



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:30 AM UTC

PDB ID : 7ZGY / pdb_00007zgy
EMDB ID : EMD-14715
Title : S-layer Deinnoxanthin Binding Complex, C3 symmetry
Authors : Farci, D.; Piano, D.
Deposited on : 2022-04-04
Resolution : 2.54 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

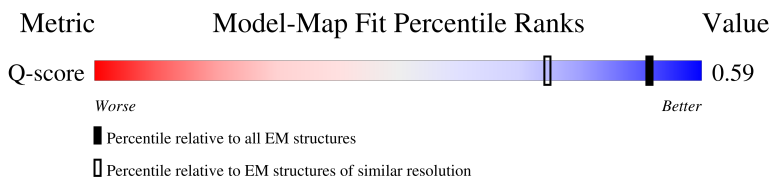
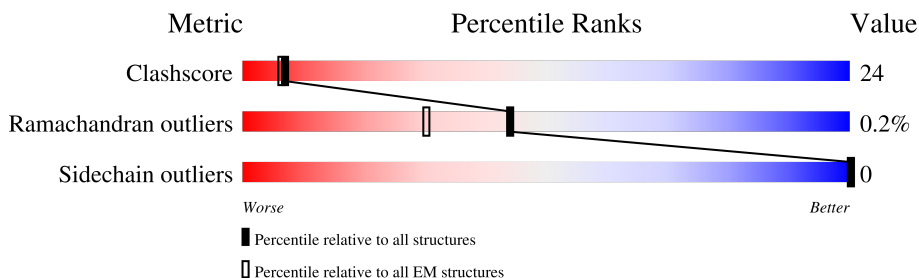
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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	7403 (2.04 - 3.04)

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	1167	 50% 31% 19%
1	B	1167	 50% 31% 19%
1	C	1167	 49% 33% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JPI	A	1201	X	-	-	-
2	JPI	B	1302	X	-	-	-
2	JPI	C	1201	X	-	-	-

2 Entry composition [i](#)

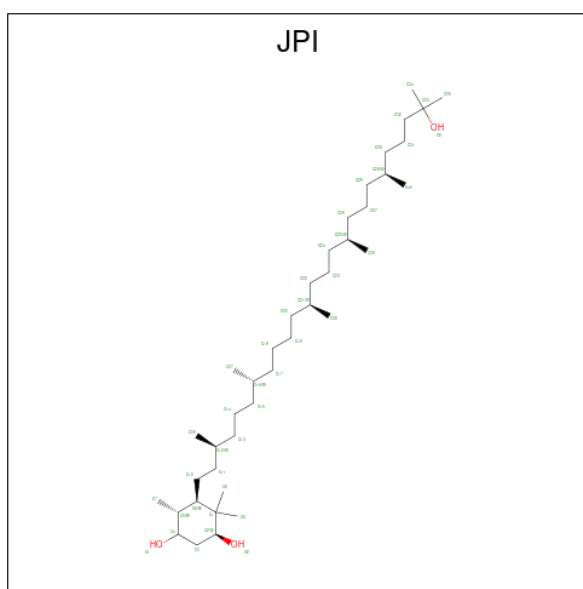
There are 6 unique types of molecules in this entry. The entry contains 22575 atoms, of which 714 are hydrogens and 0 are deuteriums.

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 S-layer protein SlpA.

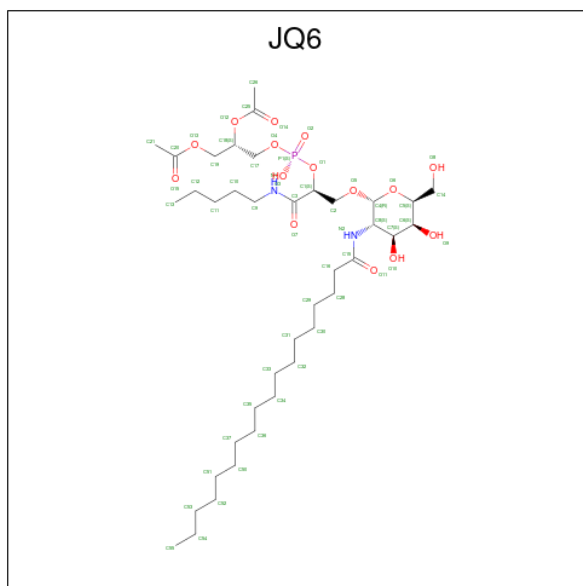
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	B	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	C	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		

- Molecule 2 is (3 {S},5 {R},6 {R})-5-[(3 {S},7 {R},12 {S},16 {S},20 {S})-3,7,12,16,20,24-hexamethyl-24-oxidanyl-pentacosyl]-4,4,6-trimethyl-cyclohexane-1,3-diol (CCD ID: JPI) (formula: C₄₀H₈₀O₃).



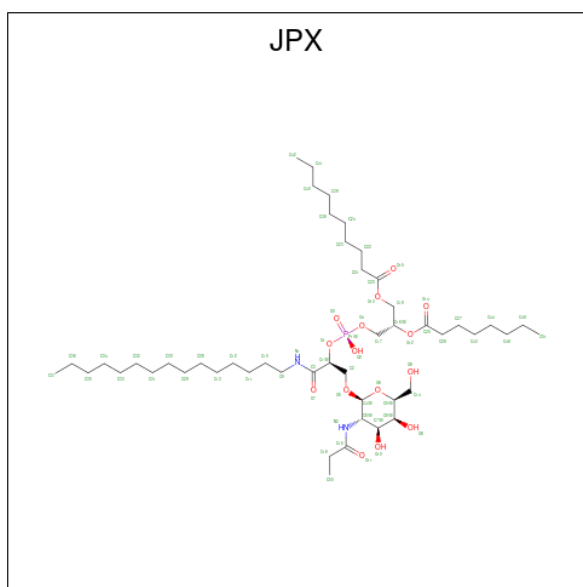
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			119	40	76	3	
2	B	1	Total	C	H	O	0
			119	40	76	3	
2	C	1	Total	C	H	O	0
			119	40	76	3	

- Molecule 3 is [(2 {S})-2-acetyloxy-3-[[[(2 {S})-3-[(2 {R},3 {S},4 {S},5 {S},6 {S})-6-(hydroxymethyl)-3-(octadecanoylamino)-4,5-bis(oxidanyl)oxan-2-yl]oxy-1-oxidanylidene-1-(pentylamino)propan-2-yl]oxy-oxidanyl-phosphoryl]oxy-propyl] ethanoate (CCD ID: JQ6) (formula: $C_{39}H_{73}N_2O_{15}P$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			129	39	72	2	15	1	
3	B	1	Total	C	H	N	O	P	0
			129	39	72	2	15	1	
3	C	1	Total	C	H	N	O	P	0
			129	39	72	2	15	1	

- Molecule 4 is [(2 {S})-3-[[[(2 {S})-3-[(2 {S},3 {S},4 {S},5 {S},6 {S})-6-(hydroxymethyl)-4,5-bis(oxidanyl)-3-(propanoylamino)oxan-2-yl]oxy-1-oxidanylidene-1-(pentadecylamino)propan-2-yl]oxy-oxidanyl-phosphoryl]oxy-2-octanoyloxy-propyl] decanoate (CCD ID: JPX) (formula: $C_{48}H_{91}N_2O_{15}P$).



Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	H	N	O	P	0	
			156	48	90	2	15	1		
4	B	1	Total	C	H	N	O	P	0	
			156	48	90	2	15	1		
4	B	1	Total	C	H	N	O	P	0	
			156	48	90	2	15	1		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	Cu	0
			3	3	
5	B	3	Total	Cu	0
			3	3	
5	C	3	Total	Cu	0
			3	3	

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Fe	0
			1	1	
6	B	1	Total	Fe	0
			1	1	

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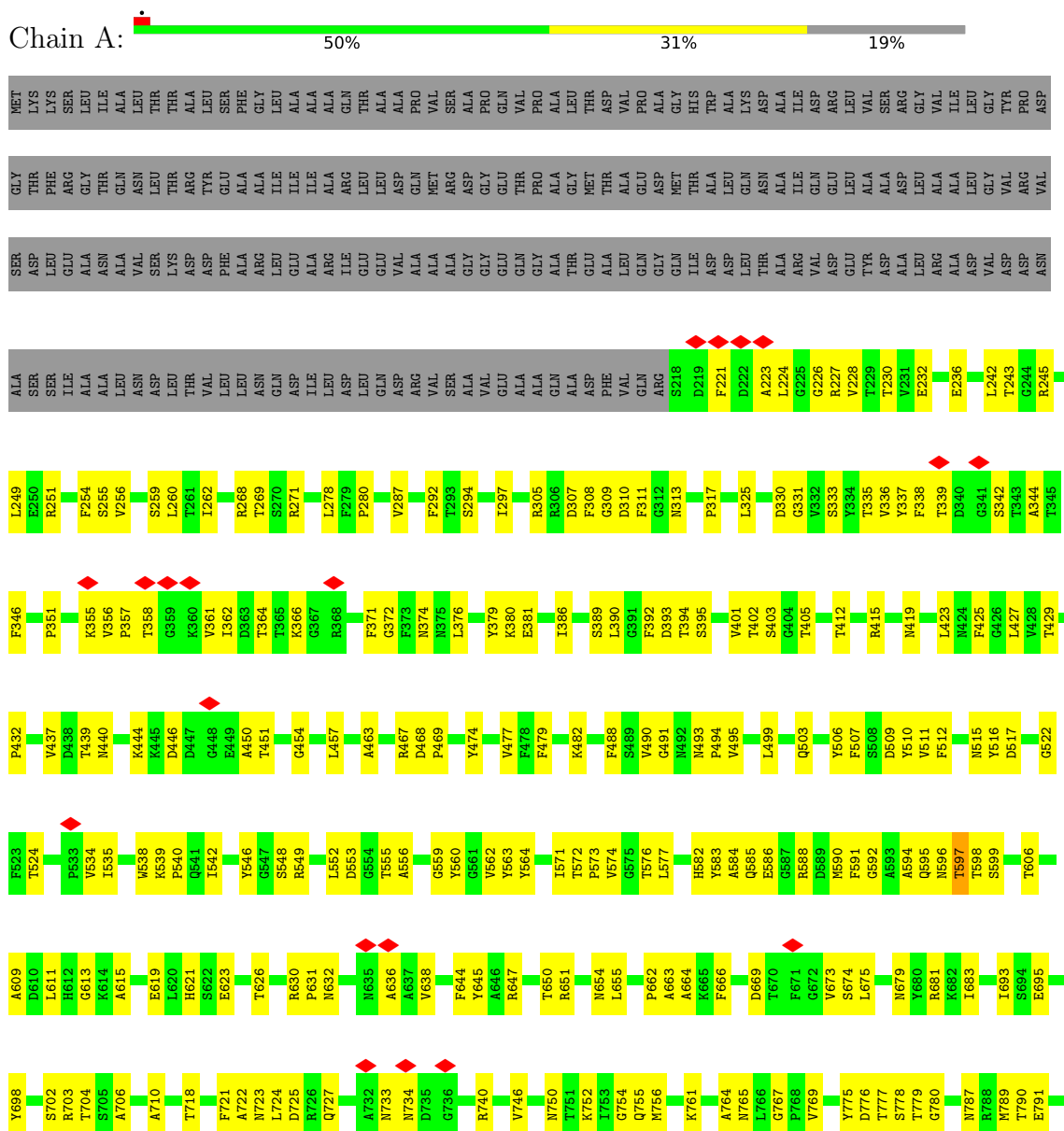
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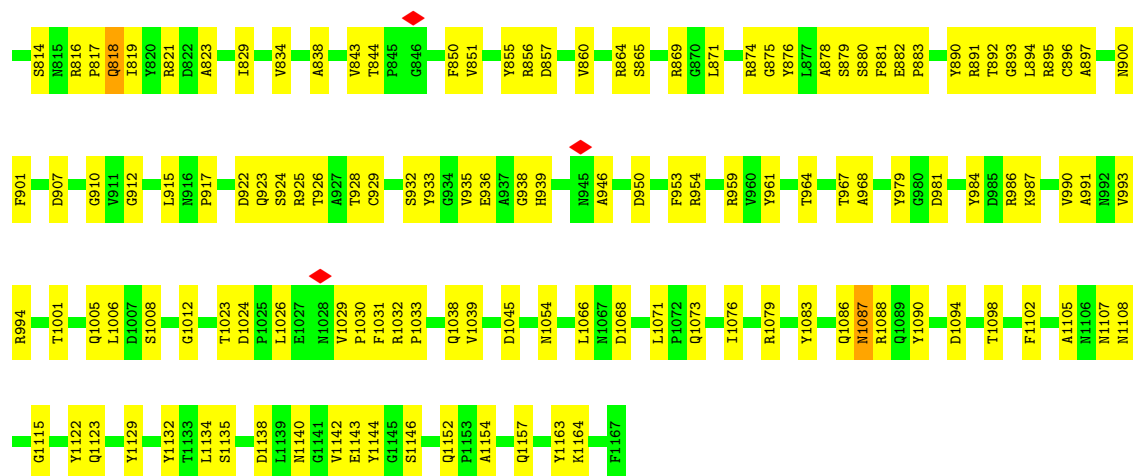
Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Fe	0
			1	1	

3 Residue-property plots

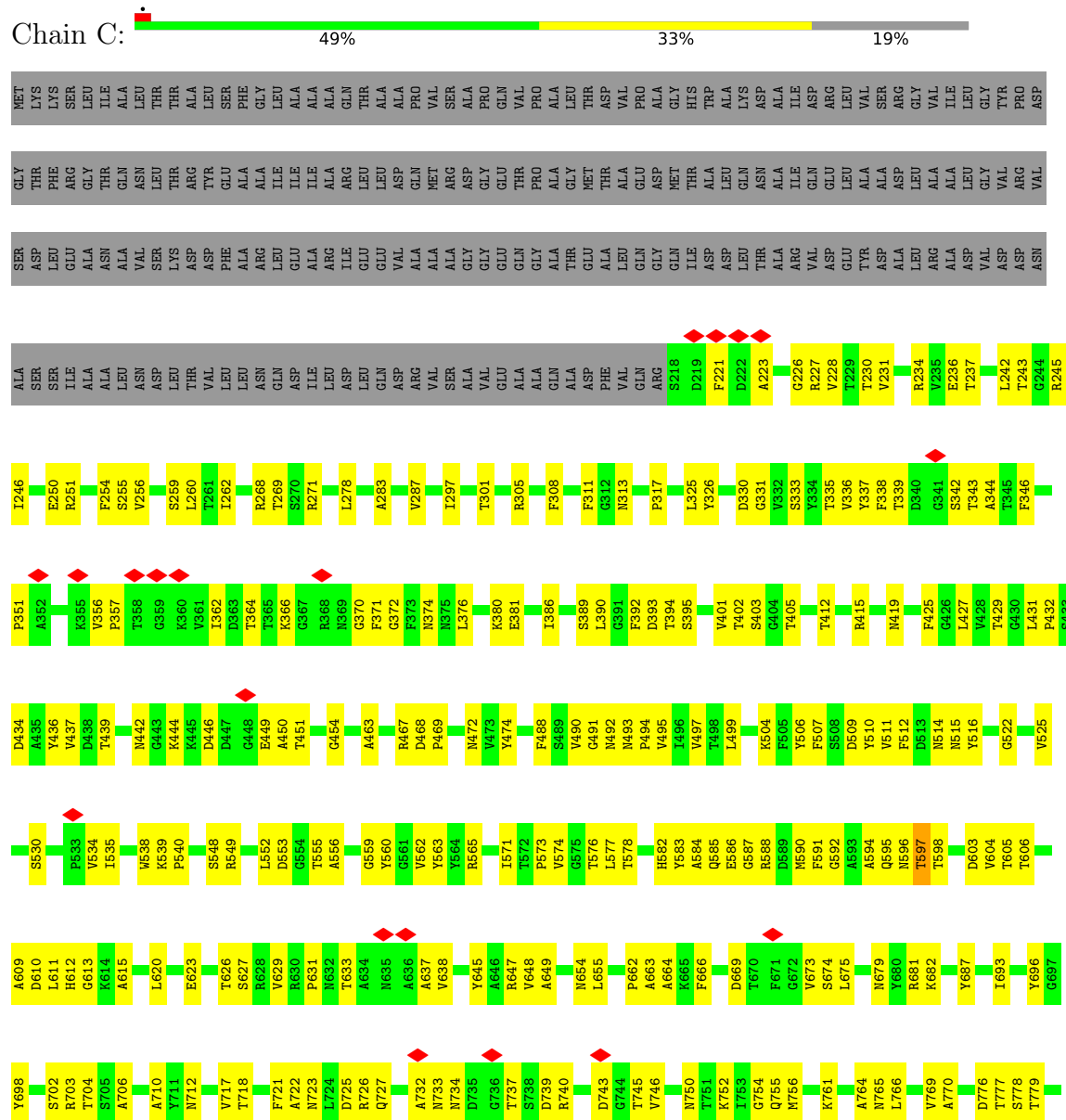
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: S-layer protein SlpA





• Molecule 1: S-layer protein SlpA



F167	G1077	A966	D784
	V1078	T967	A878
	R1079	F973	S879
	Y1080		E882
		D981	P883
	M1083		N888
	A1085	R986	A889
	Q1086	K987	Y890
	N1087	V988	R891
	R1088	G989	T892
		V990	G893
	T1091	A991	L894
		R992	R895
	G1095	V993	C896
		R994	A897
			D898
	G1100	T1001	N899
	Y1101	T1002	N900
	F1102	N1003	F901
	A1105		D907
	N1106	L1006	I908
	N1107		D909
	M1108	A1011	G910
	R1109		V911
	R1110	L1019	D822
			G912
	L1113	T1023	G913
	N1114		V914
	G1115	L1026	L915
		E1027	N916
	V1118	N1028	P917
	Y1122	V1029	D822
	Q1123	P1030	
		F1031	
		R1032	
	Y1132	P1033	
	T1133		R925
	L1134	N1036	T926
	S1135	G1037	A927
		Q1038	T928
		V1039	C929
	D1138		S932
	L1139		R856
	N1140	D1045	D857
	G1141	N1046	V858
	V1142	R1047	R859
	E1143		A937
	Y1144		G938
	G1145	N1052	H939
	S1146	Y1053	
		N1054	
		A1055	N945
	Q1152	N1056	A946
	P1153		
	A1154	F953	
		R954	
	Q1157		
		L1066	
	Y1163	L1071	R959
	K1164		V960
			Y961
			T965

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	252122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.993	Depositor
Minimum map value	-1.662	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	431.90402, 431.90402, 431.90402	wwPDB
Map dimensions	528, 528, 528	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.818, 0.818, 0.818	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, FE, JQ6, JPX, JPI

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	0.16	0/7258	0.36	2/9865 (0.0%)
1	B	0.16	0/7258	0.36	1/9865 (0.0%)
1	C	0.16	0/7258	0.35	2/9865 (0.0%)
All	All	0.16	0/21774	0.36	5/29595 (0.0%)

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
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	ASN	CB-CA-C	-6.03	109.61	116.54
1	B	597	THR	CB-CA-C	-5.58	110.16	116.63
1	A	597	THR	CB-CA-C	-5.51	110.24	116.63
1	C	597	THR	CB-CA-C	-5.49	110.26	116.63
1	C	801	SER	CB-CA-C	-5.19	110.17	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	696	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7117	0	6745	353	0
1	B	7117	0	6745	350	0
1	C	7117	0	6745	357	0
2	A	43	76	0	7	0
2	B	43	76	0	5	0
2	C	43	76	0	1	0
3	A	57	72	0	3	0
3	B	57	72	0	3	0
3	C	57	72	0	7	0
4	A	66	90	0	8	0
4	B	132	180	0	11	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	21861	714	20235	1013	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 24.

The worst 5 of 1013 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)
4:B:1301:JPX:C30	4:B:1301:JPX:O15	1.82	1.28
3:A:1202:JQ6:C20	4:A:1203:JPX:C50	2.23	1.15
4:A:1203:JPX:O15	4:A:1203:JPX:C31	2.00	1.08
3:A:1202:JQ6:C21	4:A:1203:JPX:C16	2.33	1.05
1:A:540:PRO:HB2	2:A:1201:JPI:C37	1.87	1.04

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	947/1167 (81%)	848 (90%)	97 (10%)	2 (0%)	43	56
1	B	947/1167 (81%)	846 (89%)	99 (10%)	2 (0%)	43	56
1	C	947/1167 (81%)	850 (90%)	95 (10%)	2 (0%)	43	56
All	All	2841/3501 (81%)	2544 (90%)	291 (10%)	6 (0%)	44	56

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLN
1	B	818	GLN
1	C	818	GLN
1	B	1087	ASN
1	A	1087	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/891 (82%)	726 (100%)	0	100	100
1	B	726/891 (82%)	726 (100%)	0	100	100
1	C	726/891 (82%)	726 (100%)	0	100	100
All	All	2178/2673 (82%)	2178 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	654	ASN
1	C	861	ASN
1	B	350	ASN
1	B	282	ASN
1	C	1054	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
2	JPI	C	1201	-	43,43,43	2.08	3 (6%)	53,58,58	1.85	6 (11%)
2	JPI	A	1201	-	43,43,43	2.08	3 (6%)	53,58,58	1.89	6 (11%)
2	JPI	B	1302	-	43,43,43	2.04	3 (6%)	53,58,58	1.91	7 (13%)
3	JQ6	C	1202	-	56,57,57	0.26	0	65,71,71	0.61	1 (1%)
3	JQ6	B	1304	4	56,57,57	0.29	0	65,71,71	0.53	0
4	JPX	B	1301	3	65,66,66	0.47	1 (1%)	74,80,80	0.77	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JPX	A	1203	-	65,66,66	0.45	1 (1%)	74,80,80	0.73	2 (2%)
4	JPX	B	1303	-	65,66,66	0.38	0	74,80,80	1.23	6 (8%)
3	JQ6	A	1202	-	56,57,57	0.31	0	65,71,71	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JPI	C	1201	-	4/4/11/11	13/37/61/61	0/1/1/1
2	JPI	A	1201	-	4/4/11/11	10/37/61/61	0/1/1/1
2	JPI	B	1302	-	4/4/11/11	18/37/61/61	0/1/1/1
3	JQ6	C	1202	-	-	26/58/78/78	0/1/1/1
3	JQ6	B	1304	4	-	23/58/78/78	0/1/1/1
4	JPX	B	1301	3	-	39/69/89/89	0/1/1/1
4	JPX	A	1203	-	-	32/69/89/89	0/1/1/1
4	JPX	B	1303	-	-	31/69/89/89	0/1/1/1
3	JQ6	A	1202	-	-	30/58/78/78	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	JPI	C5-C6	-9.87	1.34	1.54
2	A	1201	JPI	C5-C6	-9.77	1.34	1.54
2	B	1302	JPI	C5-C6	-9.51	1.35	1.54
2	A	1201	JPI	O1-C4	-8.88	1.24	1.43
2	B	1302	JPI	O1-C4	-8.74	1.25	1.43

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	JPI	C7-C5-C6	8.15	126.14	112.95
2	C	1201	JPI	C7-C5-C6	8.10	126.06	112.95
2	B	1302	JPI	C7-C5-C6	7.54	125.15	112.95
4	B	1303	JPX	O6-C4-O5	-6.03	95.79	110.04
2	B	1302	JPI	O1-C4-C5	5.64	122.18	110.62

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1201	JPI	C6
2	A	1201	JPI	C5
2	A	1201	JPI	C4
2	A	1201	JPI	C2
2	B	1302	JPI	C6

5 of 222 torsion outliers are listed below:

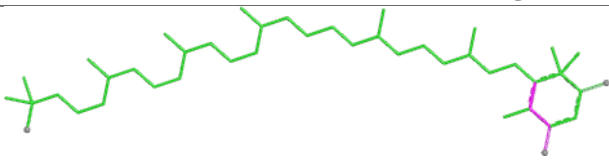
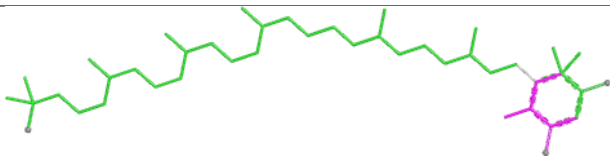
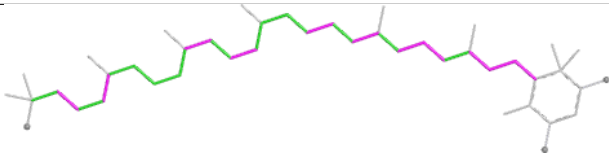
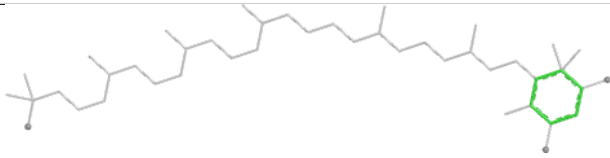
Mol	Chain	Res	Type	Atoms
2	B	1302	JPI	C6-C10-C11-C12
2	B	1302	JPI	C11-C10-C6-C1
2	C	1201	JPI	C11-C10-C6-C5
3	A	1202	JQ6	O1-C1-C2-O5
3	A	1202	JQ6	C16-C15-N2-C8

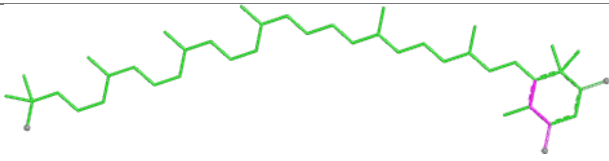
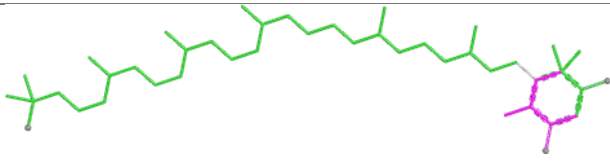
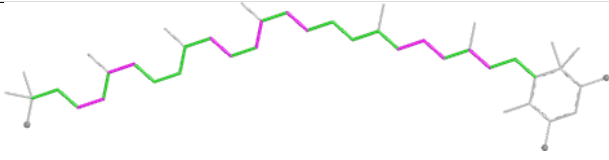
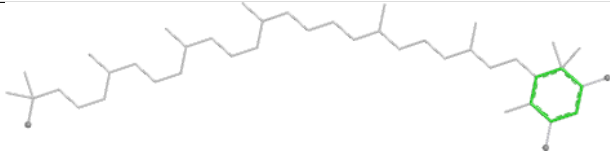
There are no ring outliers.

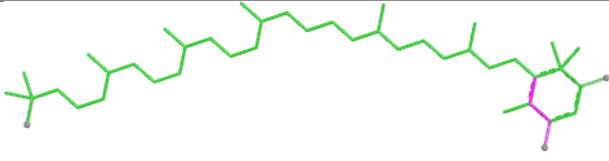
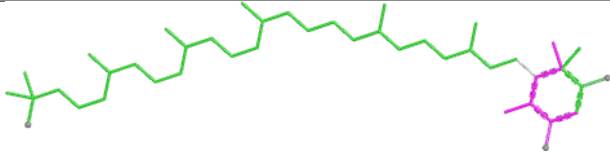
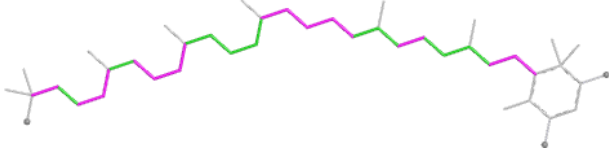
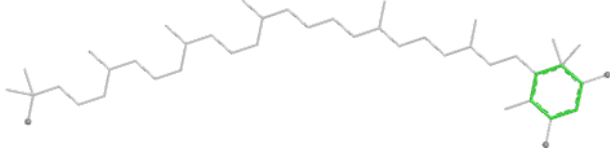
9 monomers are involved in 40 short contacts:

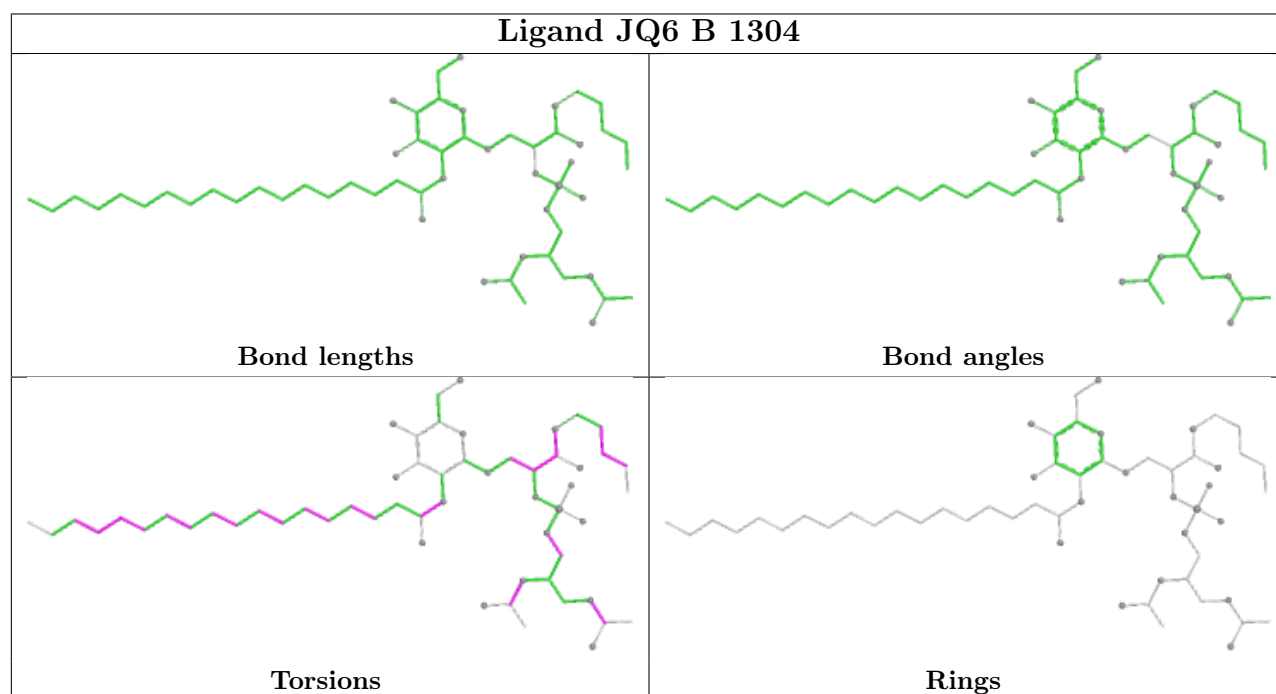
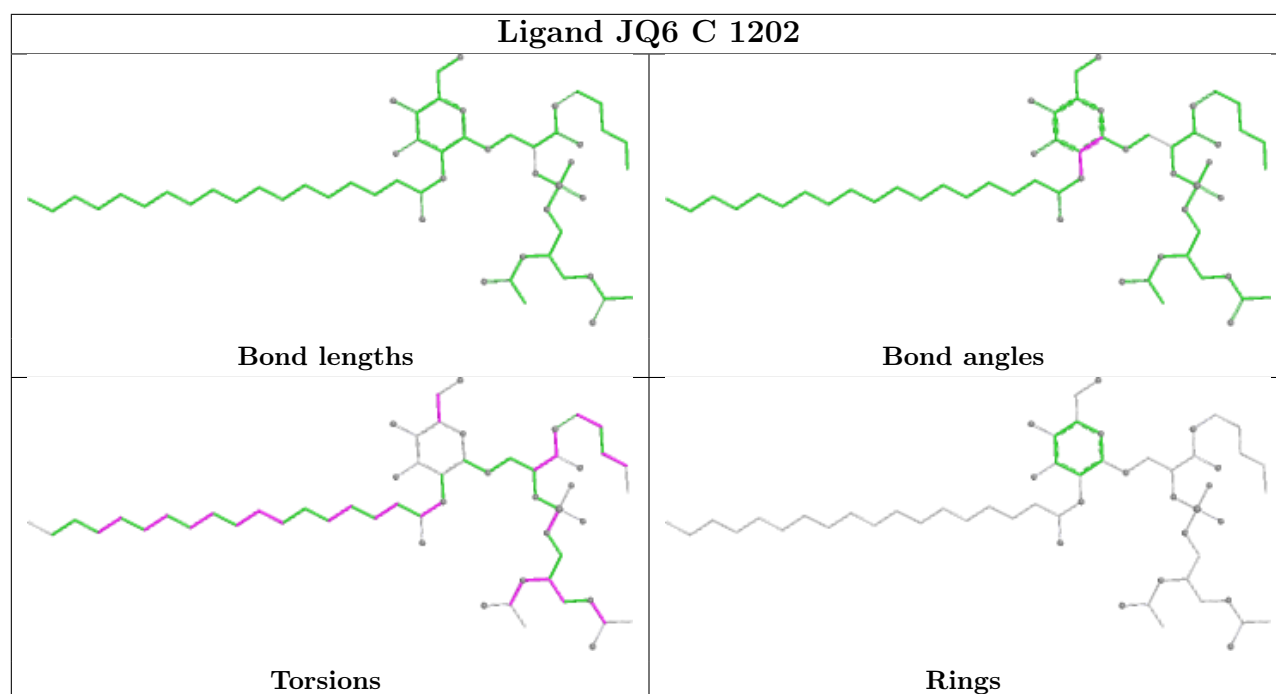
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	JPI	1	0
2	A	1201	JPI	7	0
2	B	1302	JPI	5	0
3	C	1202	JQ6	7	0
3	B	1304	JQ6	3	0
4	B	1301	JPX	8	0
4	A	1203	JPX	8	0
4	B	1303	JPX	3	0
3	A	1202	JQ6	3	0

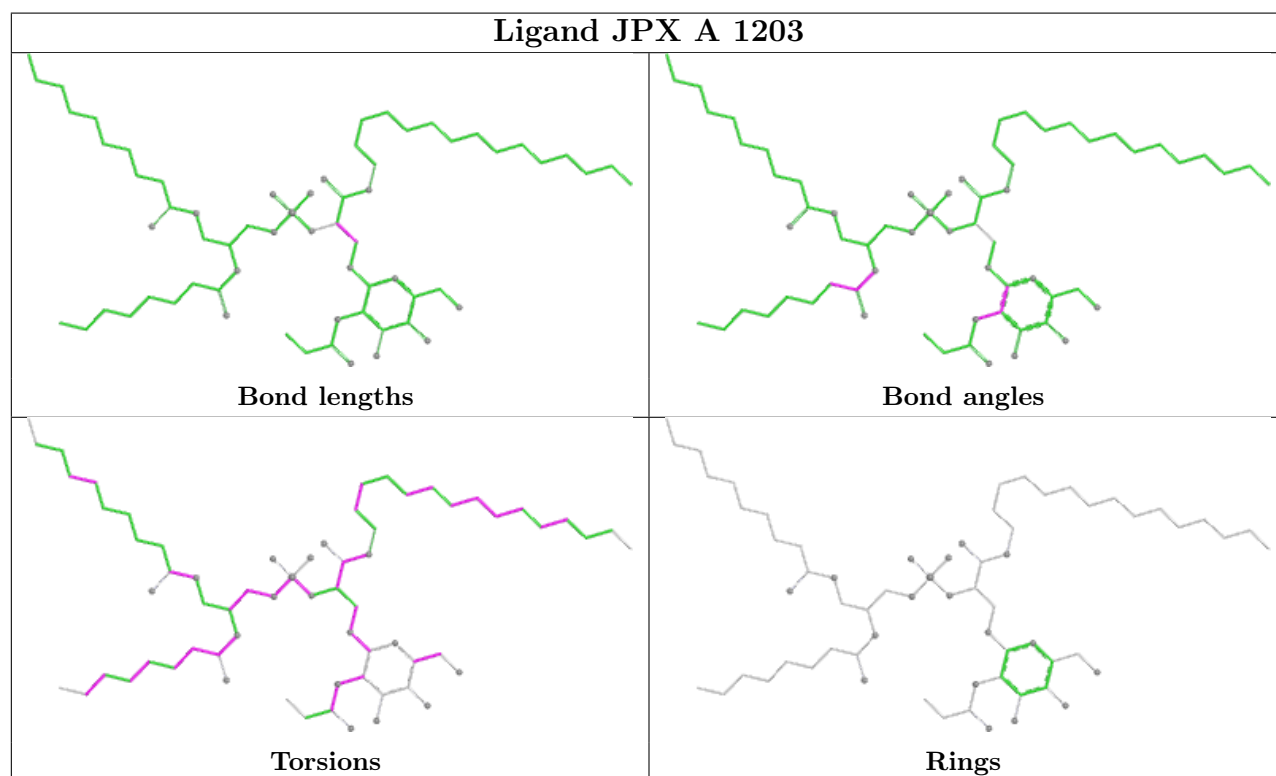
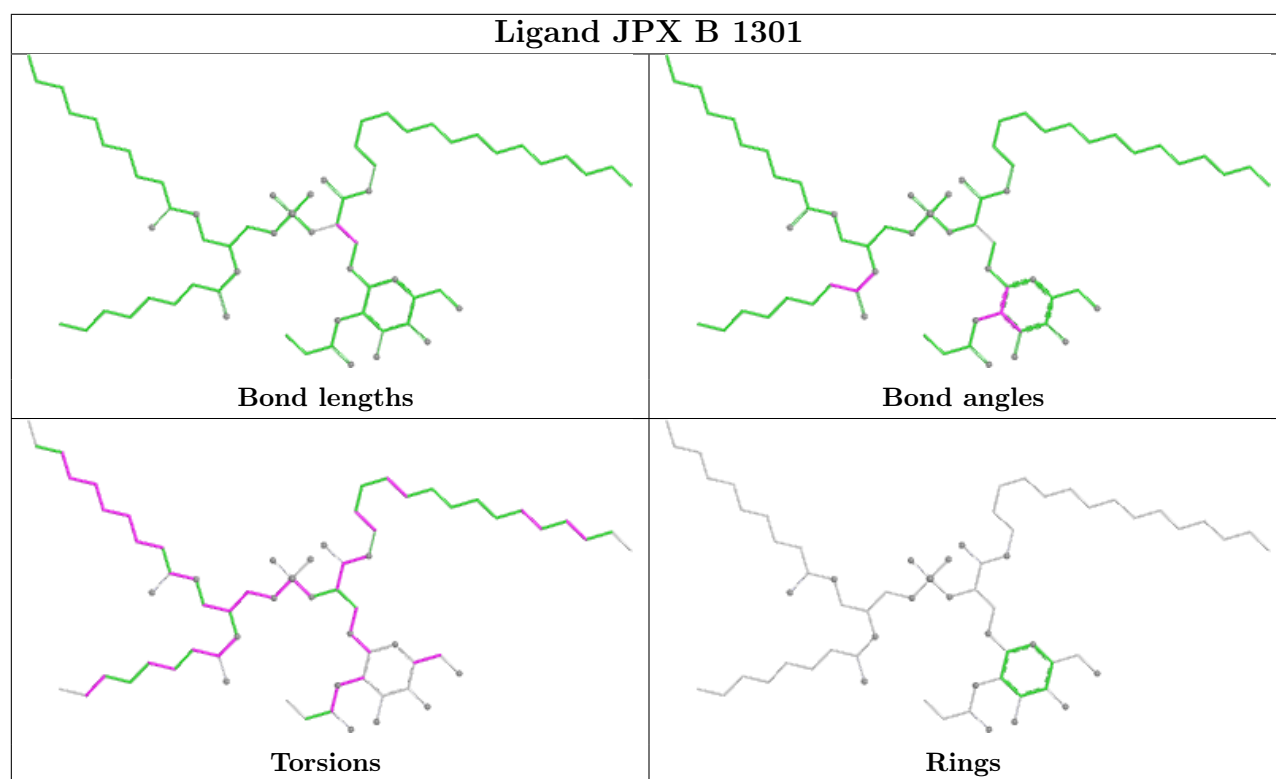
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

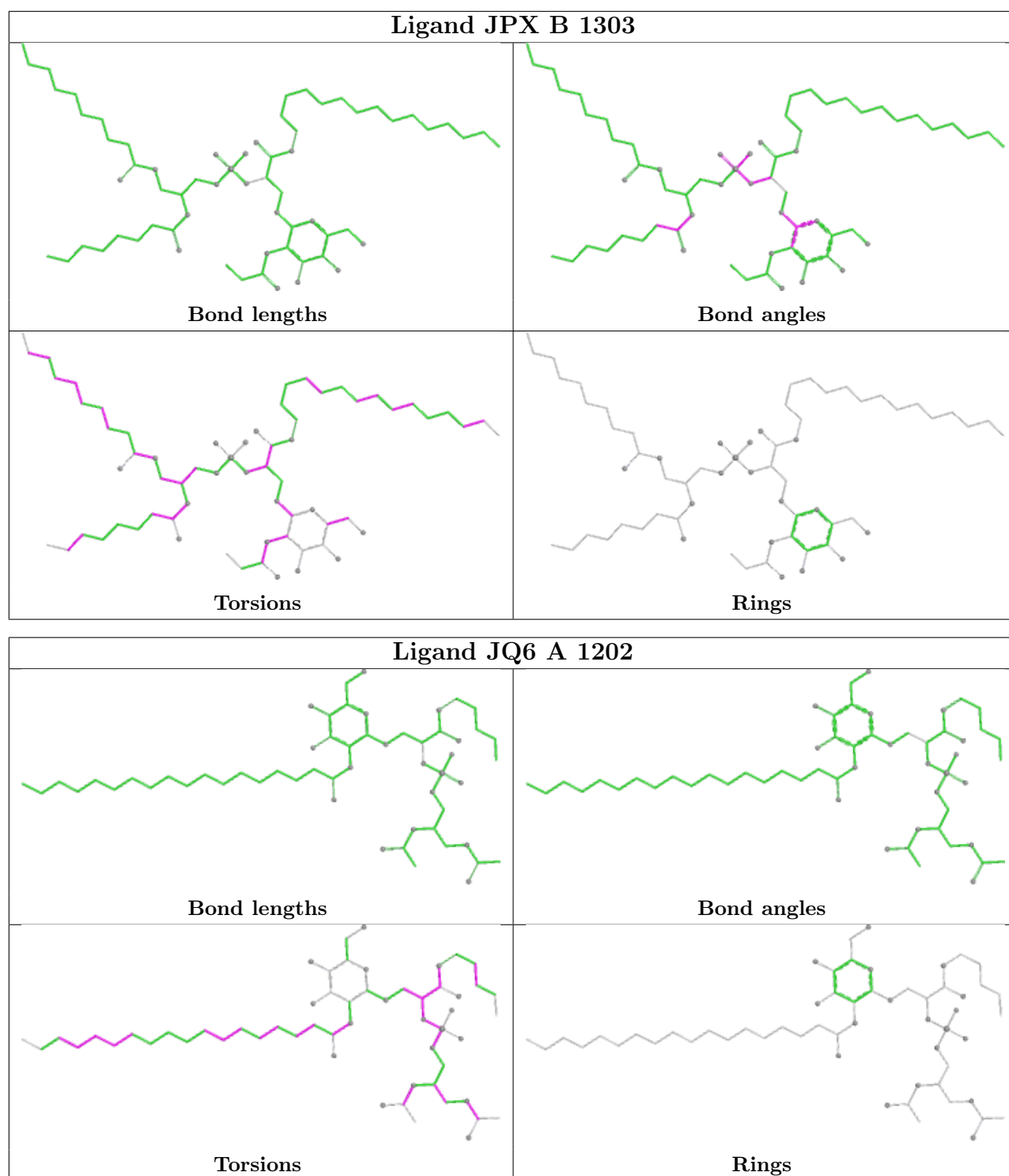
Ligand JPI C 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand JPI A 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand JPI B 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

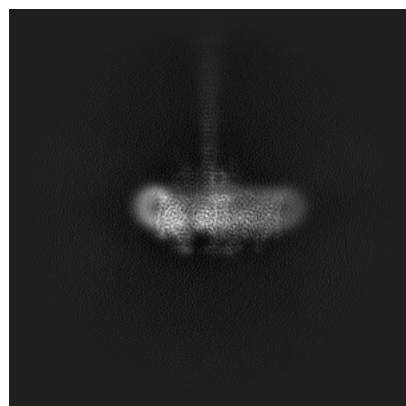
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14715. These allow visual inspection of the internal detail of the map and identification of artifacts.

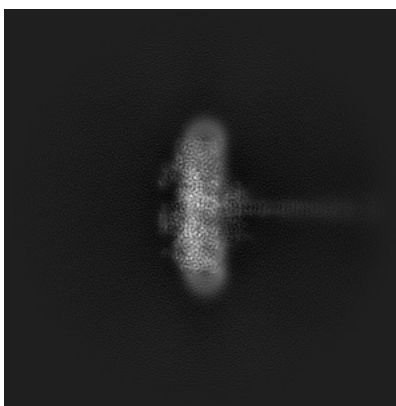
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

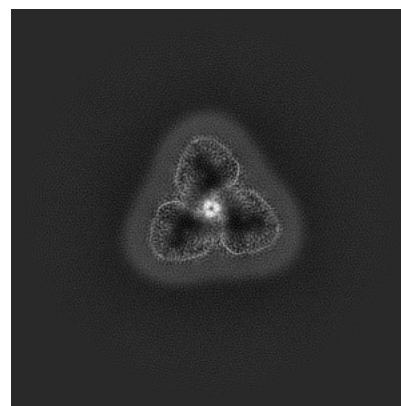
6.1.1 Primary map



X

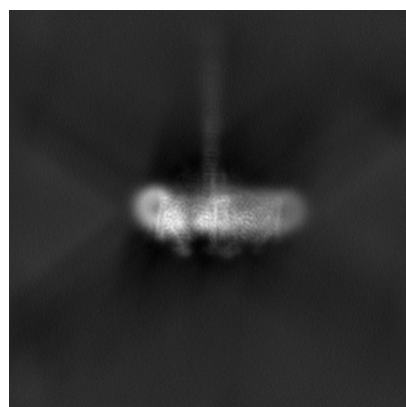


Y

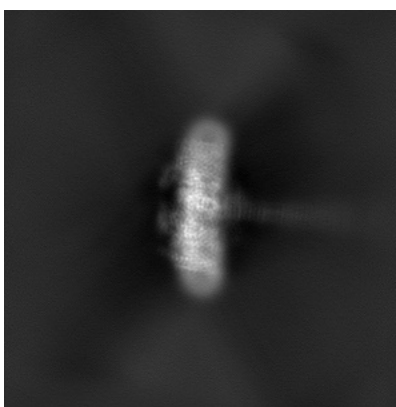


Z

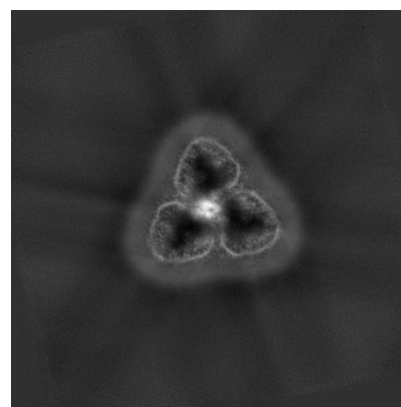
6.1.2 Raw map



X



Y

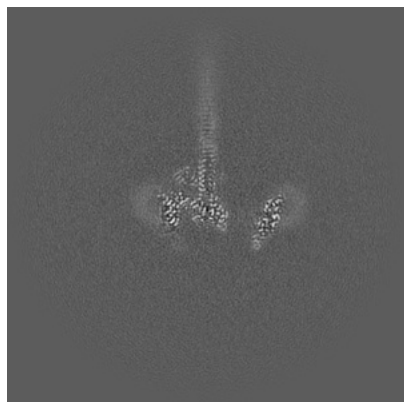


Z

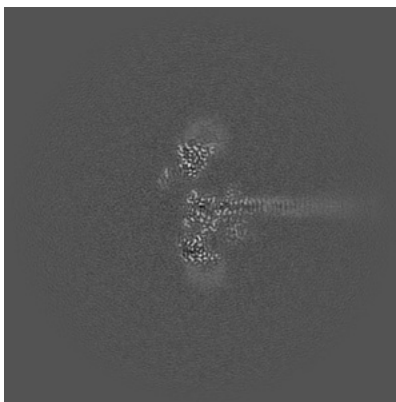
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

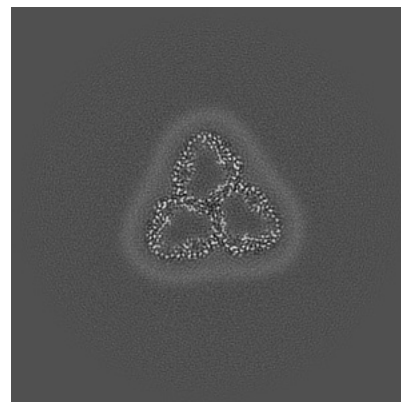
6.2.1 Primary map



X Index: 264

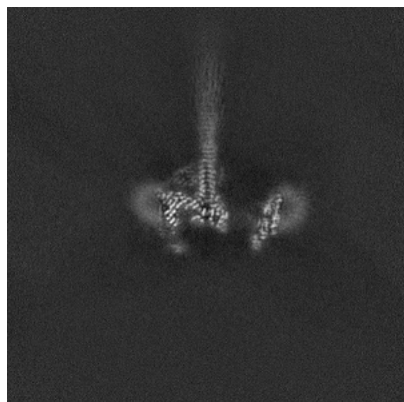


Y Index: 264

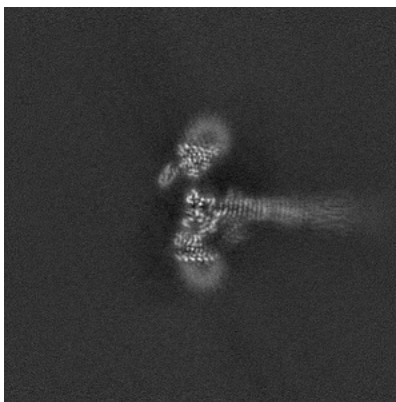


Z Index: 264

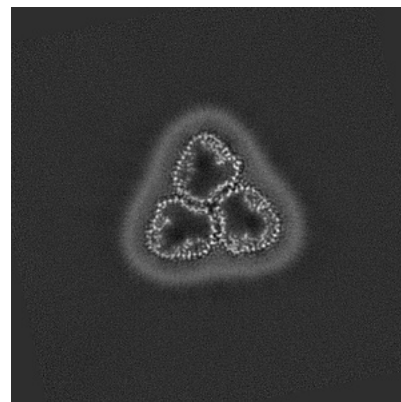
6.2.2 Raw map



X Index: 264



Y Index: 264

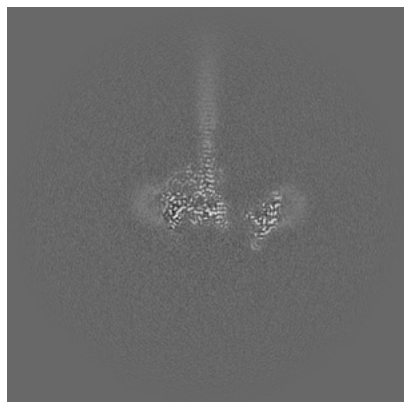


Z Index: 264

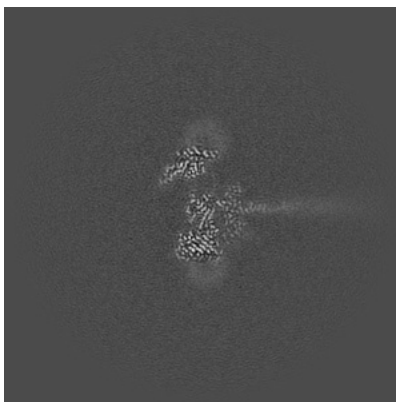
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

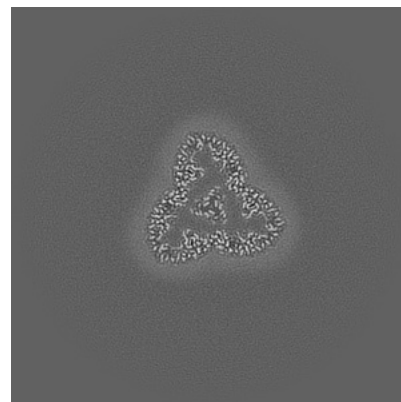
6.3.1 Primary map



X Index: 268

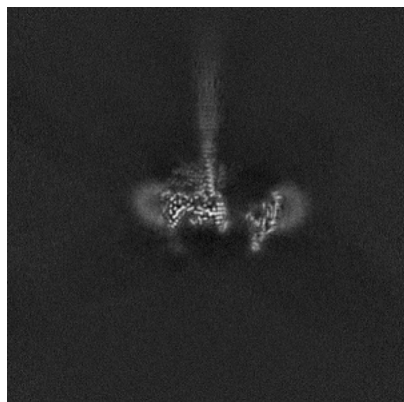


Y Index: 272

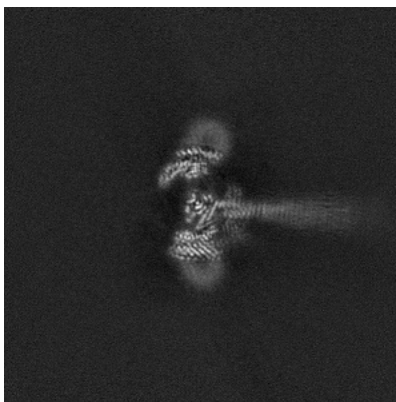


Z Index: 246

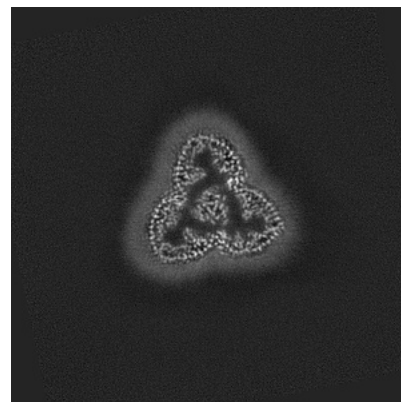
6.3.2 Raw map



X Index: 268



Y Index: 271

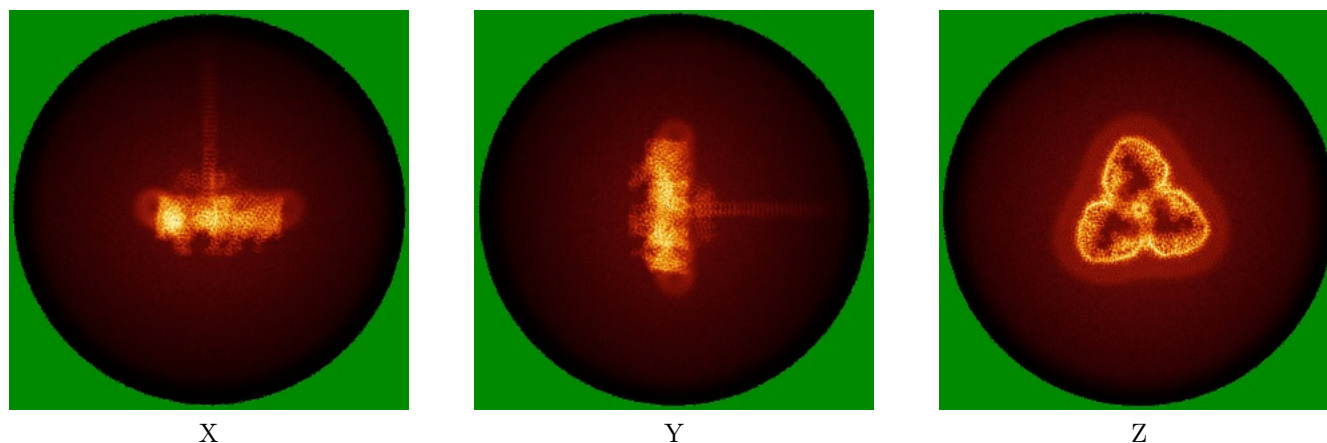


Z Index: 247

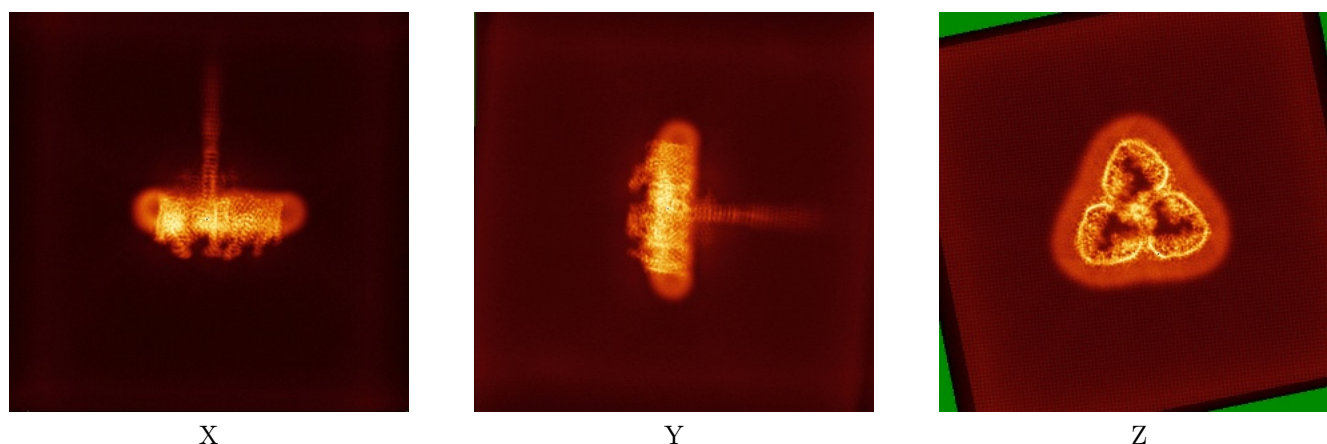
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

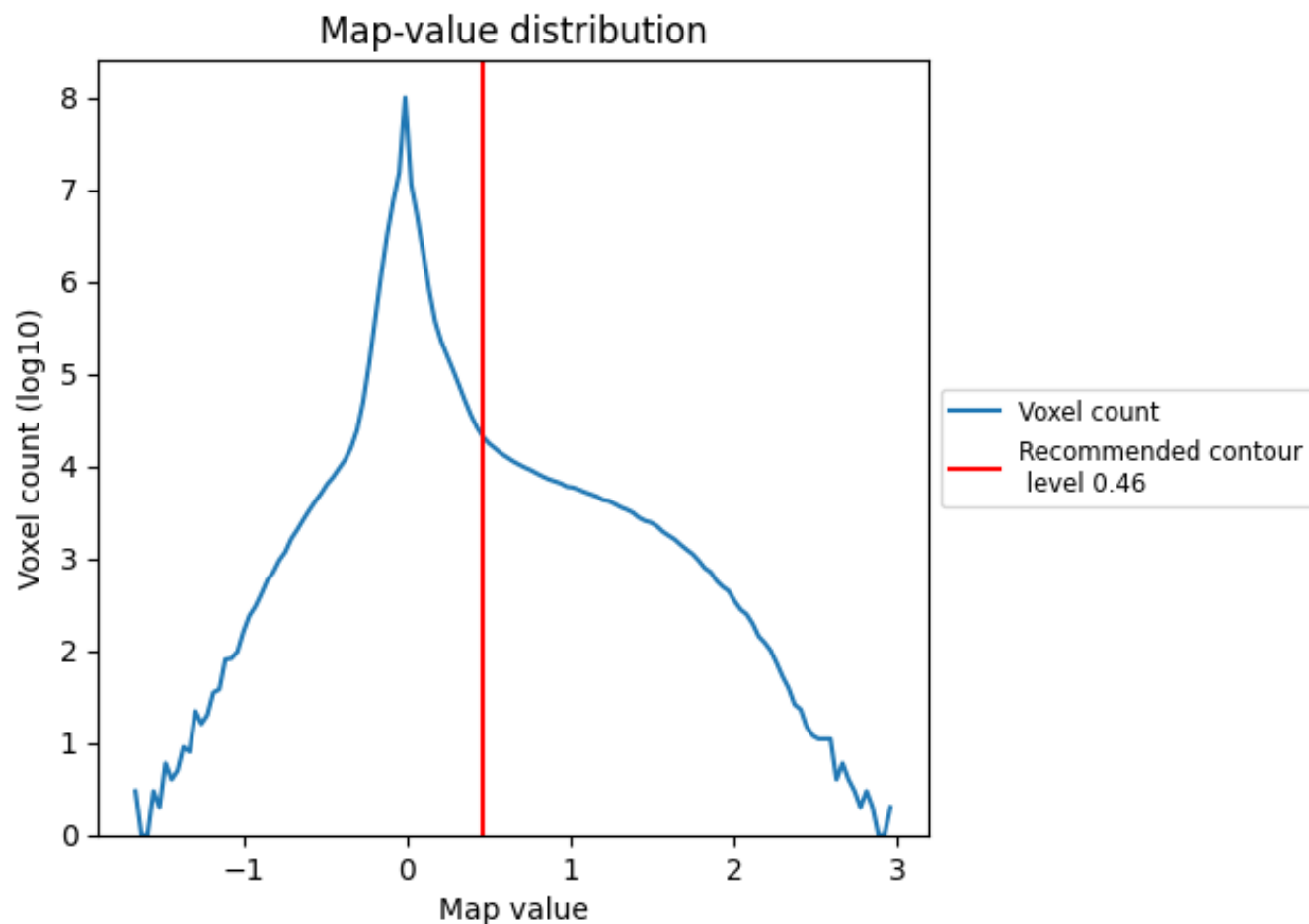
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

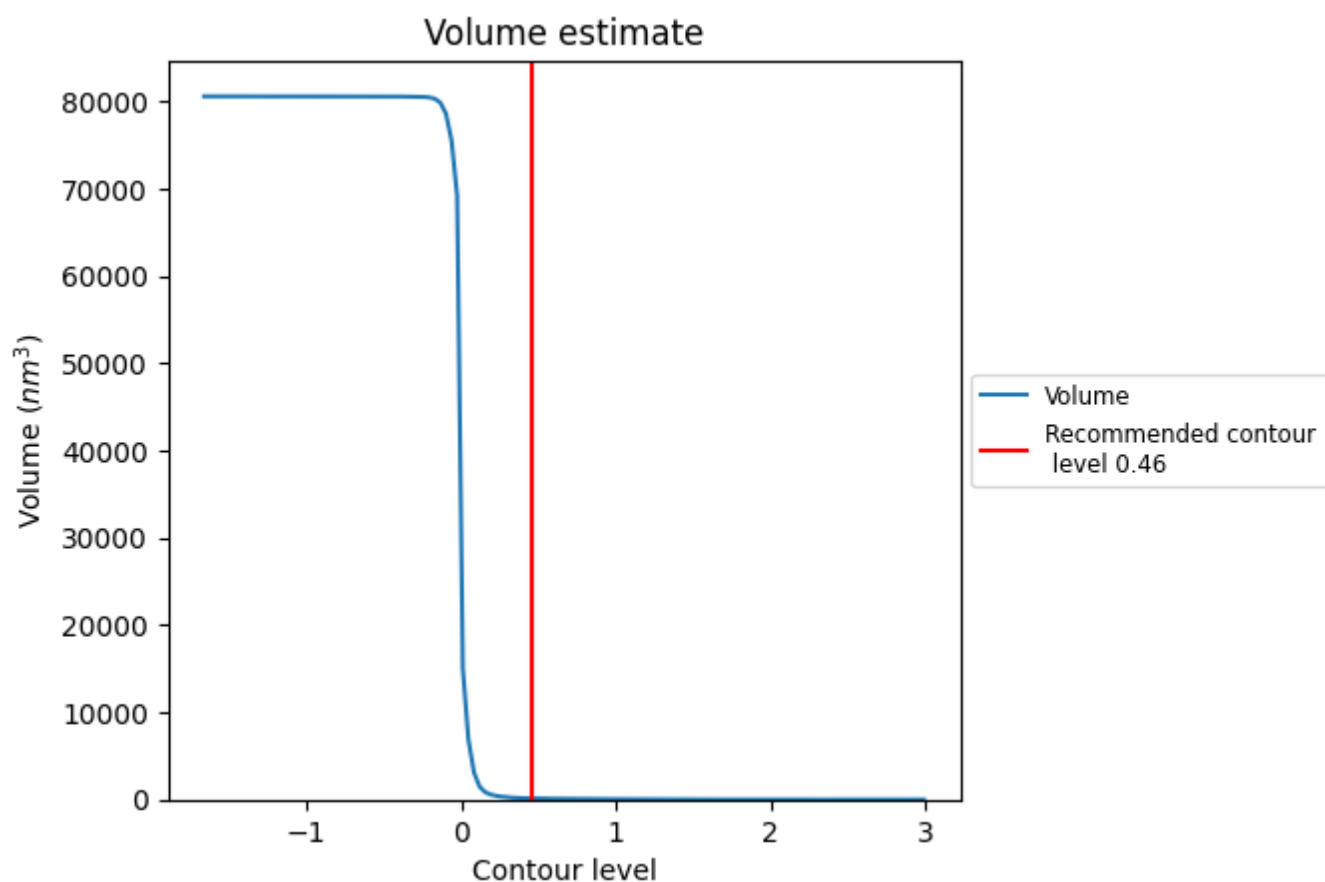
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

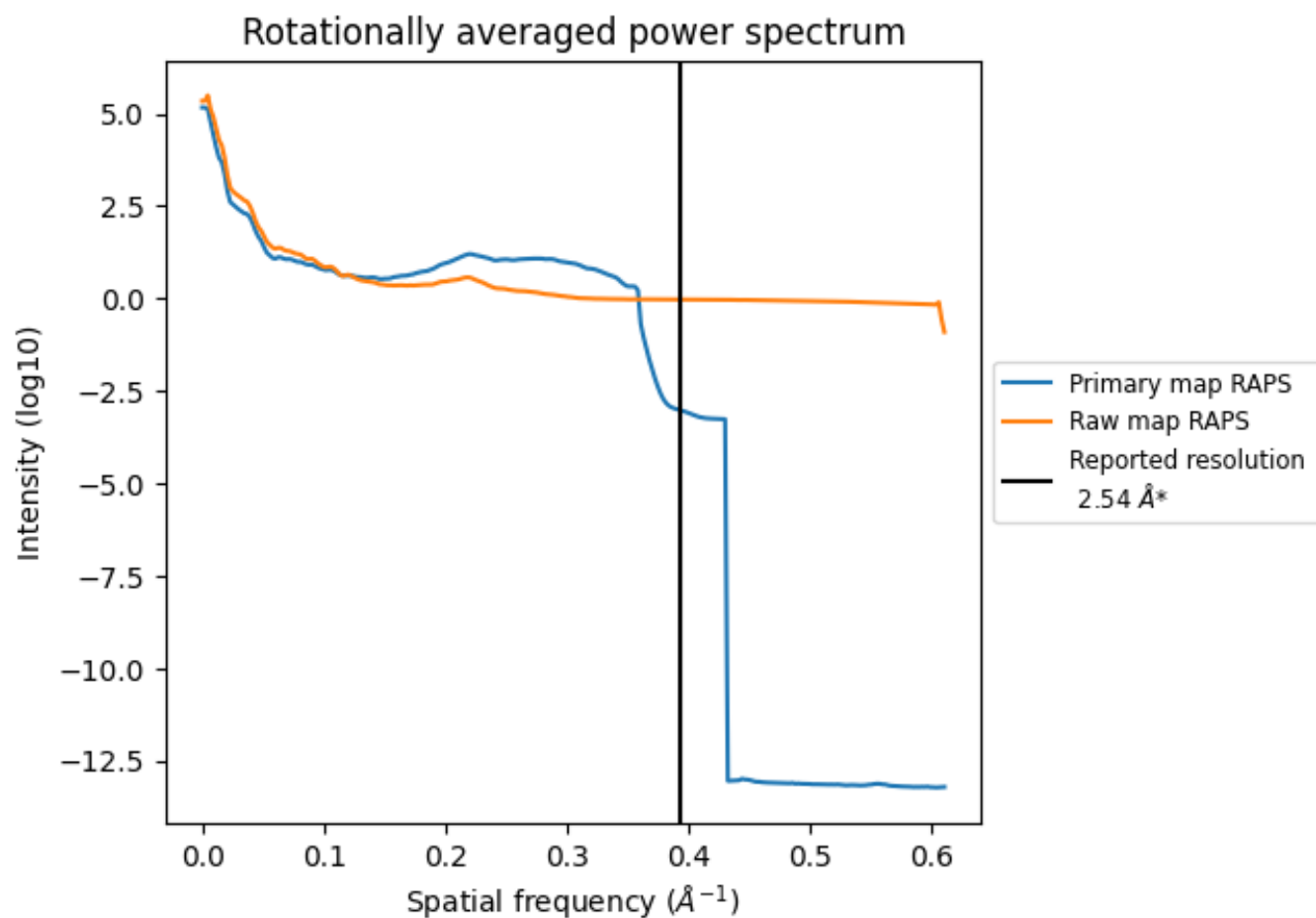
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 118 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 ⓘ

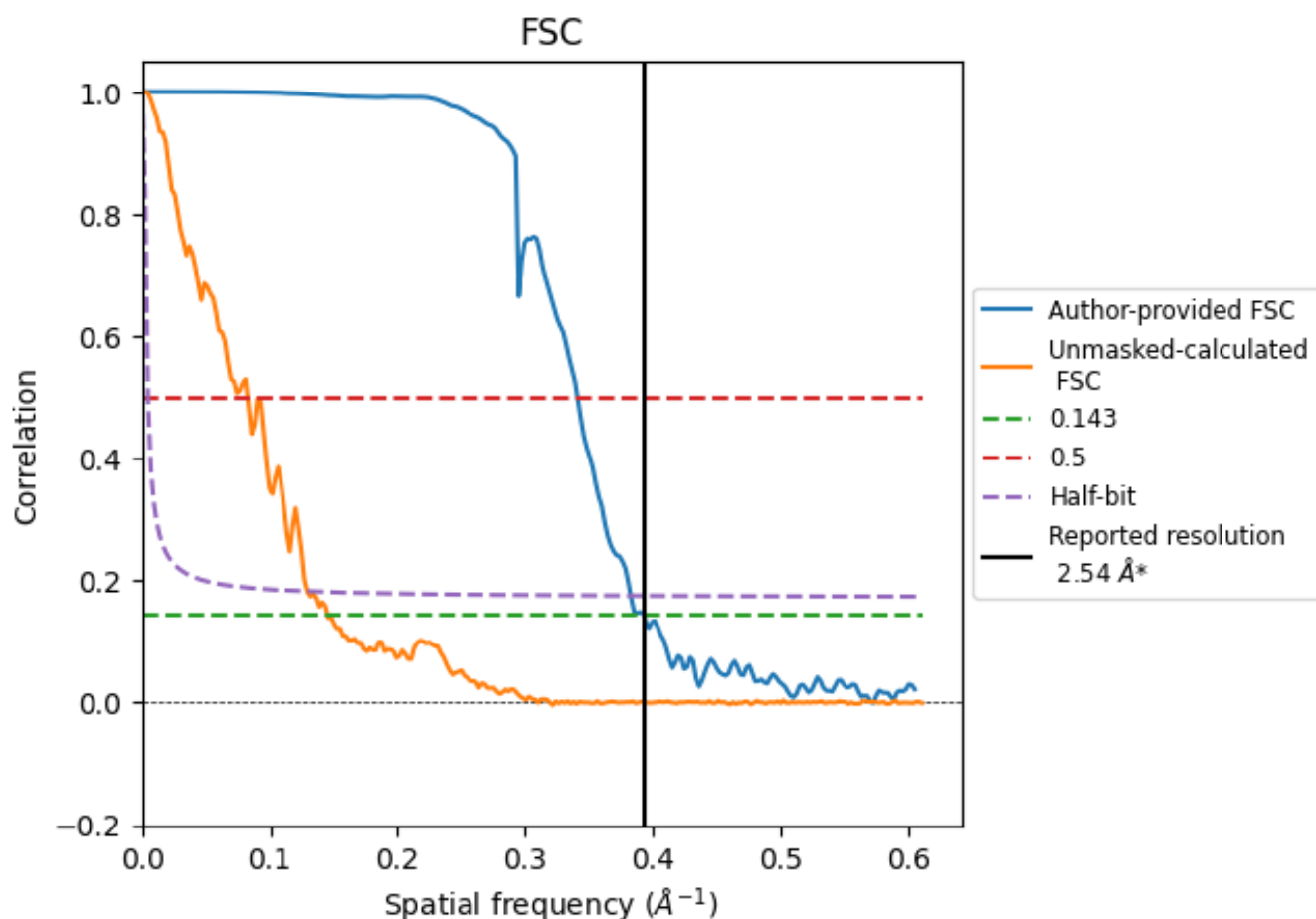


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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 0.394 Å⁻¹

8.2 Resolution estimates [i](#)

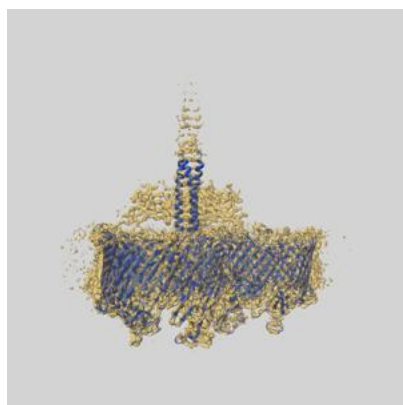
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.93	2.61
Unmasked-calculated*	6.88	12.11	7.72

*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 6.88 differs from the reported value 2.54 by more than 10 %

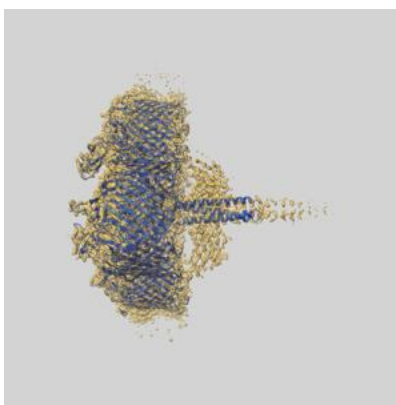
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14715 and PDB model 7ZGY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

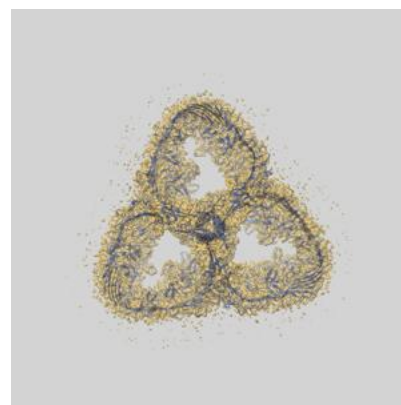
9.1 Map-model overlay [i](#)



X



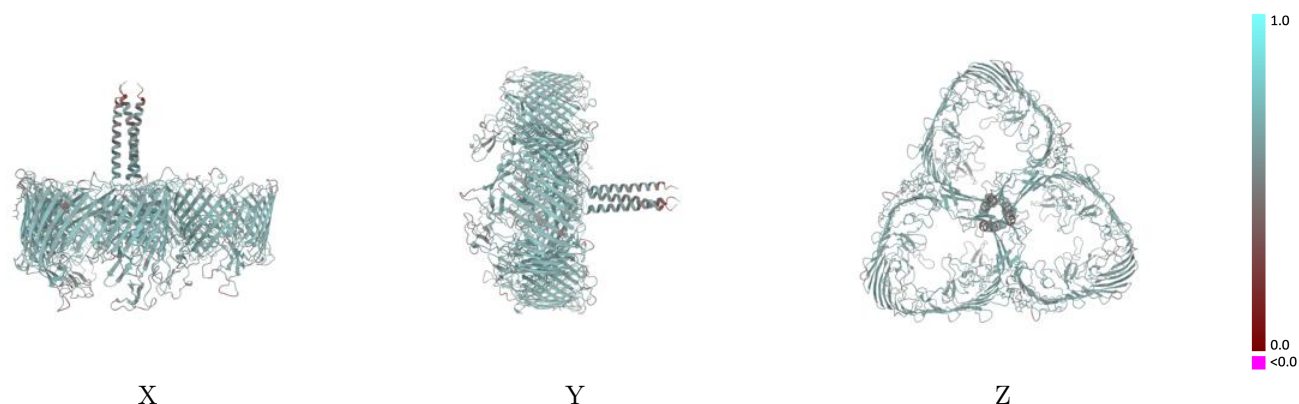
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



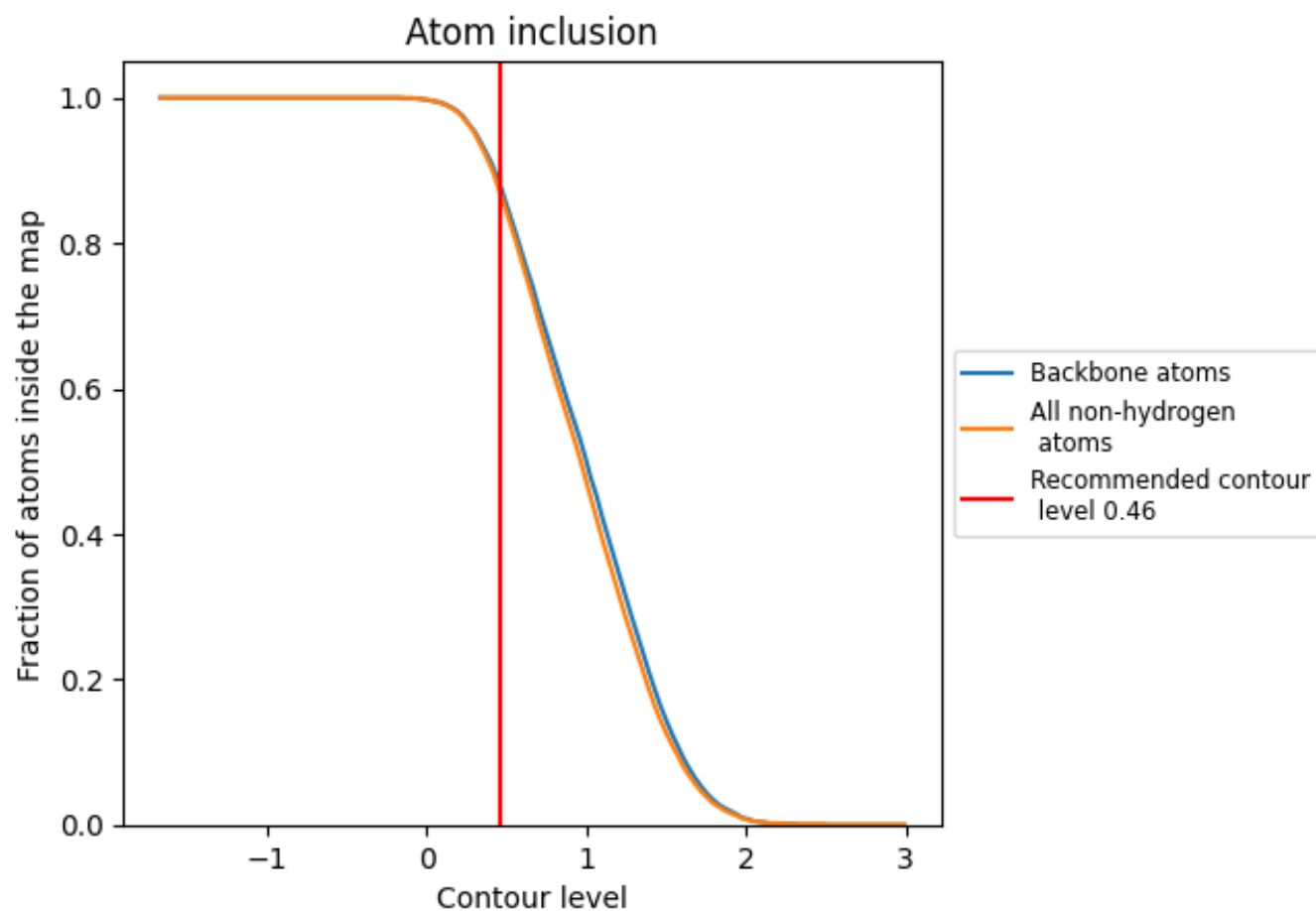
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.46).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.5900
A	0.8730	0.5900
B	0.8740	0.5910
C	0.8700	0.5890

