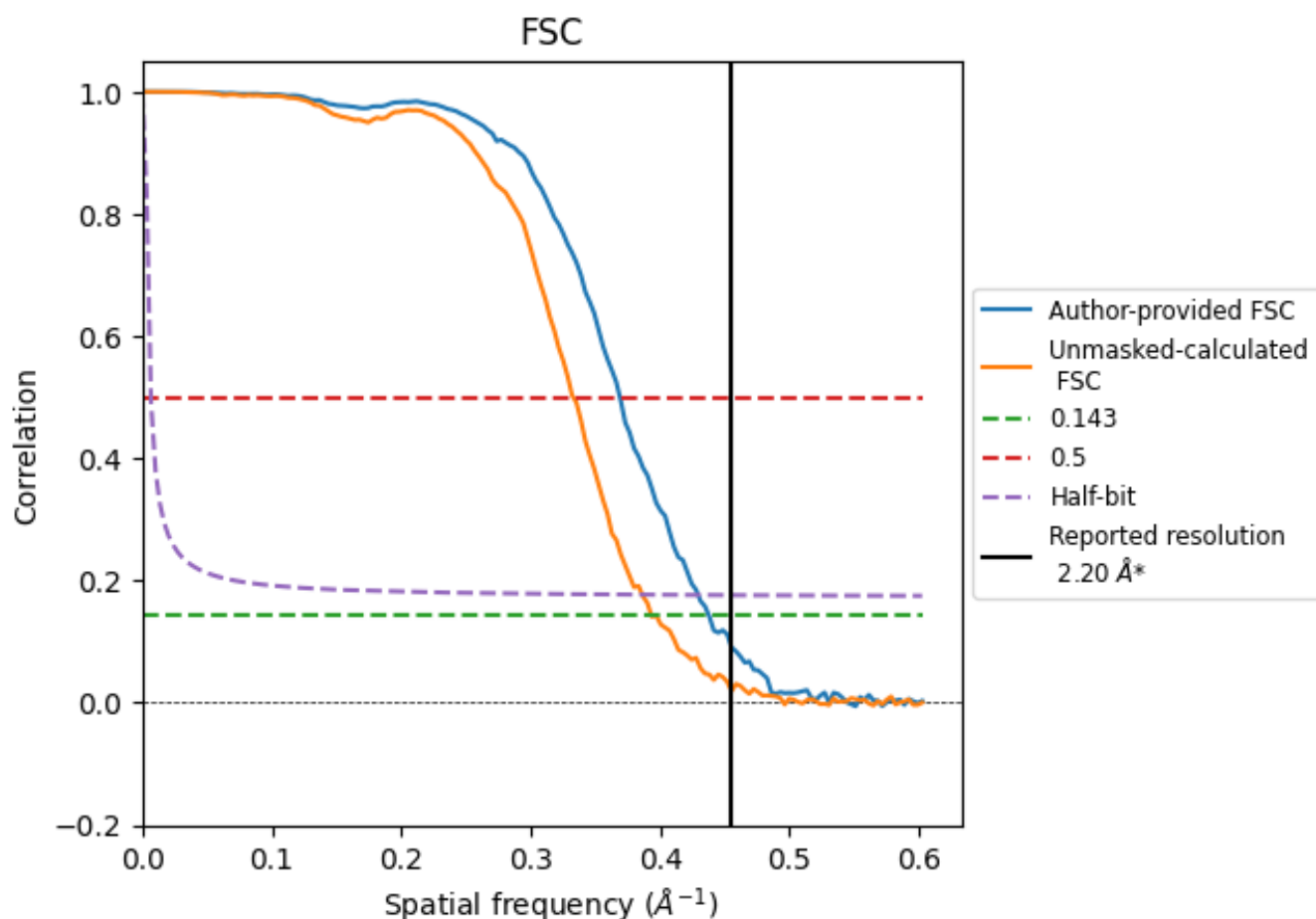


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

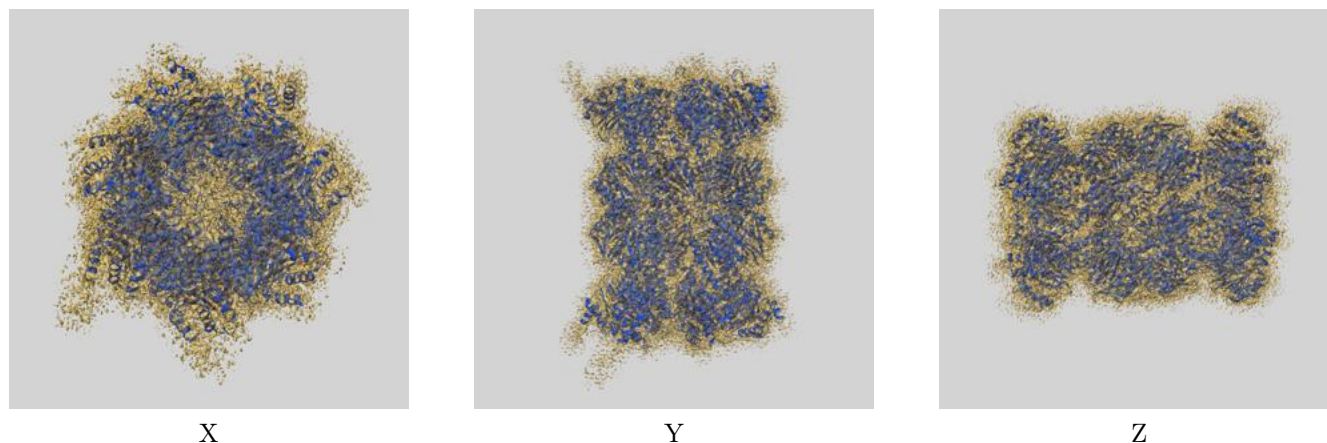
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.28	2.71	2.33
Unmasked-calculated*	2.54	3.00	2.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

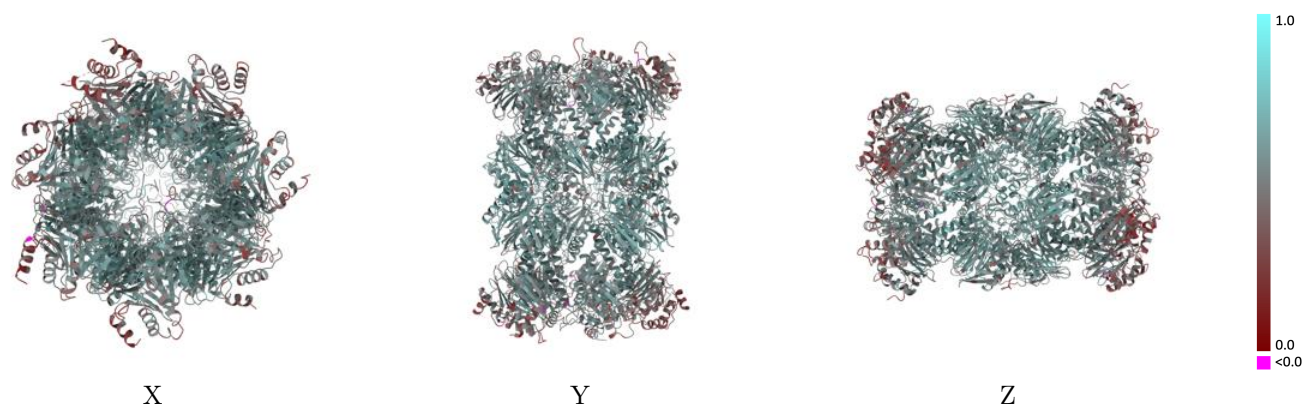
This section contains information regarding the fit between EMDB map EMD-39565 and PDB model 8YSX. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



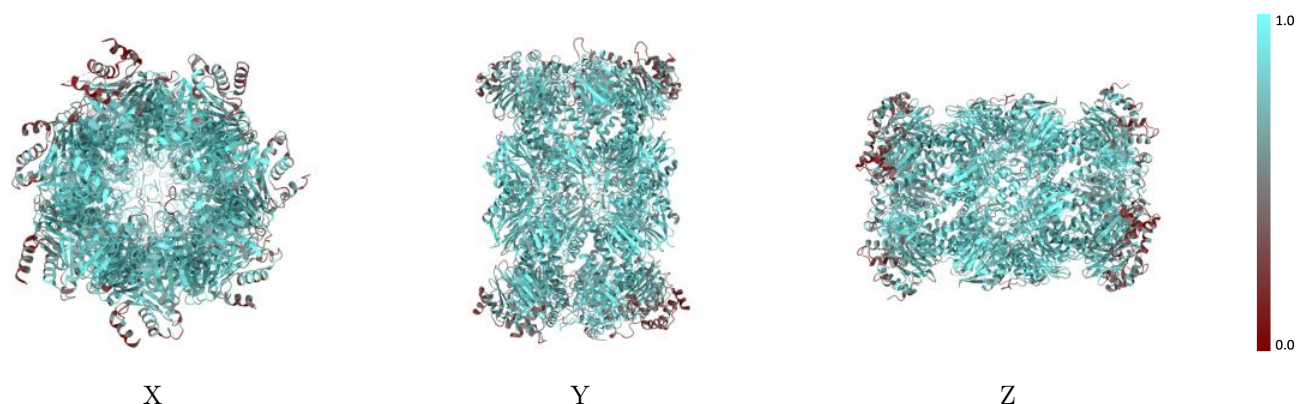
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



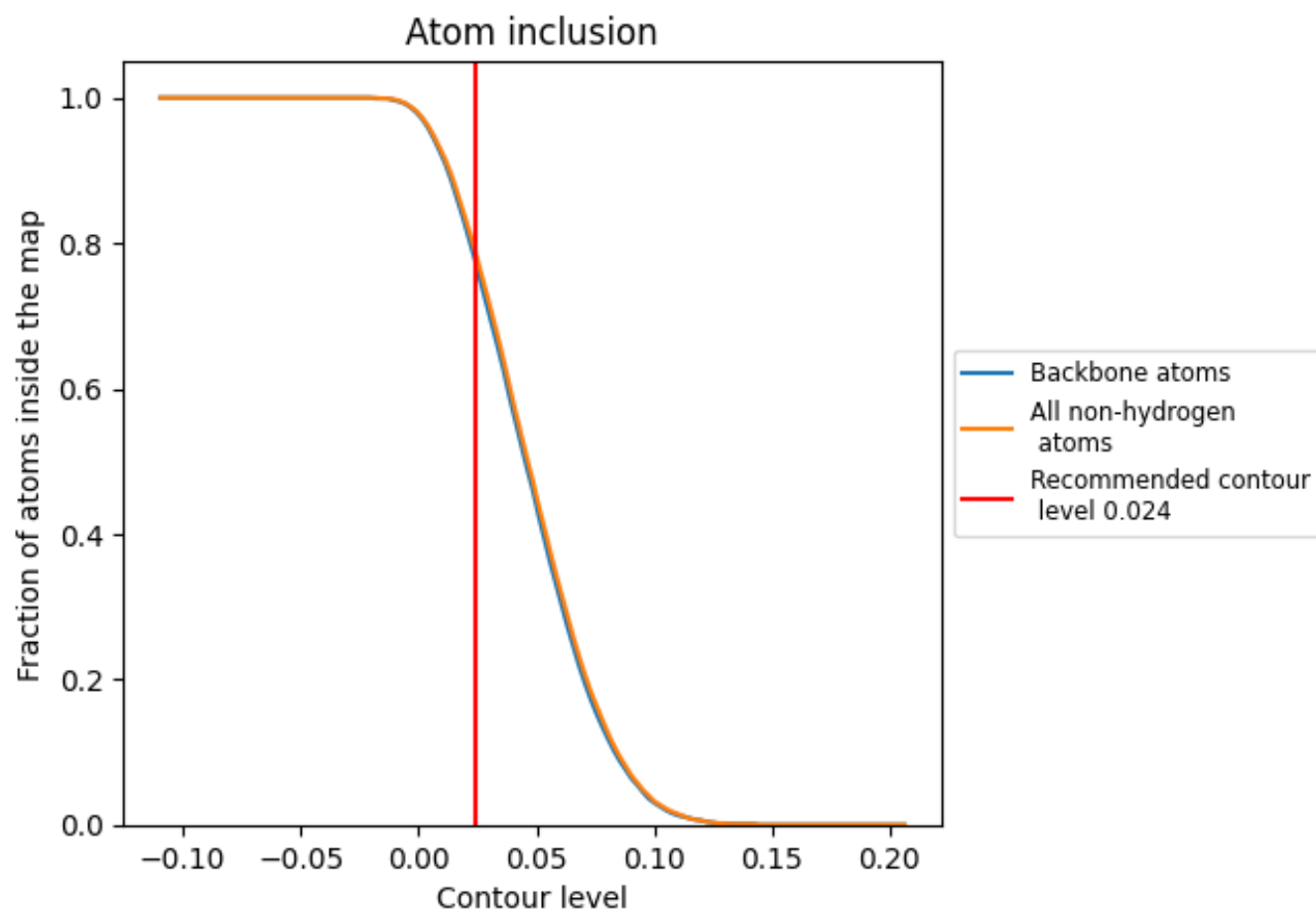
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5410
A	 0.8800	 0.6060
B	 0.8300	 0.5720
C	 0.8790	 0.5970
D	 0.8790	 0.5980
E	 0.8310	 0.5710
F	 0.8790	 0.6050
G	 0.7500	 0.5140
H	 0.7350	 0.5070
I	 0.7120	 0.4940
J	 0.7240	 0.4990
K	 0.6420	 0.4490
L	 0.7550	 0.5130
M	 0.7360	 0.5100
N	 0.7080	 0.4930
O	 0.7290	 0.4920
P	 0.7510	 0.5050
Q	 0.7240	 0.4980
R	 0.6520	 0.4630
S	 0.8700	 0.5800
T	 0.9080	 0.6140
U	 0.9000	 0.5940
V	 0.9060	 0.6120
W	 0.9060	 0.5940
X	 0.8700	 0.5810
Y	 0.9030	 0.5990
Z	 0.7290	 0.4950
a	 0.9050	 0.5950
b	 0.7500	 0.5010

