wwPDB EM Validation Summary Report

Apr 8, 2024 – 05:21 pm BST

PDB ID	:	8OIX
EMDB ID	:	EMD-16901
Title	:	CryoEM structure of 20S Trichomonas vaginalis proteasome in complex with proteasome inhibitor Salinosporamid A
Authors	:	Silhan, J.; Fajtova, P.; Boura, E.
Deposited on	:	2023-03-23
Resolution	:	2.89 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:

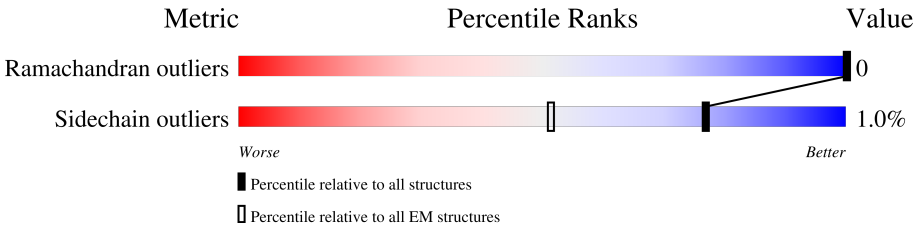
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	241	5% 99%
1	O	241	5% 99%
2	B	232	5% 98%
2	P	232	5% 98%
3	C	251	92% 6%
3	Q	251	92% 6%
4	D	235	14% 97%
4	R	235	14% 97%
5	E	251	93% 7%

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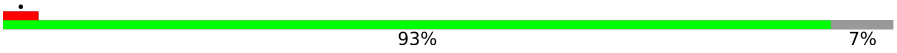
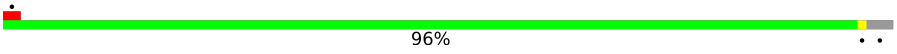
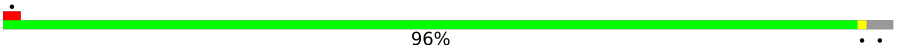
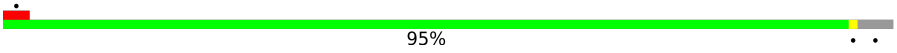
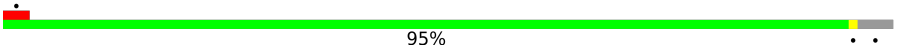
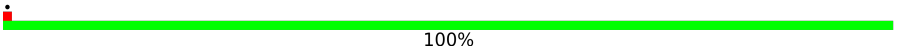
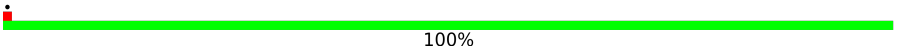
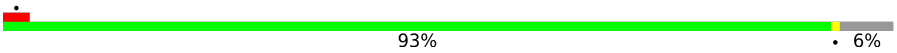
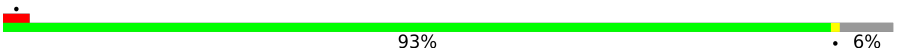
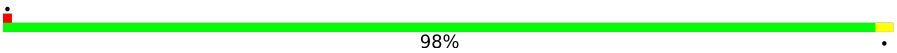
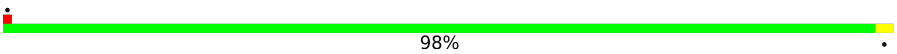
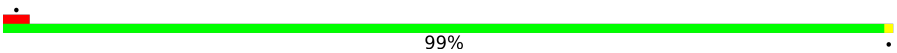
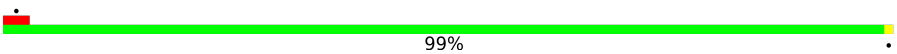
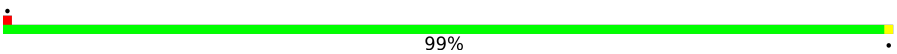
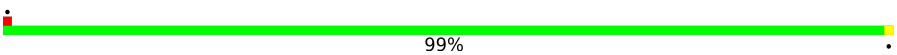
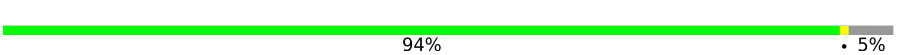
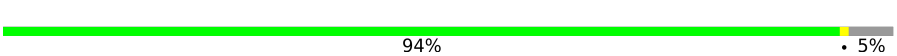
Mol	Chain	Length	Quality of chain
5	S	251	
6	F	233	
6	T	233	
7	G	240	
7	U	240	
8	H	204	
8	V	204	
9	I	244	
9	W	244	
10	J	206	
10	X	206	
11	K	191	
11	Y	191	
12	L	203	
12	Z	203	
13	M	224	
13	a	224	
14	N	244	
14	b	244	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 47786 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 Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1843	1171	304	359	9		
1	O	239	Total	C	N	O	S	0	0
			1843	1171	304	359	9		

- Molecule 2 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1770	1121	305	340	4		
2	P	229	Total	C	N	O	S	0	0
			1770	1121	305	340	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1833	1157	309	357	10		
3	Q	235	Total	C	N	O	S	0	0
			1833	1157	309	357	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	230	Total	C	N	O	S	0	0
			1801	1120	320	349	12		
4	R	230	Total	C	N	O	S	0	0
			1801	1120	320	349	12		

- 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
			1785	1111	319	345	10		
5	S	234	Total	C	N	O	S	0	0
			1785	1111	319	345	10		

- Molecule 6 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1726	1083	307	326	10		
6	T	225	Total	C	N	O	S	0	0
			1726	1083	307	326	10		

- Molecule 7 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1836	1176	310	343	7		
7	U	230	Total	C	N	O	S	0	0
			1836	1176	310	343	7		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1536	955	273	301	7		
8	V	204	Total	C	N	O	S	0	0
			1536	955	273	301	7		

- Molecule 9 is a protein called proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	230	Total	C	N	O	S	0	0
			1780	1120	312	338	10		
9	W	230	Total	C	N	O	S	0	0
			1780	1120	312	338	10		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	205	Total	C	N	O	S	0	0
			1605	1024	267	303	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	205	Total	C	N	O	S	0	0
			1605	1024	267	303	11		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	191	Total	C	N	O	S	0	0
			1499	957	249	283	10		
11	Y	191	Total	C	N	O	S	0	0
			1499	957	249	283	10		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	203	Total	C	N	O	S	0	0
			1585	1002	278	295	10		
12	Z	203	Total	C	N	O	S	0	0
			1585	1002	278	295	10		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1656	1043	283	320	10		
13	a	212	Total	C	N	O	S	0	0
			1656	1043	283	320	10		

- Molecule 14 is a protein called Family T1, proteasome beta subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	208	Total	C	N	O	S	0	0
			1598	1015	271	304	8		
14	b	208	Total	C	N	O	S	0	0
			1598	1015	271	304	8		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	215	SER	-	expression tag	UNP A2F3X4
N	216	ALA	-	expression tag	UNP A2F3X4
N	217	TRP	-	expression tag	UNP A2F3X4
N	218	SER	-	expression tag	UNP A2F3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	219	HIS	-	expression tag	UNP A2F3X4
N	220	PRO	-	expression tag	UNP A2F3X4
N	221	GLN	-	expression tag	UNP A2F3X4
N	222	PHE	-	expression tag	UNP A2F3X4
N	223	GLU	-	expression tag	UNP A2F3X4
N	224	LYS	-	expression tag	UNP A2F3X4
N	225	GLY	-	expression tag	UNP A2F3X4
N	226	GLY	-	expression tag	UNP A2F3X4
N	227	GLY	-	expression tag	UNP A2F3X4
N	228	SER	-	expression tag	UNP A2F3X4
N	229	GLY	-	expression tag	UNP A2F3X4
N	230	GLY	-	expression tag	UNP A2F3X4
N	231	GLY	-	expression tag	UNP A2F3X4
N	232	SER	-	expression tag	UNP A2F3X4
N	233	GLY	-	expression tag	UNP A2F3X4
N	234	GLY	-	expression tag	UNP A2F3X4
N	235	SER	-	expression tag	UNP A2F3X4
N	236	ALA	-	expression tag	UNP A2F3X4
N	237	TRP	-	expression tag	UNP A2F3X4
N	238	SER	-	expression tag	UNP A2F3X4
N	239	HIS	-	expression tag	UNP A2F3X4
N	240	PRO	-	expression tag	UNP A2F3X4
N	241	GLN	-	expression tag	UNP A2F3X4
N	242	PHE	-	expression tag	UNP A2F3X4
N	243	GLU	-	expression tag	UNP A2F3X4
N	244	LYS	-	expression tag	UNP A2F3X4
b	215	SER	-	expression tag	UNP A2F3X4
b	216	ALA	-	expression tag	UNP A2F3X4
b	217	TRP	-	expression tag	UNP A2F3X4
b	218	SER	-	expression tag	UNP A2F3X4
b	219	HIS	-	expression tag	UNP A2F3X4
b	220	PRO	-	expression tag	UNP A2F3X4
b	221	GLN	-	expression tag	UNP A2F3X4
b	222	PHE	-	expression tag	UNP A2F3X4
b	223	GLU	-	expression tag	UNP A2F3X4
b	224	LYS	-	expression tag	UNP A2F3X4
b	225	GLY	-	expression tag	UNP A2F3X4
b	226	GLY	-	expression tag	UNP A2F3X4
b	227	GLY	-	expression tag	UNP A2F3X4
b	228	SER	-	expression tag	UNP A2F3X4
b	229	GLY	-	expression tag	UNP A2F3X4
b	230	GLY	-	expression tag	UNP A2F3X4

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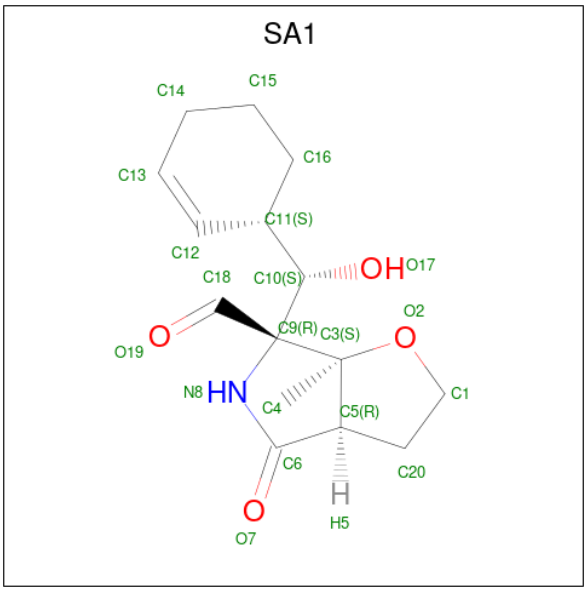
Chain	Residue	Modelled	Actual	Comment	Reference
b	231	GLY	-	expression tag	UNP A2F3X4
b	232	SER	-	expression tag	UNP A2F3X4
b	233	GLY	-	expression tag	UNP A2F3X4
b	234	GLY	-	expression tag	UNP A2F3X4
b	235	SER	-	expression tag	UNP A2F3X4
b	236	ALA	-	expression tag	UNP A2F3X4
b	237	TRP	-	expression tag	UNP A2F3X4
b	238	SER	-	expression tag	UNP A2F3X4
b	239	HIS	-	expression tag	UNP A2F3X4
b	240	PRO	-	expression tag	UNP A2F3X4
b	241	GLN	-	expression tag	UNP A2F3X4
b	242	PHE	-	expression tag	UNP A2F3X4
b	243	GLU	-	expression tag	UNP A2F3X4
b	244	LYS	-	expression tag	UNP A2F3X4

- Molecule 15 is (3AR,6R,6AS)-6-((S)-((S)-CYCLOHEX-2-ENYL)(HYDROXY)METHYL)-6A-METHYL-4-OXO-HEXAHYDRO-2H-FURO[3,2-C]PYRROLE-6-CARBALDEHYDE (three-letter code: SA1) (formula: $C_{15}H_{21}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
15	H	1	Total C N O 20 15 1 4	0
15	I	1	Total C N O 20 15 1 4	0
15	V	1	Total C N O 20 15 1 4	0

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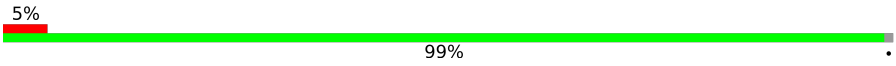
Mol	Chain	Residues	Atoms				AltConf
15	W	1	Total	C	N	O	0
			20	15	1	4	

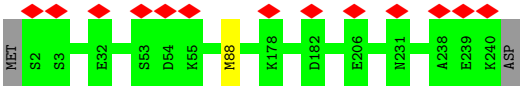
3 Residue-property plots (i)

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: Family T1, proteasome alpha subunit, threonine peptidase

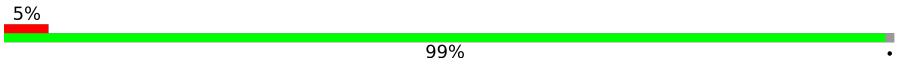
Chain A:

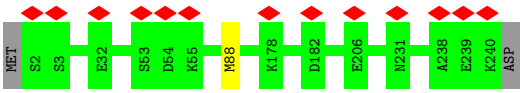




• Molecule 1: Family T1, proteasome alpha subunit, threonine peptidase

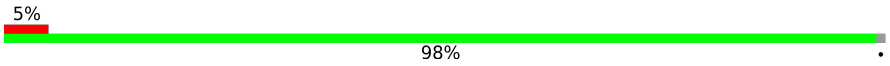
Chain O:

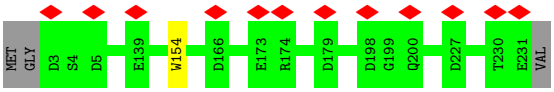




• Molecule 2: Family T1, proteasome alpha subunit, threonine peptidase

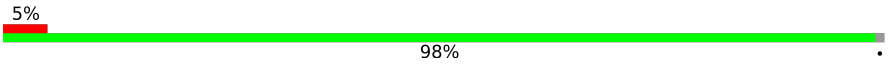
Chain B:

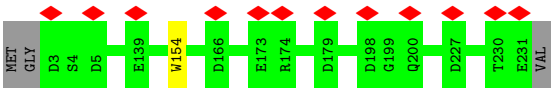




• Molecule 2: Family T1, proteasome alpha subunit, threonine peptidase

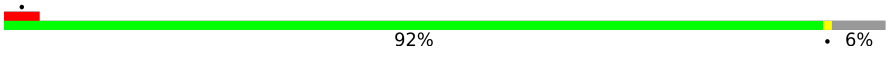
Chain P:

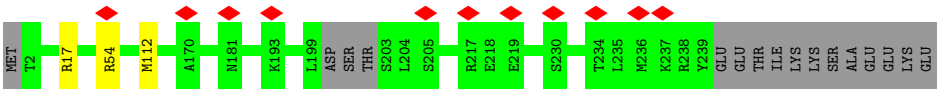




• Molecule 3: Proteasome subunit alpha type

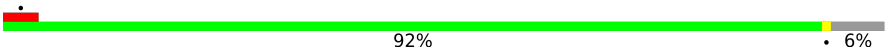
Chain C:

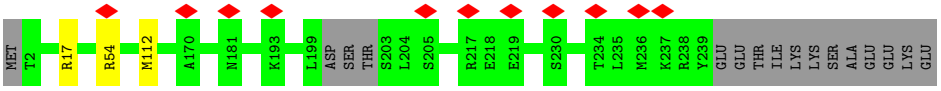




• Molecule 3: Proteasome subunit alpha type

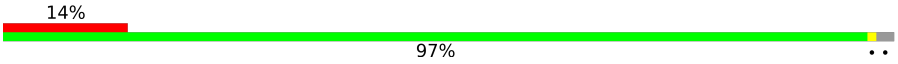
Chain Q:

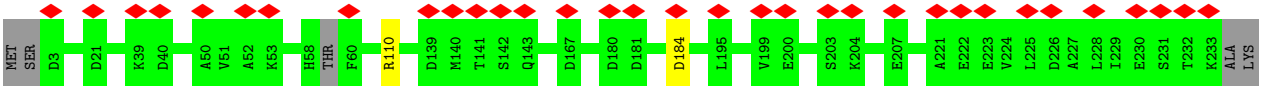




• Molecule 4: Proteasome subunit alpha type

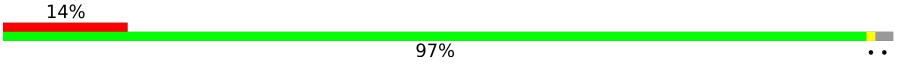
Chain D:

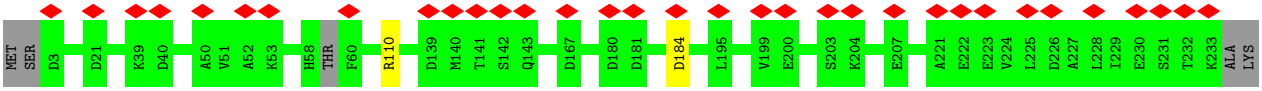




• Molecule 4: Proteasome subunit alpha type

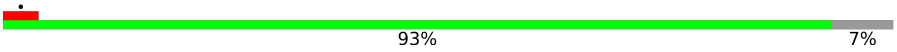
Chain R:

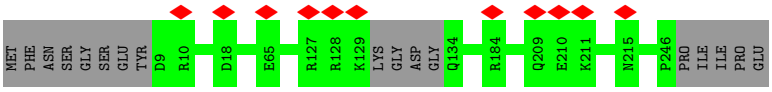




• Molecule 5: Proteasome subunit alpha type

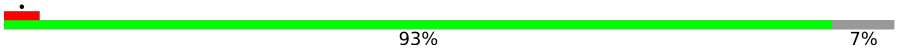
Chain E:

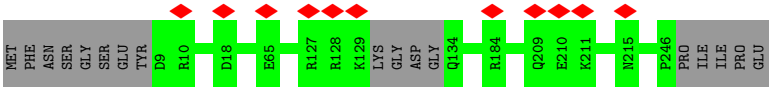




• Molecule 5: Proteasome subunit alpha type

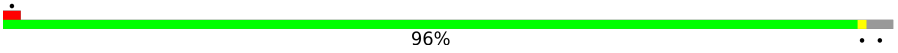
Chain S:

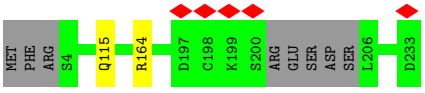




• Molecule 6: Family T1, proteasome alpha subunit, threonine peptidase

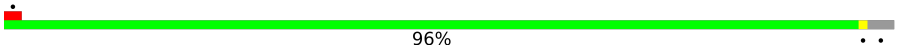
Chain F:

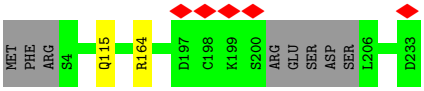




• Molecule 6: Family T1, proteasome alpha subunit, threonine peptidase

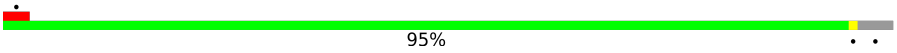
Chain T:

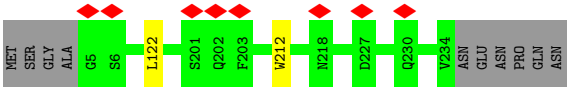




• Molecule 7: Family T1, proteasome alpha subunit, threonine peptidase

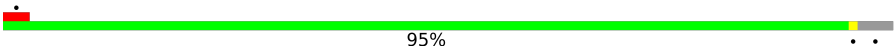
Chain G:

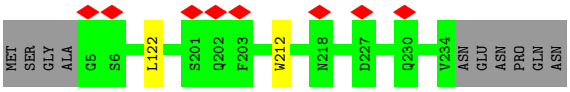




• Molecule 7: Family T1, proteasome alpha subunit, threonine peptidase

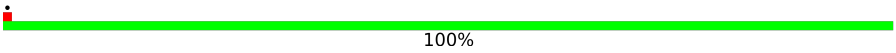
Chain U:

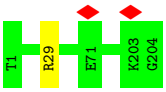




• Molecule 8: Proteasome subunit beta

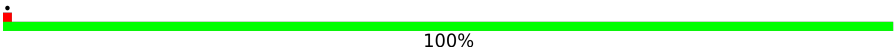
Chain H:

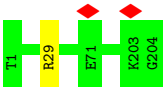




• Molecule 8: Proteasome subunit beta

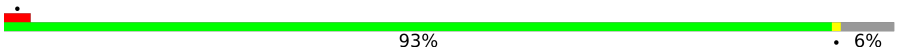
Chain V:

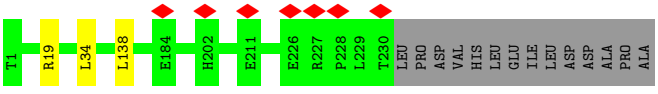




• Molecule 9: proteasome endopeptidase complex

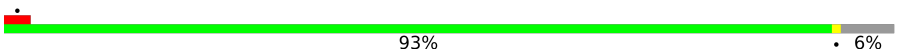
Chain I:

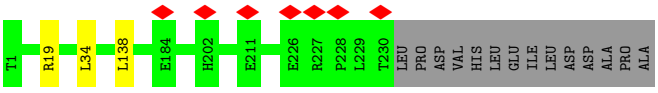




• Molecule 9: proteasome endopeptidase complex

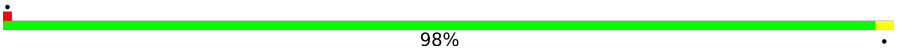
Chain W:

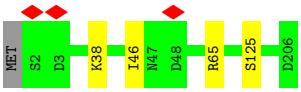




• Molecule 10: Proteasome subunit beta

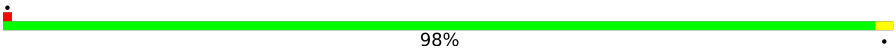
Chain J:

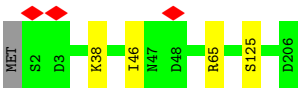




• Molecule 10: Proteasome subunit beta

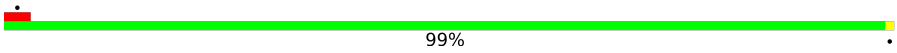
Chain X:

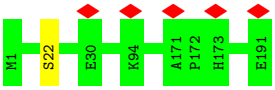




• Molecule 11: Proteasome subunit beta

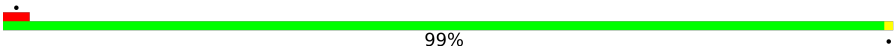
Chain K:

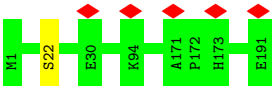




• Molecule 11: Proteasome subunit beta

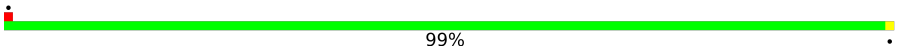
Chain Y:

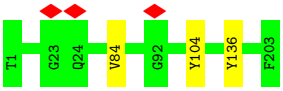




• Molecule 12: Proteasome subunit beta

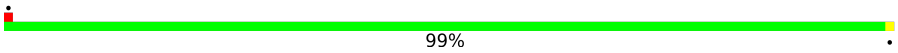
Chain L:

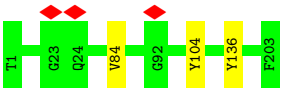




• Molecule 12: Proteasome subunit beta

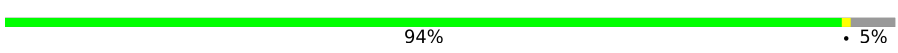
Chain Z:

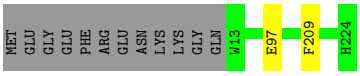




• Molecule 13: Proteasome subunit beta

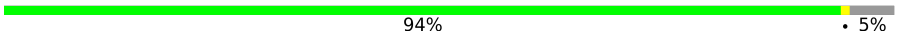
Chain M:

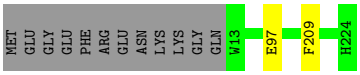




• Molecule 13: Proteasome subunit beta

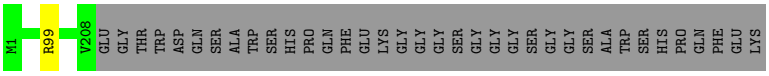
Chain a:





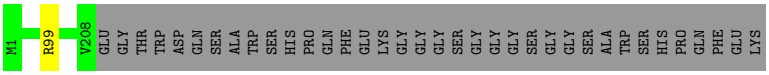
• Molecule 14: Family T1, proteasome beta subunit, threonine peptidase

Chain N:



• Molecule 14: Family T1, proteasome beta subunit, threonine peptidase

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	14257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.828	Depositor
Minimum map value	-0.480	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.133	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7, 0.7, 0.7	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SA1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/1875	0.47	0/2538
1	O	0.29	0/1875	0.47	0/2538
2	B	0.27	0/1801	0.51	0/2434
2	P	0.27	0/1801	0.51	0/2434
3	C	0.27	0/1862	0.50	0/2516
3	Q	0.27	0/1862	0.50	0/2516
4	D	0.26	0/1831	0.52	0/2471
4	R	0.26	0/1831	0.52	0/2471
5	E	0.29	0/1809	0.52	0/2441
5	S	0.29	0/1809	0.53	0/2441
6	F	0.28	0/1758	0.49	0/2373
6	T	0.28	0/1758	0.49	0/2373
7	G	0.28	0/1884	0.49	0/2553
7	U	0.28	0/1884	0.49	0/2553
8	H	0.27	0/1555	0.52	0/2106
8	V	0.27	0/1555	0.52	0/2106
9	I	0.28	0/1814	0.51	0/2462
9	W	0.28	0/1814	0.51	0/2462
10	J	0.32	0/1635	0.51	0/2212
10	X	0.32	0/1635	0.52	0/2212
11	K	0.27	0/1529	0.48	0/2062
11	Y	0.27	0/1529	0.48	0/2062
12	L	0.29	0/1620	0.52	0/2190
12	Z	0.29	0/1620	0.52	0/2190
13	M	0.29	0/1695	0.53	0/2295
13	a	0.29	0/1695	0.53	0/2295
14	N	0.29	0/1631	0.48	0/2213
14	b	0.29	0/1631	0.48	0/2213
All	All	0.28	0/48598	0.50	0/65732

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
9	I	0	1
9	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	19	ARG	Sidechain
9	W	19	ARG	Sidechain

5.2 Too-close contacts (i)

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

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	237/241 (98%)	232 (98%)	5 (2%)	0	100	100
1	O	237/241 (98%)	232 (98%)	5 (2%)	0	100	100
2	B	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
2	P	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
3	C	231/251 (92%)	227 (98%)	4 (2%)	0	100	100
3	Q	231/251 (92%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	228/235 (97%)	222 (97%)	6 (3%)	0	100	100
4	R	228/235 (97%)	222 (97%)	6 (3%)	0	100	100
5	E	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
5	S	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
6	F	221/233 (95%)	220 (100%)	1 (0%)	0	100	100
6	T	221/233 (95%)	220 (100%)	1 (0%)	0	100	100
7	G	228/240 (95%)	221 (97%)	7 (3%)	0	100	100
7	U	228/240 (95%)	221 (97%)	7 (3%)	0	100	100
8	H	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
8	V	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
9	I	228/244 (93%)	220 (96%)	8 (4%)	0	100	100
9	W	228/244 (93%)	220 (96%)	8 (4%)	0	100	100
10	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
10	X	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
11	K	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
11	Y	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
12	L	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
12	Z	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
13	M	210/224 (94%)	205 (98%)	5 (2%)	0	100	100
13	a	210/224 (94%)	206 (98%)	4 (2%)	0	100	100
14	N	206/244 (84%)	202 (98%)	4 (2%)	0	100	100
14	b	206/244 (84%)	202 (98%)	4 (2%)	0	100	100
All	All	6082/6398 (95%)	5943 (98%)	139 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/207 (99%)	204 (100%)	1 (0%)	88	96
1	O	205/207 (99%)	204 (100%)	1 (0%)	88	96
2	B	194/196 (99%)	193 (100%)	1 (0%)	88	96
2	P	194/196 (99%)	193 (100%)	1 (0%)	88	96
3	C	197/212 (93%)	194 (98%)	3 (2%)	65	87
3	Q	197/212 (93%)	194 (98%)	3 (2%)	65	87
4	D	193/198 (98%)	191 (99%)	2 (1%)	76	92
4	R	193/198 (98%)	191 (99%)	2 (1%)	76	92
5	E	190/204 (93%)	190 (100%)	0	100	100
5	S	190/204 (93%)	190 (100%)	0	100	100
6	F	184/193 (95%)	182 (99%)	2 (1%)	73	92
6	T	184/193 (95%)	182 (99%)	2 (1%)	73	92
7	G	196/204 (96%)	194 (99%)	2 (1%)	76	92
7	U	196/204 (96%)	194 (99%)	2 (1%)	76	92
8	H	164/164 (100%)	163 (99%)	1 (1%)	86	96
8	V	164/164 (100%)	163 (99%)	1 (1%)	86	96
9	I	191/203 (94%)	189 (99%)	2 (1%)	76	92
9	W	191/203 (94%)	189 (99%)	2 (1%)	76	92
10	J	176/177 (99%)	172 (98%)	4 (2%)	50	80
10	X	176/177 (99%)	172 (98%)	4 (2%)	50	80
11	K	162/163 (99%)	161 (99%)	1 (1%)	86	96
11	Y	162/163 (99%)	161 (99%)	1 (1%)	86	96
12	L	168/168 (100%)	165 (98%)	3 (2%)	59	85
12	Z	168/168 (100%)	165 (98%)	3 (2%)	59	85
13	M	180/190 (95%)	178 (99%)	2 (1%)	73	92
13	a	180/190 (95%)	178 (99%)	2 (1%)	73	92
14	N	173/198 (87%)	172 (99%)	1 (1%)	86	96
14	b	173/198 (87%)	172 (99%)	1 (1%)	86	96
All	All	5146/5354 (96%)	5096 (99%)	50 (1%)	77	92

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	54	ARG
7	U	212	TRP
14	b	99	ARG
3	Q	112	MET
6	T	115	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	149	GLN
11	Y	61	GLN
2	P	32	GLN
14	b	149	GLN
9	W	140	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	SA1	I	301	9	18,22,22	0.94	2 (11%)	24,34,34	1.79	6 (25%)
15	SA1	H	301	8	18,22,22	0.89	1 (5%)	24,34,34	1.56	3 (12%)
15	SA1	V	301	8	18,22,22	0.89	0	24,34,34	1.57	3 (12%)
15	SA1	W	301	9	18,22,22	0.94	2 (11%)	24,34,34	1.79	6 (25%)

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	SA1	I	301	9	-	0/4/52/52	0/3/3/3
15	SA1	H	301	8	-	0/4/52/52	0/3/3/3
15	SA1	V	301	8	-	0/4/52/52	0/3/3/3
15	SA1	W	301	9	-	0/4/52/52	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	301	SA1	O2-C3	-2.34	1.42	1.45
15	I	301	SA1	O2-C3	-2.32	1.42	1.45
15	I	301	SA1	C5-C6	-2.17	1.49	1.52
15	W	301	SA1	C5-C6	-2.17	1.49	1.52
15	H	301	SA1	O2-C3	-2.01	1.43	1.45

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	301	SA1	C14-C13-C12	-4.30	115.95	123.61
15	W	301	SA1	C14-C13-C12	-4.25	116.04	123.61
15	H	301	SA1	C14-C13-C12	-4.22	116.10	123.61
15	V	301	SA1	C14-C13-C12	-4.22	116.10	123.61
15	W	301	SA1	O2-C1-C20	-3.73	101.29	106.53

There are no chirality outliers.

There are no torsion outliers.

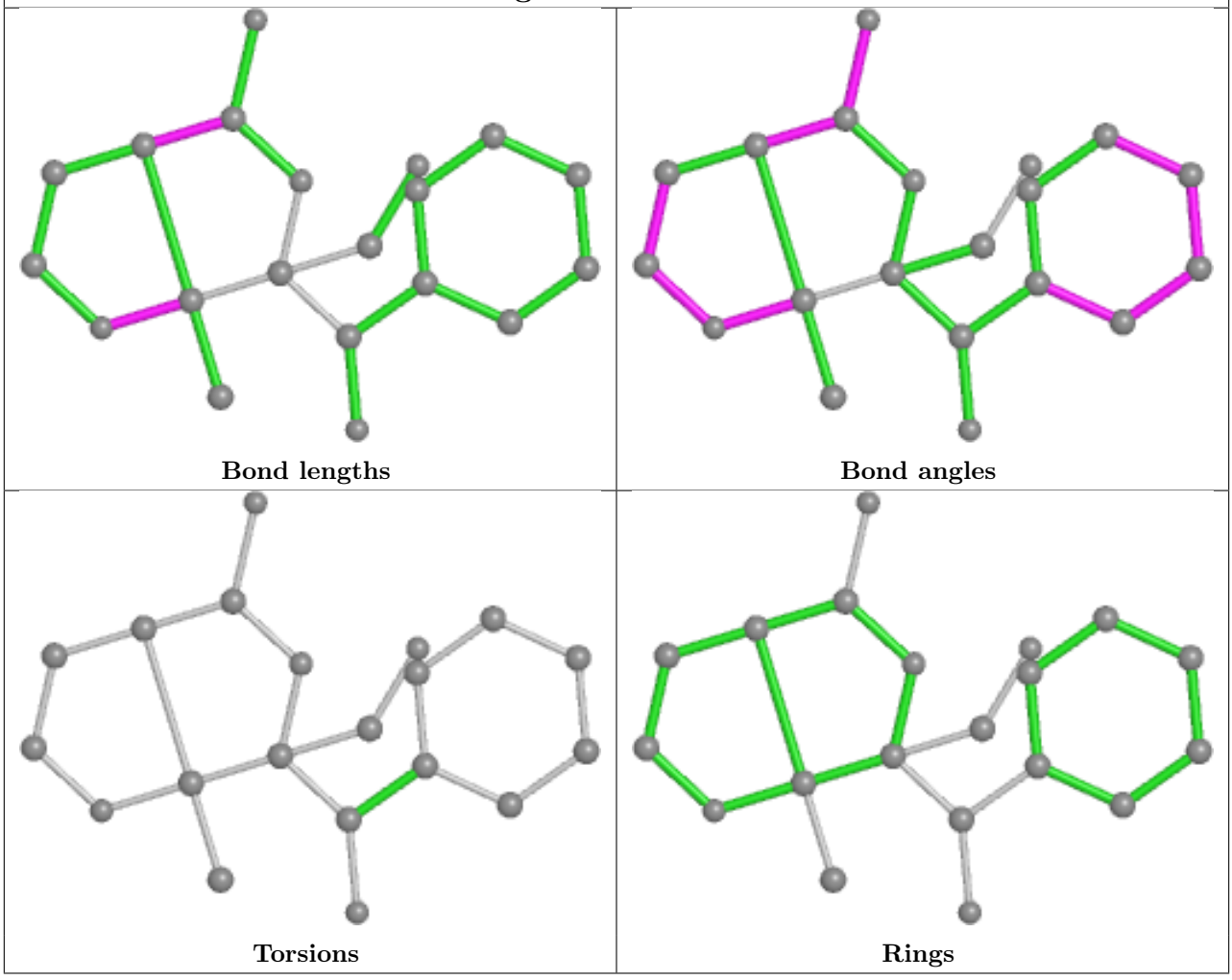
There are no ring outliers.

No monomer is involved in short contacts.

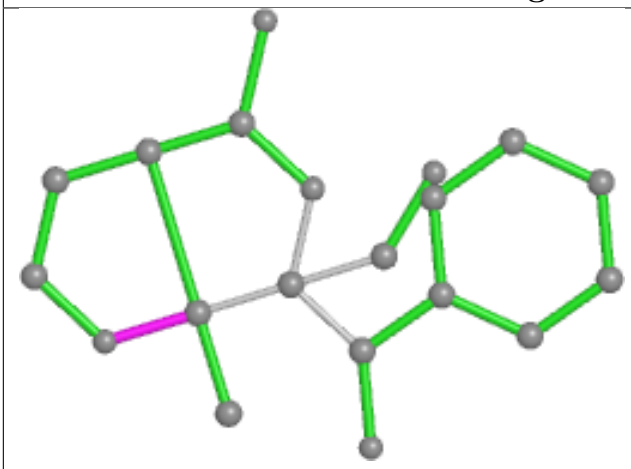
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

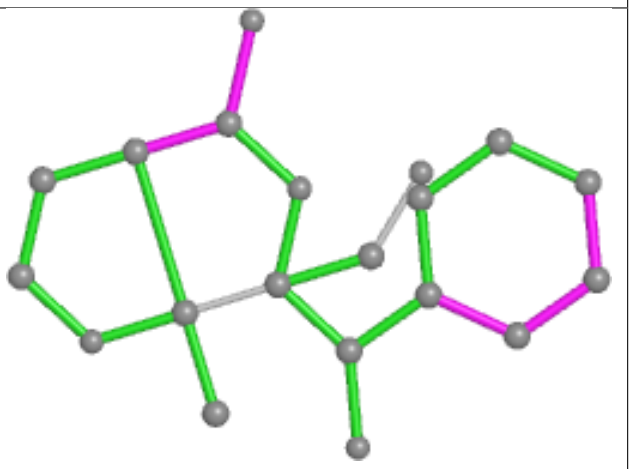
Ligand SA1 I 301



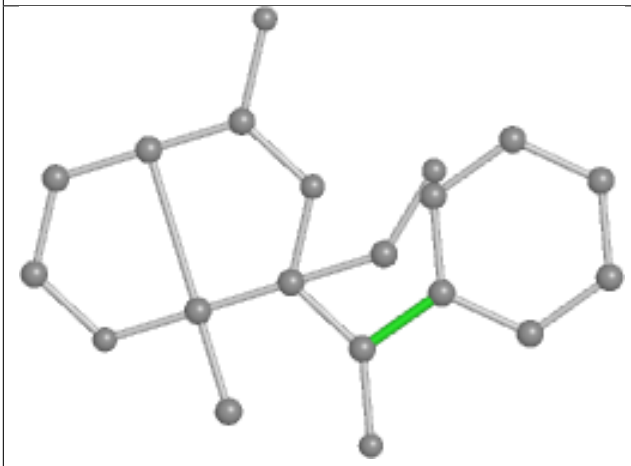
Ligand SA1 H 301



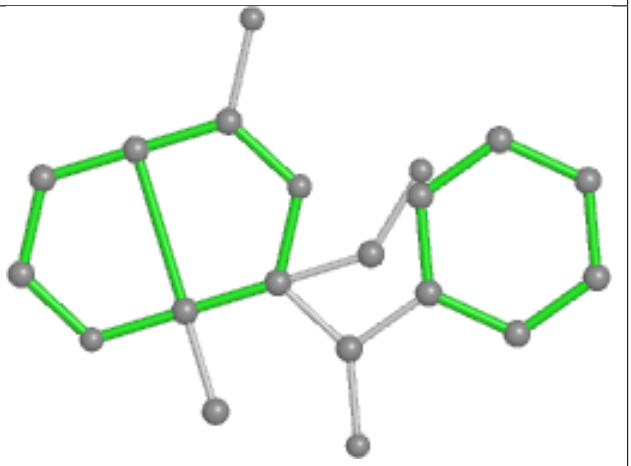
Bond lengths



Bond angles

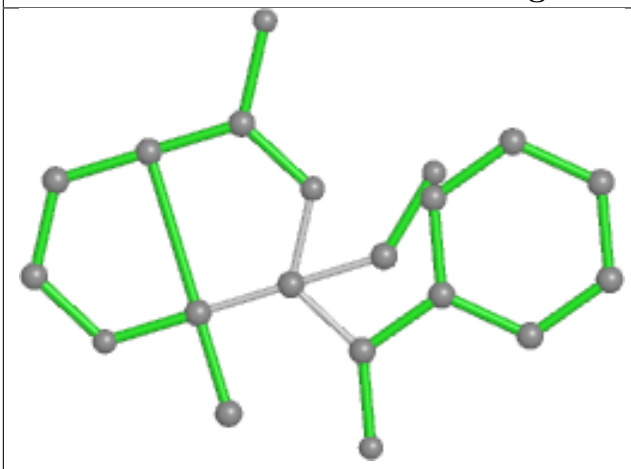


Torsions

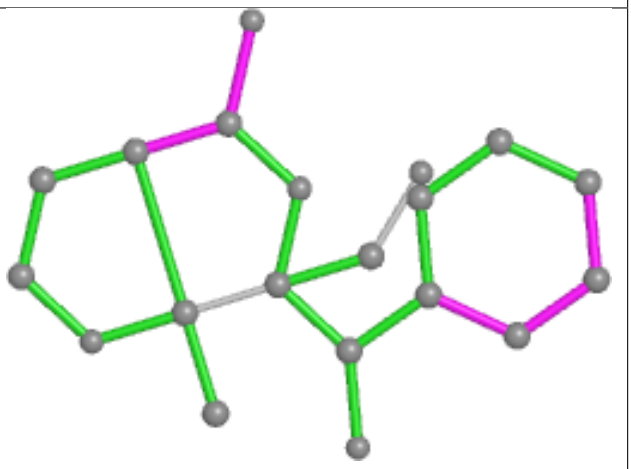


Rings

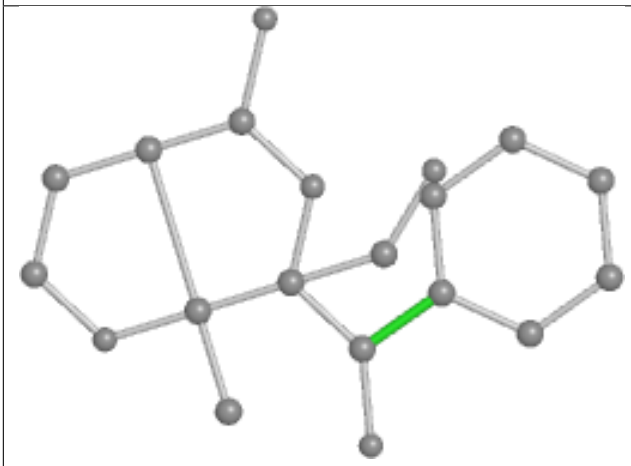
Ligand SA1 V 301



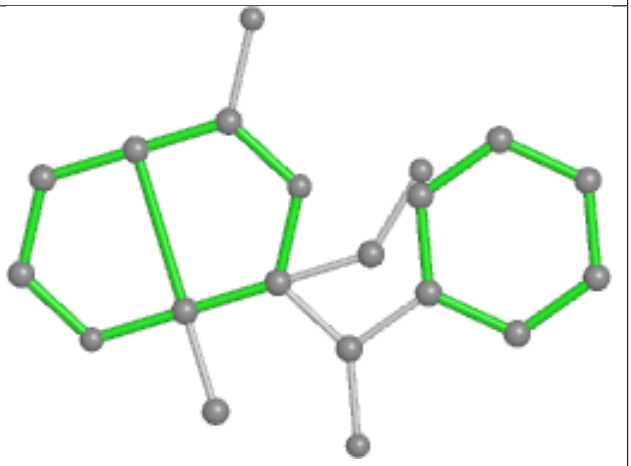
Bond lengths



Bond angles

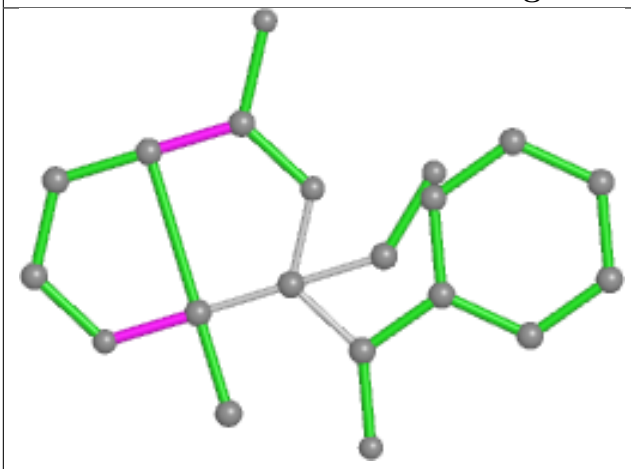


Torsions

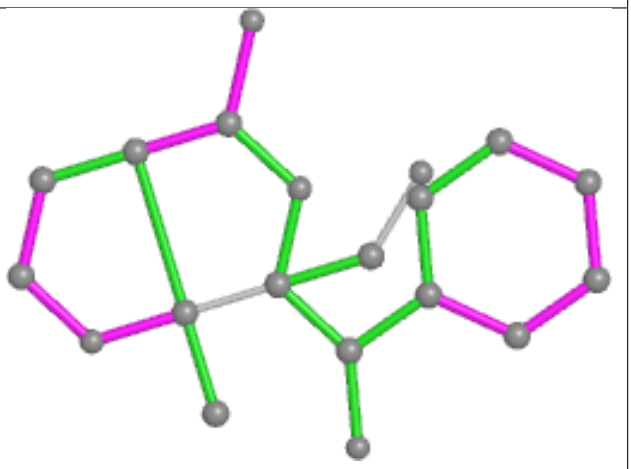


Rings

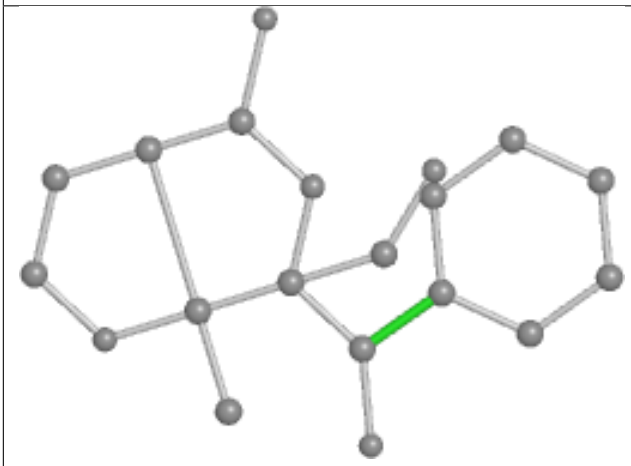
Ligand SA1 W 301



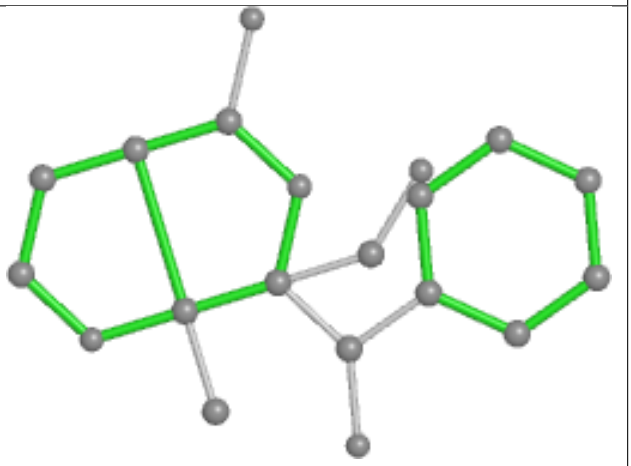
Bond lengths



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.

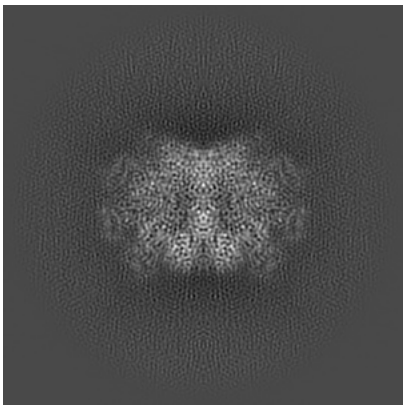
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16901. These allow visual inspection of the internal detail of the map and identification of artifacts.

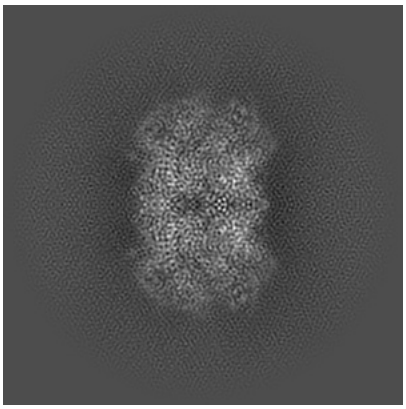
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

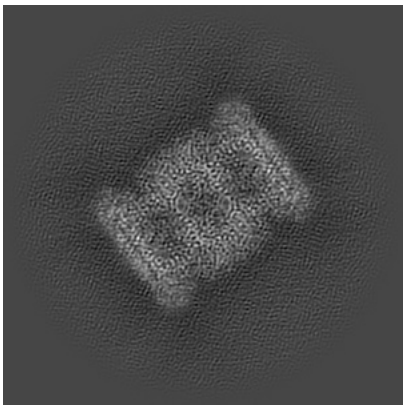
6.1.1 Primary map



X

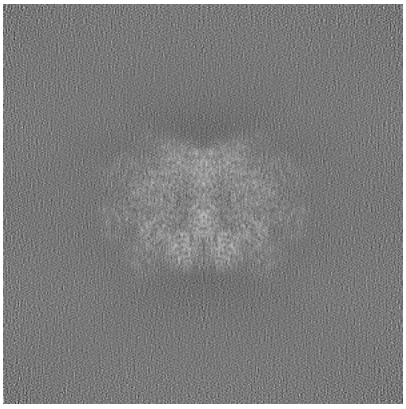


Y

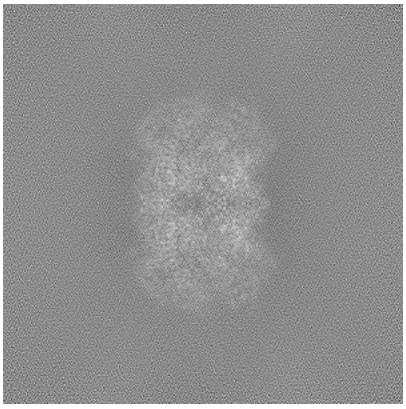


Z

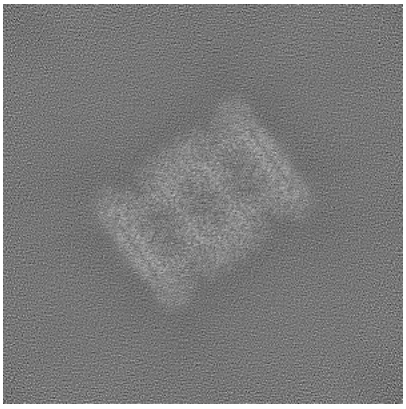
6.1.2 Raw map



X



Y

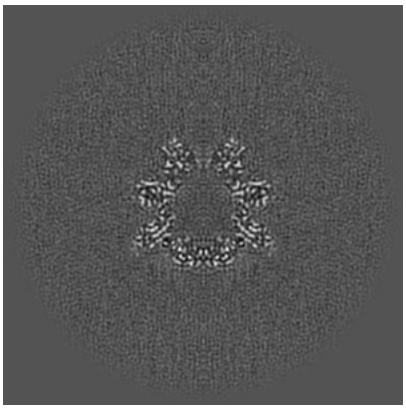


Z

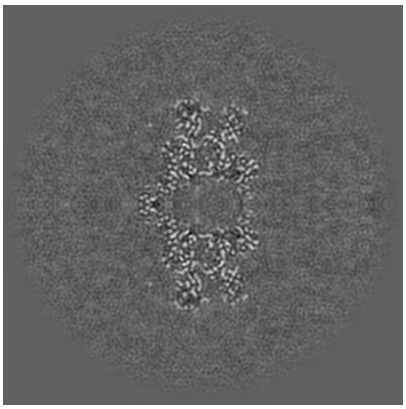
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

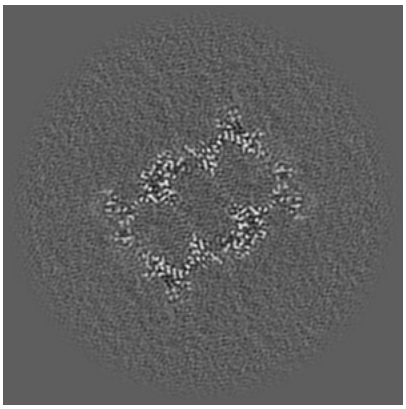
6.2.1 Primary map



X Index: 220

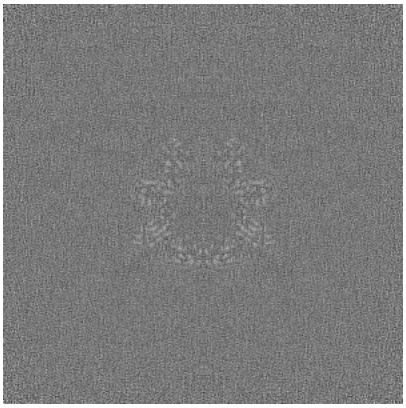


Y Index: 220

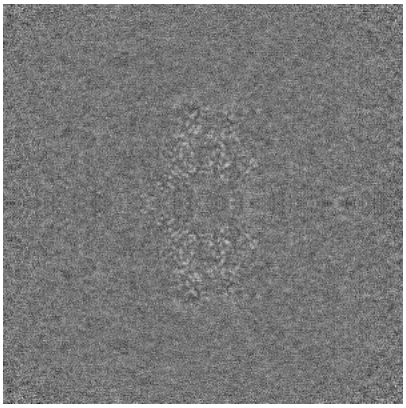


Z Index: 220

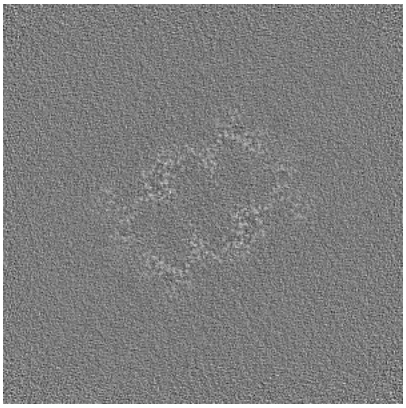
6.2.2 Raw map



X Index: 220



Y Index: 220

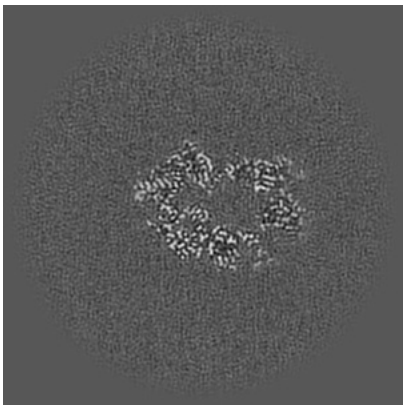


Z Index: 220

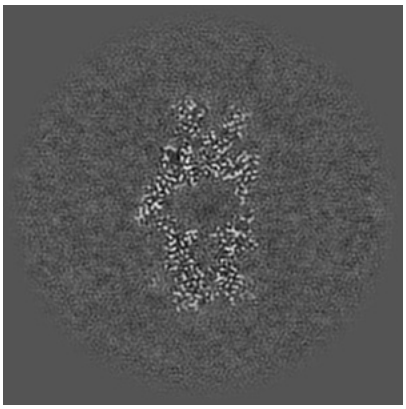
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

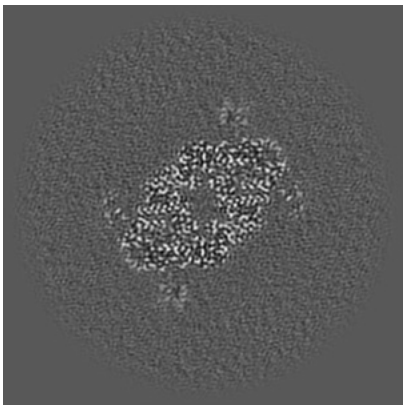
6.3.1 Primary map



X Index: 249

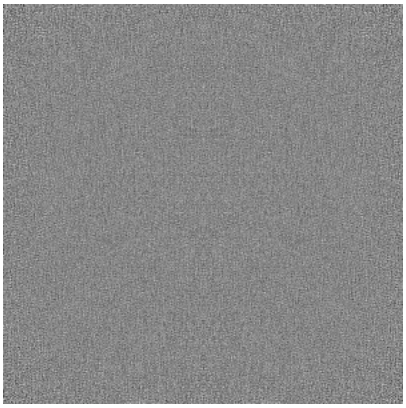


Y Index: 217

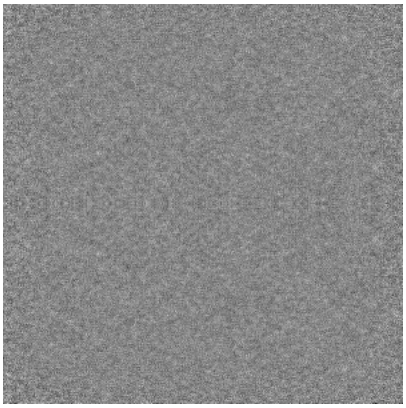


Z Index: 186

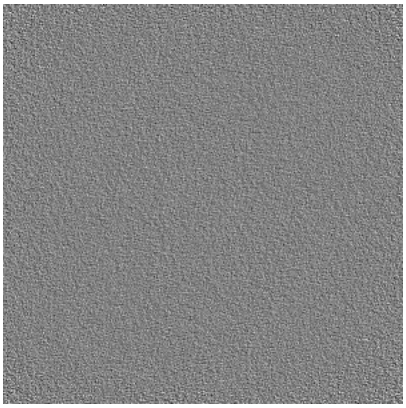
6.3.2 Raw map



X Index: 0



Y Index: 0

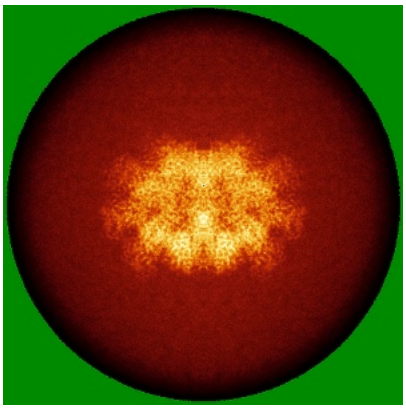


Z Index: 0

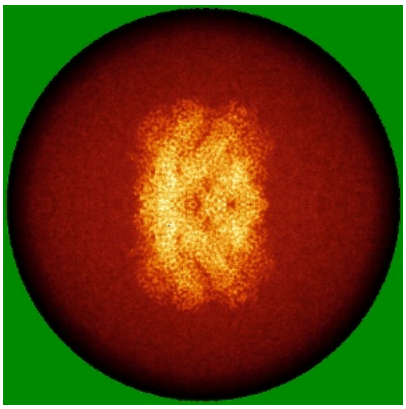
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

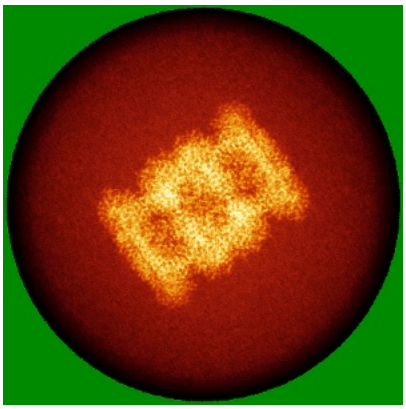
6.4.1 Primary map



X

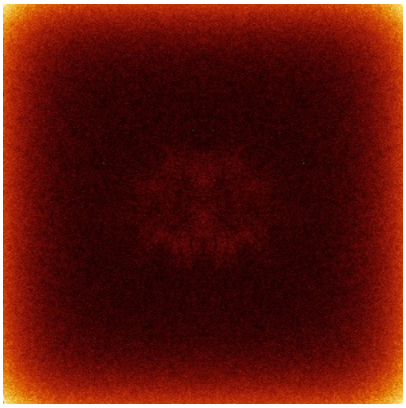


Y

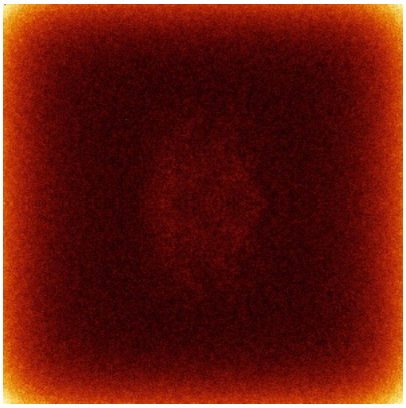


Z

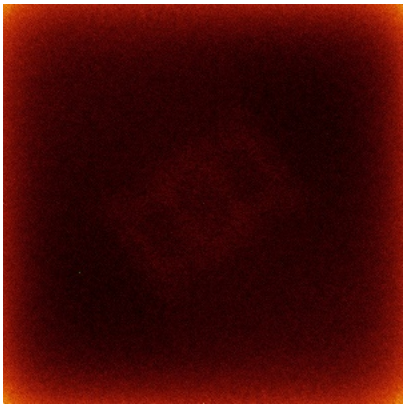
6.4.2 Raw map



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.

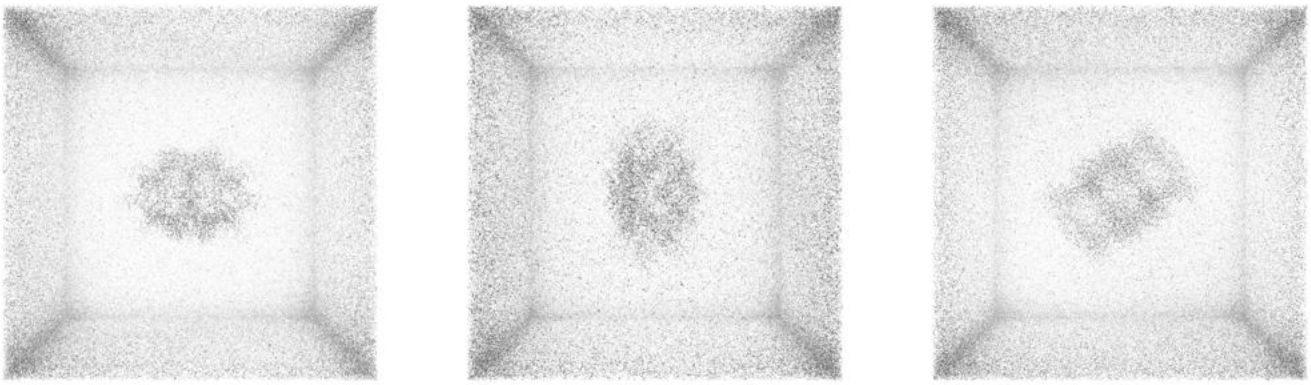
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.133. 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.

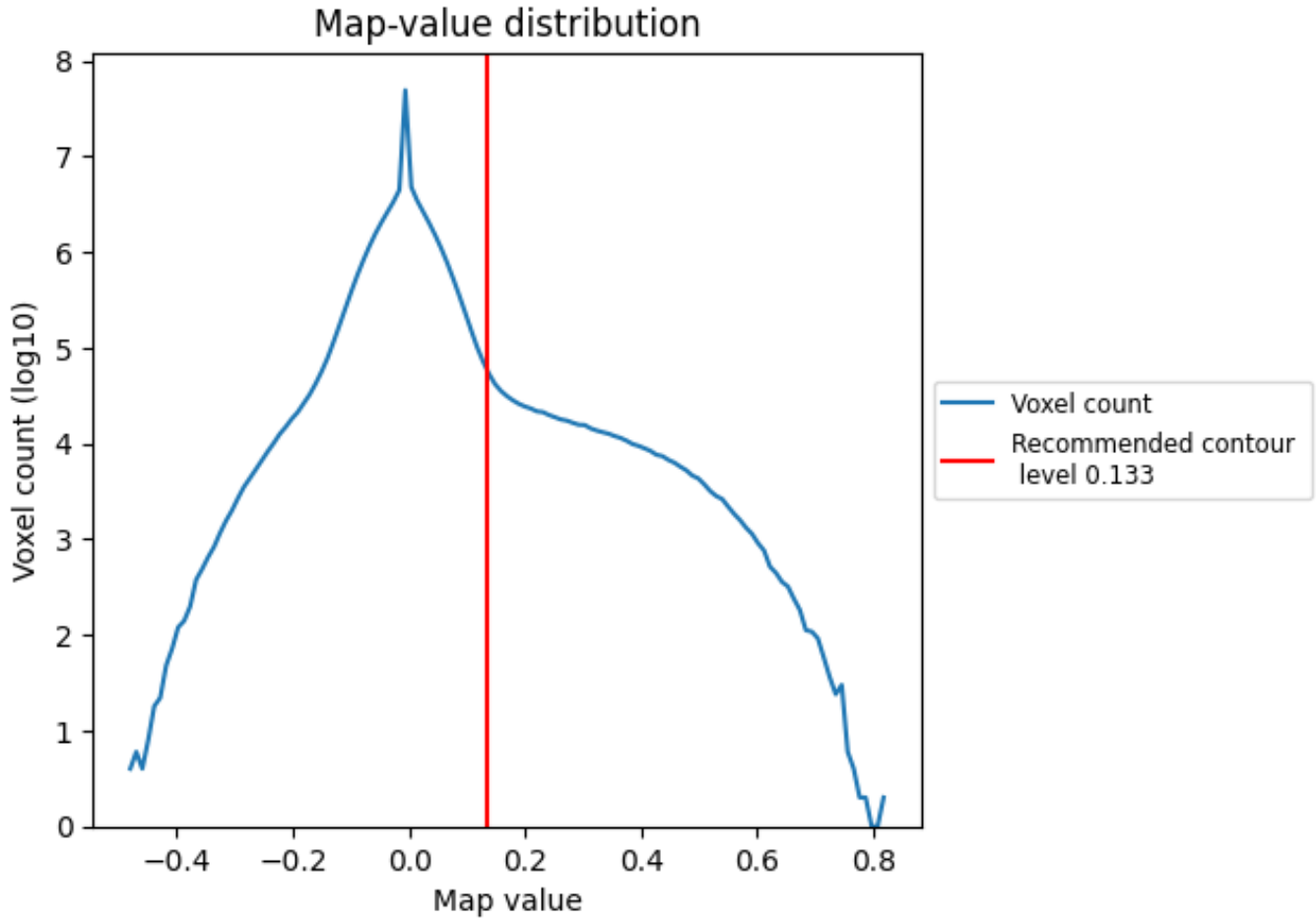
6.6 Mask visualisation (i)

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

7 Map analysis

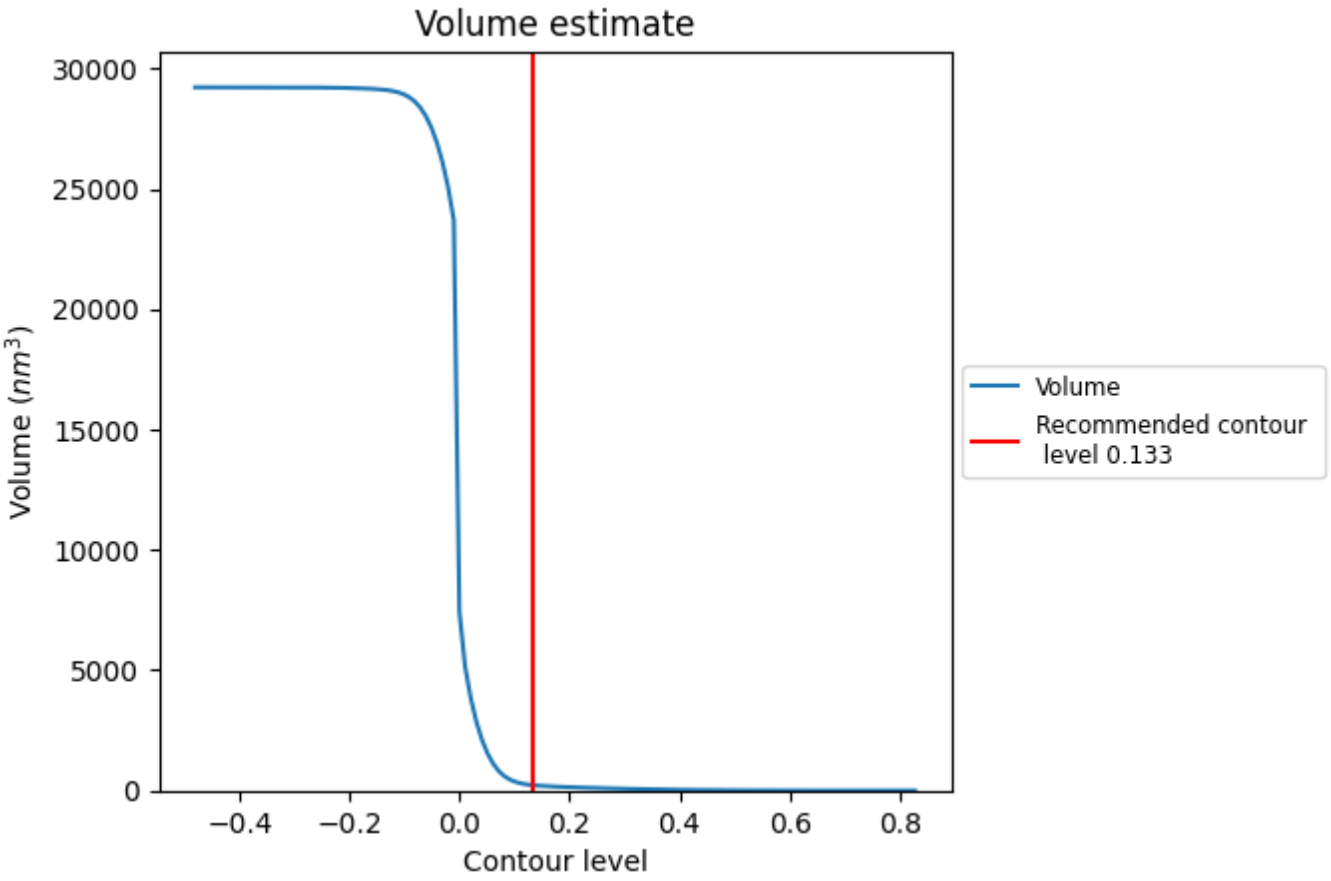
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

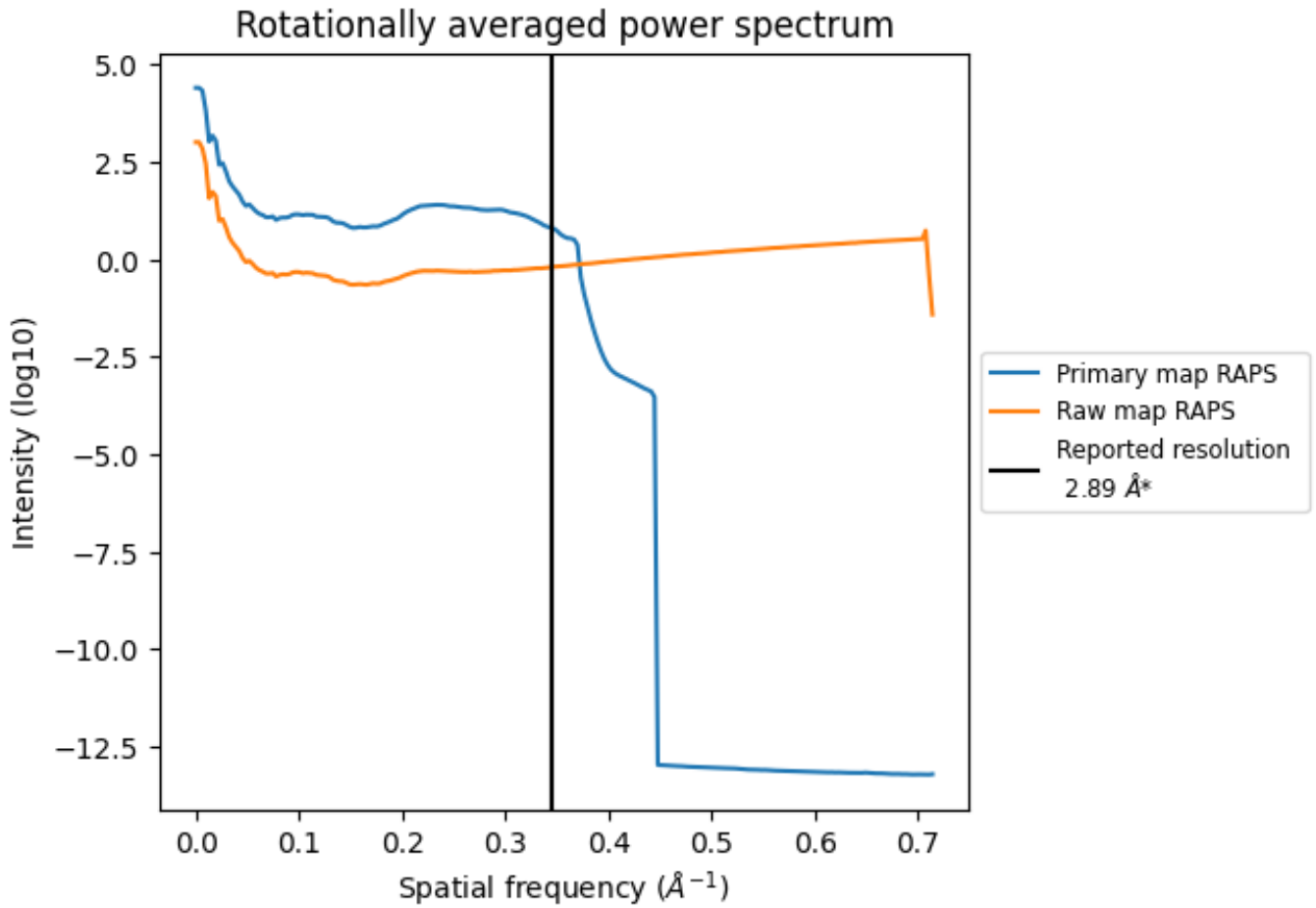
7.2 Volume estimate (i)



The volume at the recommended contour level is 225 nm^3; this corresponds to an approximate mass of 203 kDa.

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

7.3 Rotationally averaged power spectrum (i)

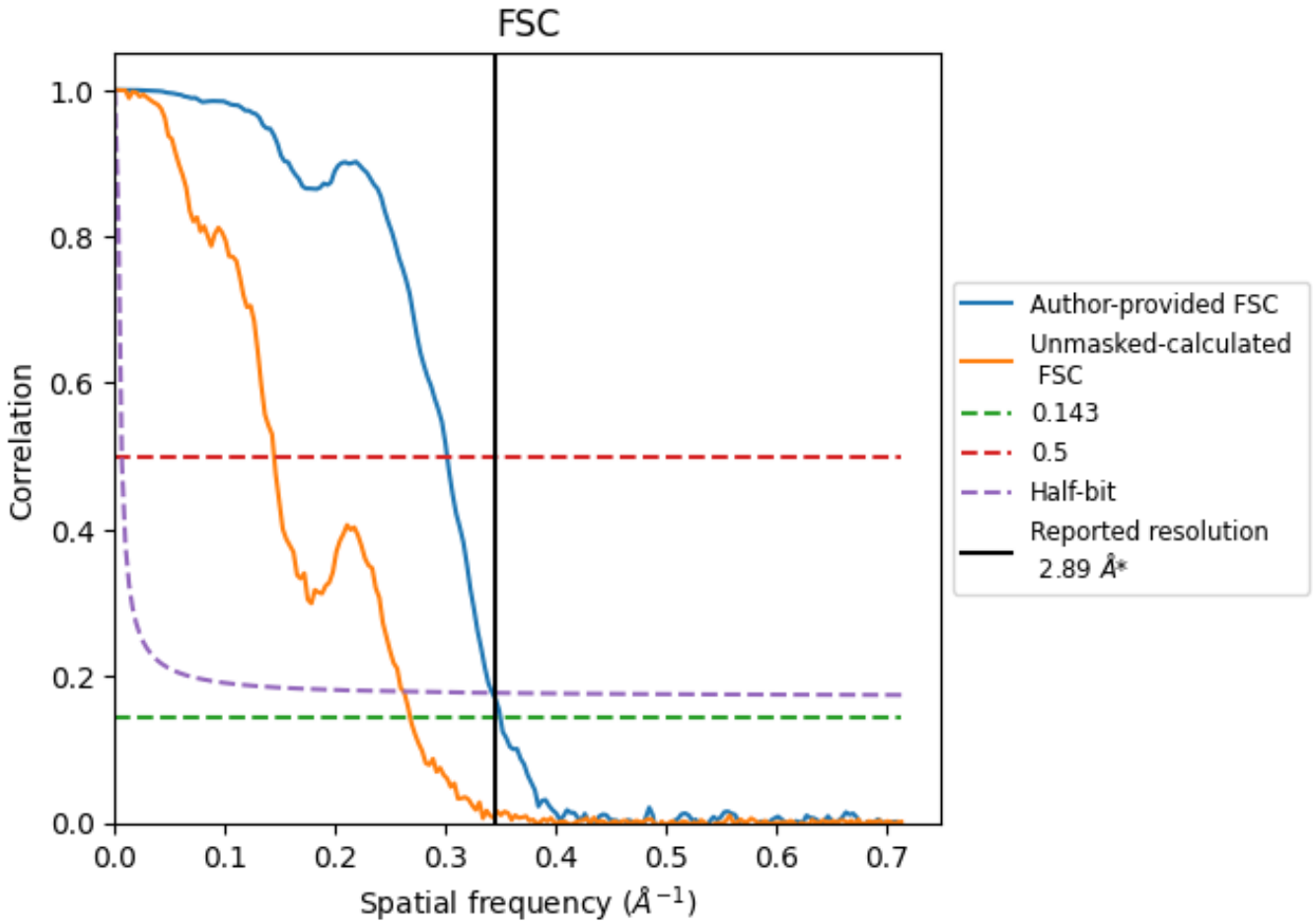


*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

8.2 Resolution estimates (i)

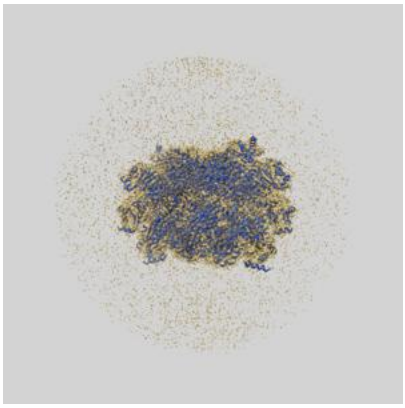
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.86	3.31	2.92
Unmasked-calculated*	3.73	6.91	3.81

*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 3.73 differs from the reported value 2.89 by more than 10 %

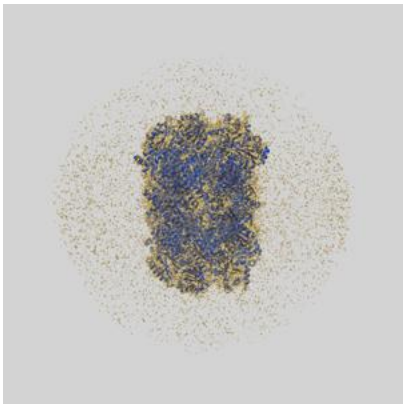
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16901 and PDB model 8OIX. Per-residue inclusion information can be found in section 3 on page 10.

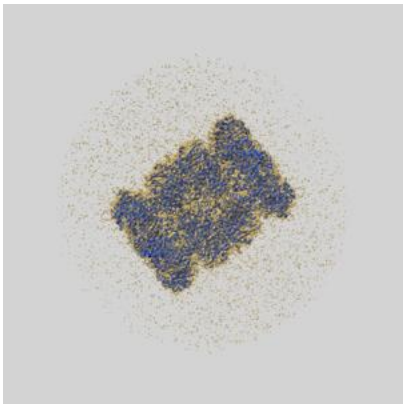
9.1 Map-model overlay



X



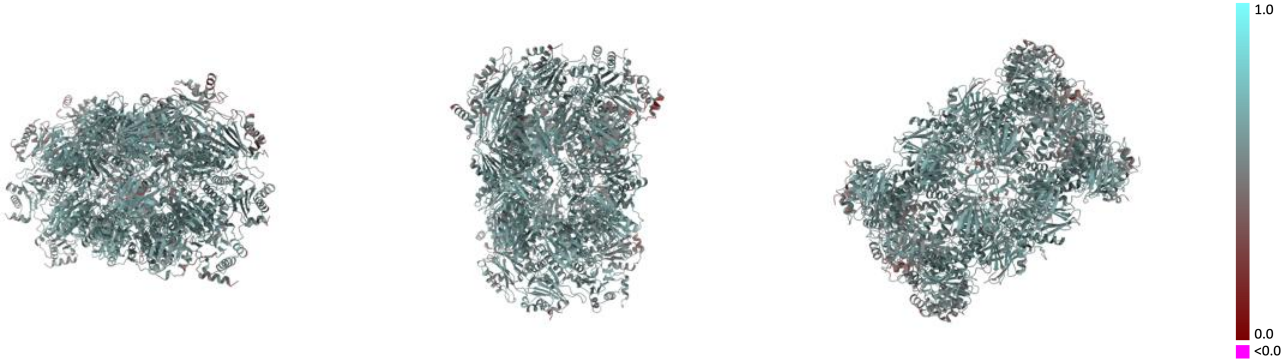
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.133 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.

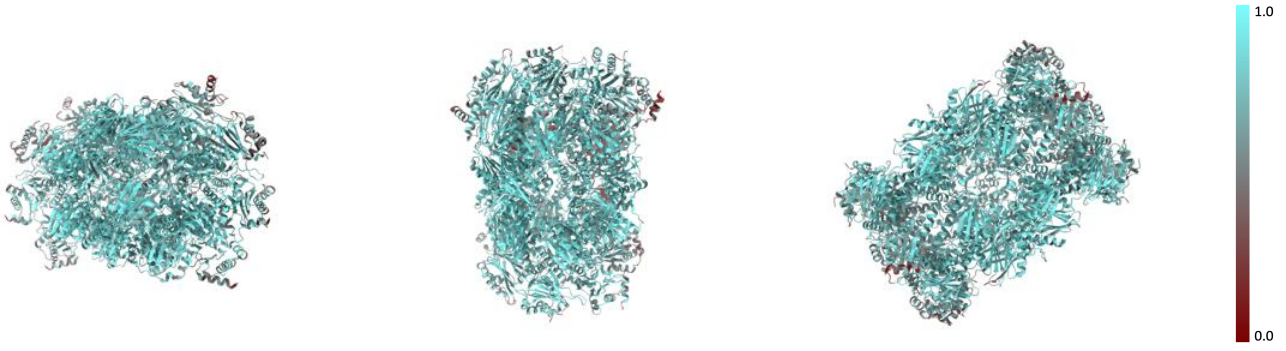
9.2 Q-score mapped to coordinate model



X Y Z

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.

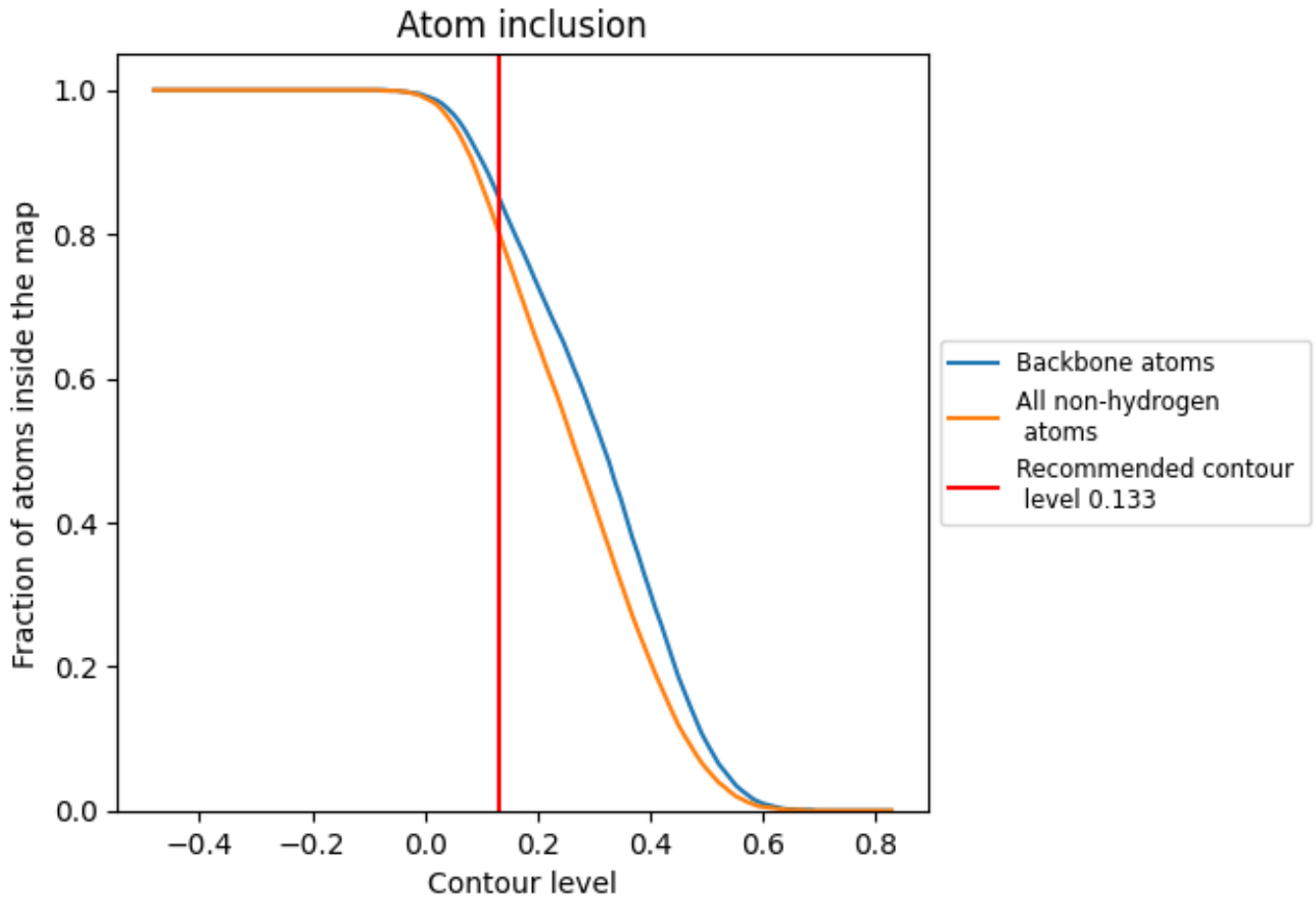
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.133).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5810
A	0.7590	0.5650
B	0.7570	0.5730
C	0.7400	0.5600
D	0.6690	0.5240
E	0.7530	0.5710
F	0.7880	0.5750
G	0.7920	0.5710
H	0.8510	0.6060
I	0.8490	0.6030
J	0.8570	0.6020
K	0.8220	0.5880
L	0.8400	0.5970
M	0.8660	0.6020
N	0.8780	0.6080
O	0.7590	0.5660
P	0.7570	0.5720
Q	0.7400	0.5610
R	0.6690	0.5250
S	0.7530	0.5730
T	0.7880	0.5760
U	0.7920	0.5690
V	0.8520	0.6060
W	0.8500	0.6040
X	0.8570	0.6020
Y	0.8220	0.5870
Z	0.8400	0.5910
a	0.8660	0.6030
b	0.8780	0.6100