



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 07:56 AM UTC

PDB ID : 9E8Y / pdb_00009e8y
EMDB ID : EMD-47735
Title : Complex fibril structure of MSA alpha-synuclein with CNS-11g at 15 hours
Authors : Lu, J.; Sawaya, M.R.; Ge, P.; Boyer, D.R.; Eisenberg, D.S.
Deposited on : 2024-11-06
Resolution : 2.90 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:

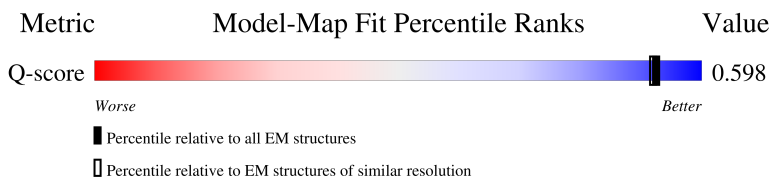
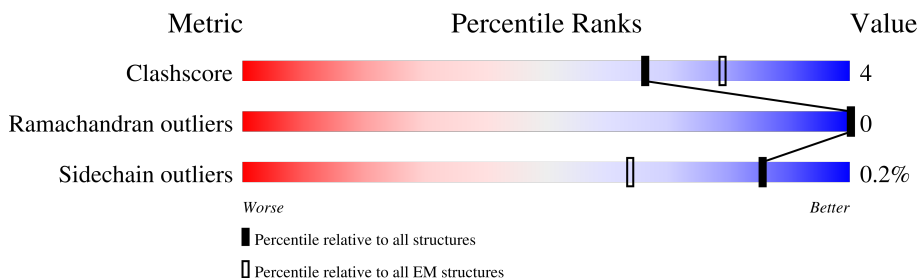
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 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.





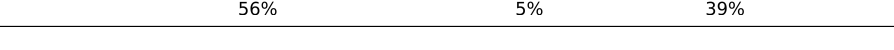
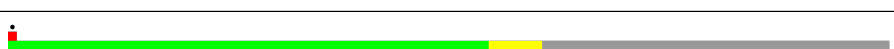


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	140	
1	B	140	
1	C	140	
1	D	140	

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Mol	Chain	Length	Quality of chain
1	E	140	
1	F	140	
1	G	140	
1	H	140	
1	I	140	
1	J	140	

2 Entry composition

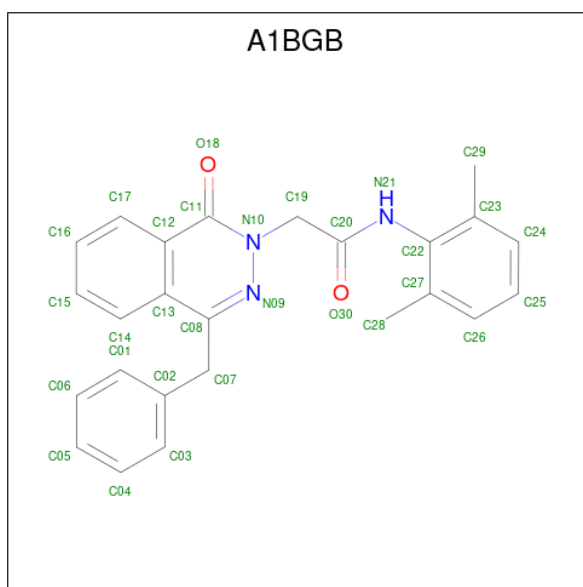
There are 2 unique types of molecules in this entry. The entry contains 5805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-synuclein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	85	Total	C	N	O	0	0
			582	362	102	118		
1	B	79	Total	C	N	O	0	0
			549	341	97	111		
1	C	85	Total	C	N	O	0	0
			582	362	102	118		
1	D	79	Total	C	N	O	0	0
			549	341	97	111		
1	E	85	Total	C	N	O	0	0
			582	362	102	118		
1	F	79	Total	C	N	O	0	0
			549	341	97	111		
1	G	85	Total	C	N	O	0	0
			582	362	102	118		
1	H	79	Total	C	N	O	0	0
			549	341	97	111		
1	I	85	Total	C	N	O	0	0
			582	362	102	118		
1	J	79	Total	C	N	O	0	0
			549	341	97	111		

- Molecule 2 is 2-(4-benzyl-1-oxophthalazin-2(1H)-yl)-N-(2,6-dimethylphenyl)acetamide (CCD ID: A1BGB) (formula: C₂₅H₂₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			30	25	3	2	
2	A	1	Total	C	N	O	0
			30	25	3	2	
2	C	1	Total	C	N	O	0
			30	25	3	2	
2	E	1	Total	C	N	O	0
			30	25	3	2	
2	I	1	Total	C	N	O	0
			30	25	3	2	

MET	ASP	VAL	PHE	MET	LYS	GLY	LEU	SER	LYS	ALA	LYS	GLU	G14	V15	T22	K23	A29	V37	V71	I88	T92	G93	D98	G98	G99	G100	G101	G102	G103	G104	G105	G106	G107	G108	G109	G110	G111	G112	G113	G114	G115	G116	G117	G118	G119	G120	G121	G122	G123	G124	G125	G126	G127	G128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180	G181	G182	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588
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PRO
SER
GLU
GLY
TYR
GLN
ASP
TYR
GLU
PRO
GLU
ALA

● Molecule 1: Alpha-synuclein



MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA LYS GLY VAL VAL ALA ALA ALA GLU K21 T22 K23 K32 E46 G68 I88 A89 Q99 LEU GLY LYS ASN GLU GLY GLY PRO GLN GLY ILE LEU GLU ASP MET PRO VAL ASP PRO ASP ASN GLU TYR

GLU MET PRO SER GLU GLY TYR GLN ASP TYR GLU PRO GLU ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-1.436°, rise=4.79 Å, axial sym=C1	Depositor
Number of segments used	5659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	18.413	Depositor
Minimum map value	-10.316	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.06	Depositor
Map size (Å)	300.8, 300.8, 300.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93999994, 0.93999994, 0.93999994	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: A1BGB

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	0.09	0/584	0.24	0/787
1	B	0.08	0/551	0.22	0/741
1	C	0.09	0/584	0.24	0/787
1	D	0.08	0/551	0.22	0/741
1	E	0.09	0/584	0.24	0/787
1	F	0.08	0/551	0.23	0/741
1	G	0.09	0/584	0.24	0/787
1	H	0.08	0/551	0.23	0/741
1	I	0.09	0/584	0.24	0/787
1	J	0.08	0/551	0.23	0/741
All	All	0.08	0/5675	0.23	0/7640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	582	0	612	7	0
1	B	549	0	578	10	0
1	C	582	0	612	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	549	0	578	10	0
1	E	582	0	612	8	0
1	F	549	0	578	10	0
1	G	582	0	612	4	0
1	H	549	0	578	5	0
1	I	582	0	612	6	0
1	J	549	0	578	7	0
2	A	60	0	0	0	0
2	C	30	0	0	0	0
2	E	30	0	0	0	0
2	I	30	0	0	0	0
All	All	5805	0	5950	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 46 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:OE1	1:H:80:LYS:NZ	2.35	0.58
1:B:46:GLU:OE1	1:D:80:LYS:NZ	2.35	0.57
1:B:80:LYS:NZ	1:F:46:GLU:OE1	2.35	0.57
1:F:80:LYS:NZ	1:J:46:GLU:OE1	2.35	0.56
1:C:71:VAL:HG21	1:C:88:ILE:HG22	1.93	0.52

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	83/140 (59%)	80 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	77/140 (55%)	76 (99%)	1 (1%)	0	100	100
1	C	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	D	77/140 (55%)	76 (99%)	1 (1%)	0	100	100
1	E	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	F	77/140 (55%)	76 (99%)	1 (1%)	0	100	100
1	G	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	H	77/140 (55%)	76 (99%)	1 (1%)	0	100	100
1	I	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	J	77/140 (55%)	76 (99%)	1 (1%)	0	100	100
All	All	800/1400 (57%)	780 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	57/103 (55%)	57 (100%)	0	100	100
1	B	55/103 (53%)	55 (100%)	0	100	100
1	C	57/103 (55%)	57 (100%)	0	100	100
1	D	55/103 (53%)	55 (100%)	0	100	100
1	E	57/103 (55%)	57 (100%)	0	100	100
1	F	55/103 (53%)	55 (100%)	0	100	100
1	G	57/103 (55%)	57 (100%)	0	100	100
1	H	55/103 (53%)	54 (98%)	1 (2%)	51	80
1	I	57/103 (55%)	57 (100%)	0	100	100
1	J	55/103 (53%)	55 (100%)	0	100	100
All	All	560/1030 (54%)	559 (100%)	1 (0%)	85	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	99	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	79	GLN
1	I	65	ASN
1	F	65	ASN
1	I	79	GLN
1	H	50	HIS

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](#)

5 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	$\# Z > 2$
2	A1BGB	A	201	-	33,33,33	2.57	8 (24%)	41,46,46	1.36	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1BGB	E	201	-	33,33,33	2.57	8 (24%)	41,46,46	1.36	4 (9%)
2	A1BGB	C	201	-	33,33,33	2.56	8 (24%)	41,46,46	1.36	3 (7%)
2	A1BGB	A	202	-	33,33,33	2.56	8 (24%)	41,46,46	1.36	3 (7%)
2	A1BGB	I	201	-	33,33,33	2.56	8 (24%)	41,46,46	1.36	3 (7%)

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	A1BGB	A	201	-	-	0/12/12/12	0/4/4/4
2	A1BGB	E	201	-	-	0/12/12/12	0/4/4/4
2	A1BGB	C	201	-	-	0/12/12/12	0/4/4/4
2	A1BGB	A	202	-	-	0/12/12/12	0/4/4/4
2	A1BGB	I	201	-	-	0/12/12/12	0/4/4/4

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	A1BGB	C08-N09	10.85	1.46	1.29
2	A	201	A1BGB	C08-N09	10.84	1.46	1.29
2	C	201	A1BGB	C08-N09	10.80	1.46	1.29
2	I	201	A1BGB	C08-N09	10.79	1.46	1.29
2	A	202	A1BGB	C08-N09	10.79	1.46	1.29

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	A1BGB	C19-N10-N09	4.54	120.11	114.27
2	I	201	A1BGB	C19-N10-N09	4.53	120.10	114.27
2	C	201	A1BGB	C19-N10-N09	4.51	120.07	114.27
2	A	201	A1BGB	C19-N10-N09	4.51	120.07	114.27
2	E	201	A1BGB	C19-N10-N09	4.50	120.06	114.27

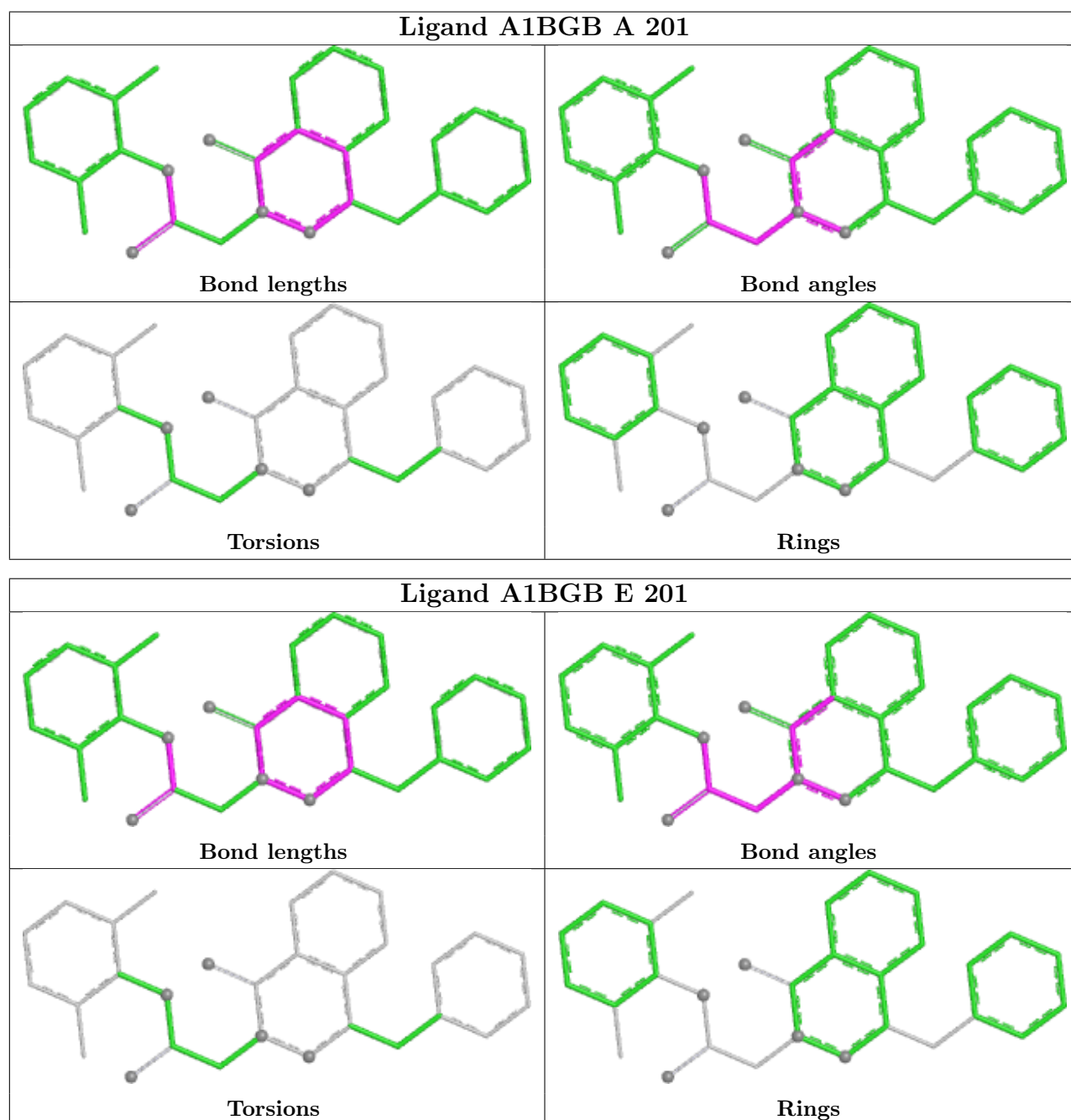
There are no chirality outliers.

There are no torsion outliers.

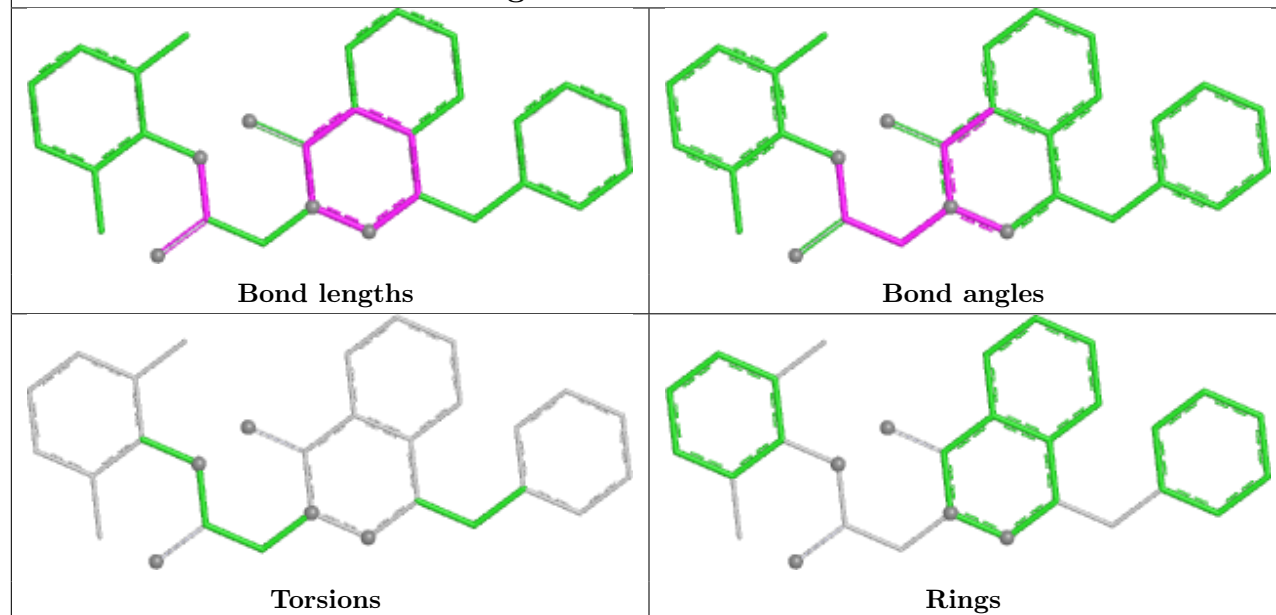
There are no ring outliers.

No monomer is involved in short contacts.

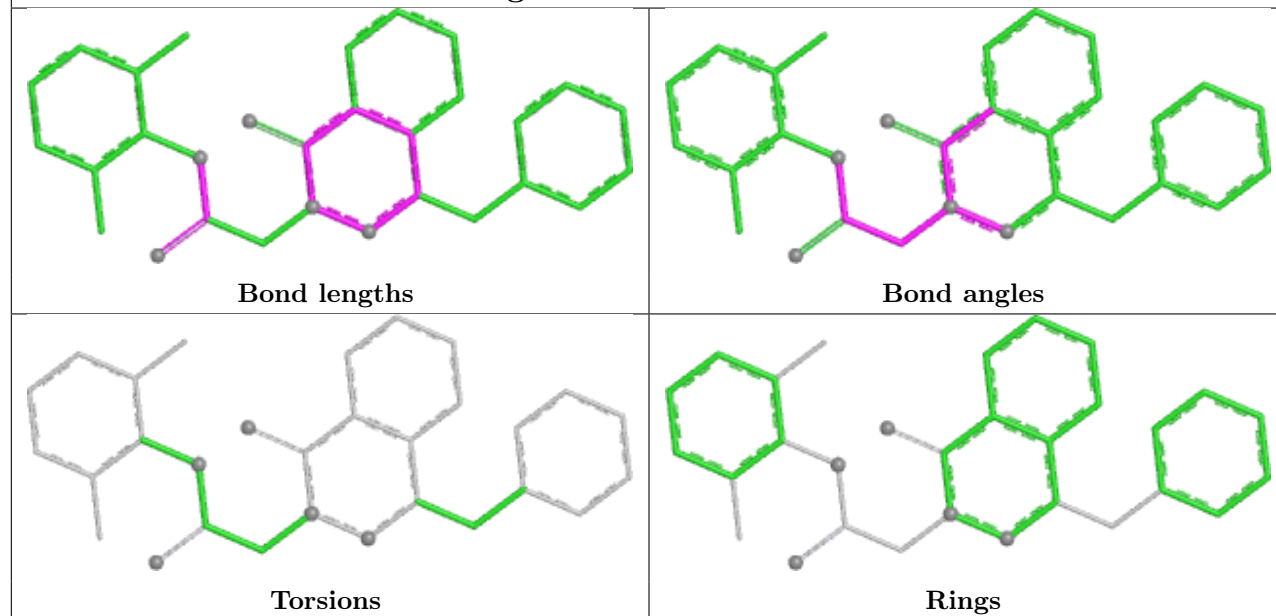
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

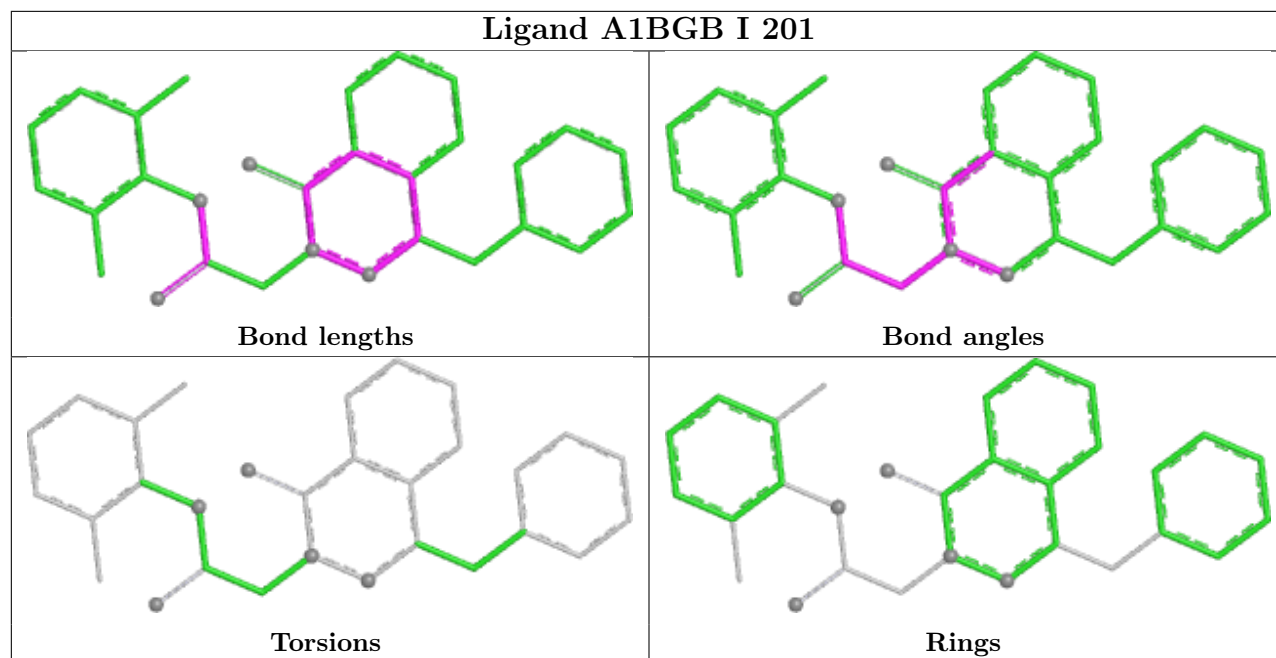


Ligand A1BGB C 201



Ligand A1BGB A 202





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.

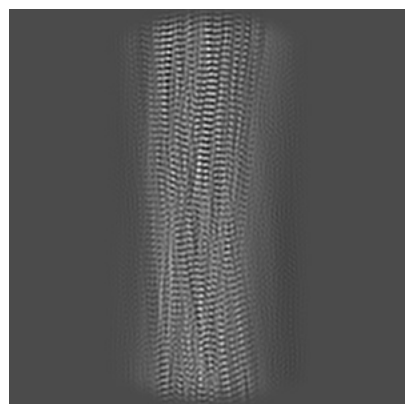
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47735. These allow visual inspection of the internal detail of the map and identification of artifacts.

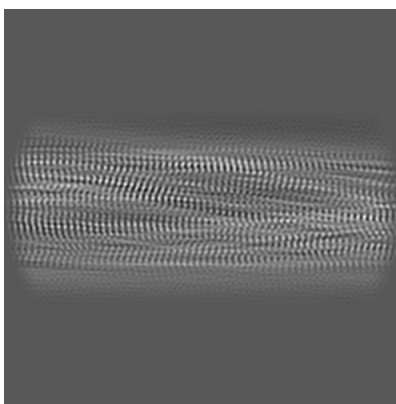
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

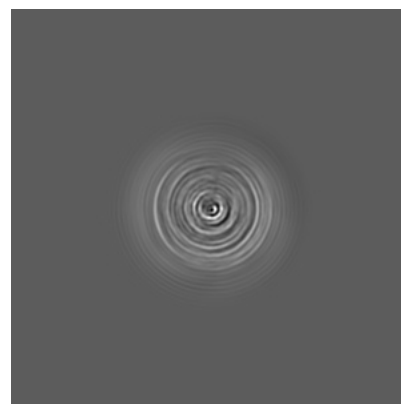
6.1.1 Primary map



X

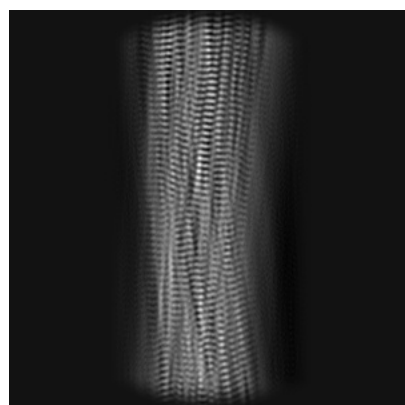


Y

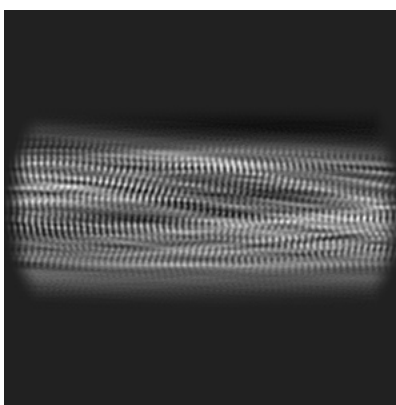


Z

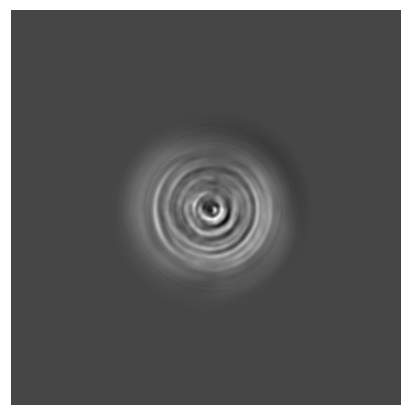
6.1.2 Raw map



X



Y

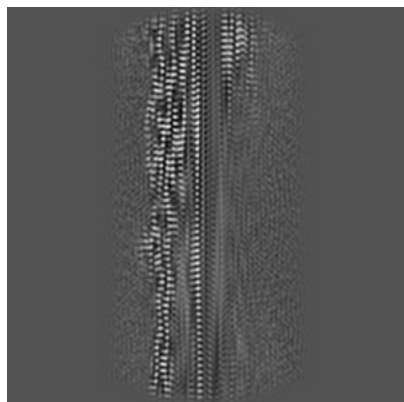


Z

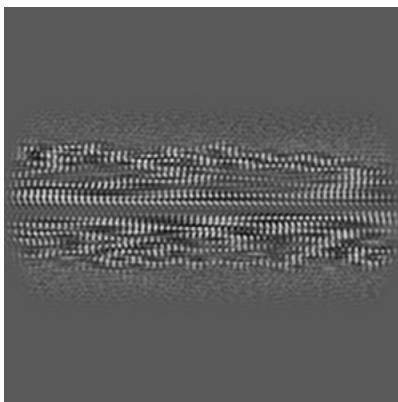
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

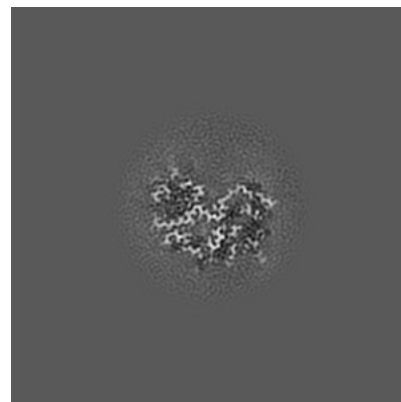
6.2.1 Primary map



X Index: 160

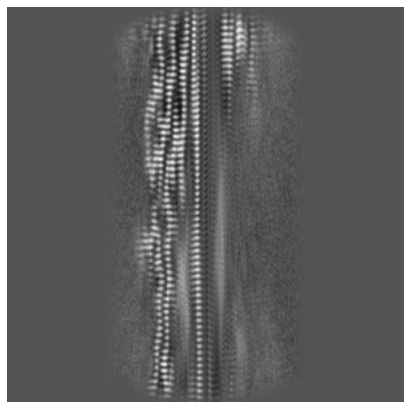


Y Index: 160

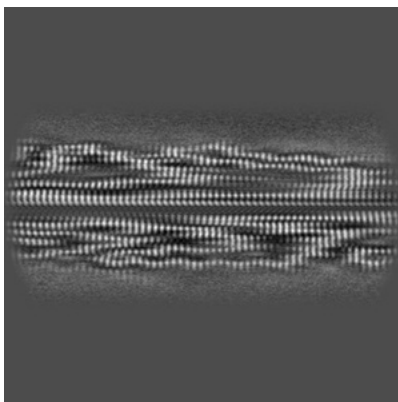


Z Index: 160

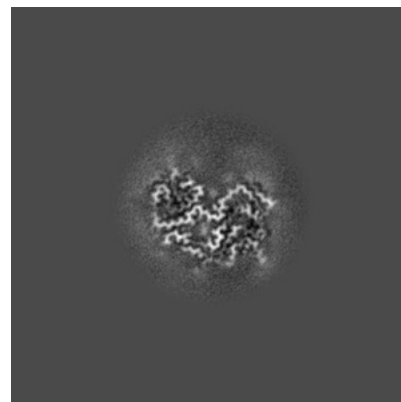
6.2.2 Raw map



X Index: 160



Y Index: 160

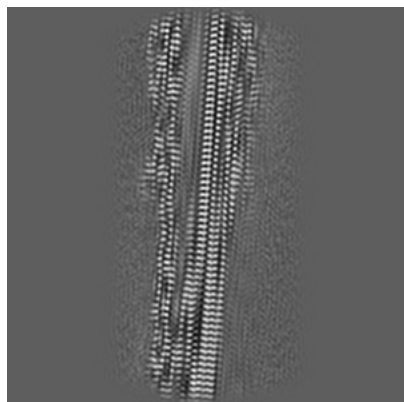


Z Index: 160

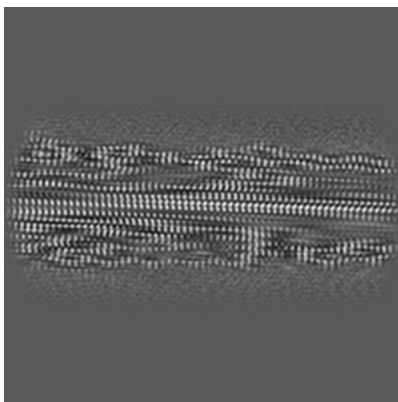
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

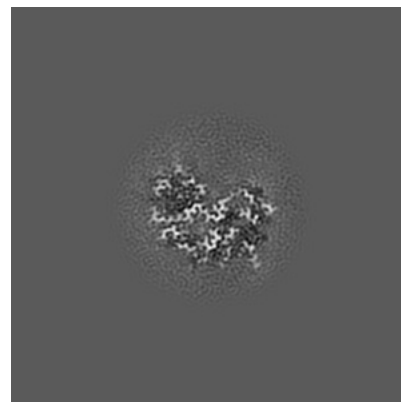
6.3.1 Primary map



X Index: 146

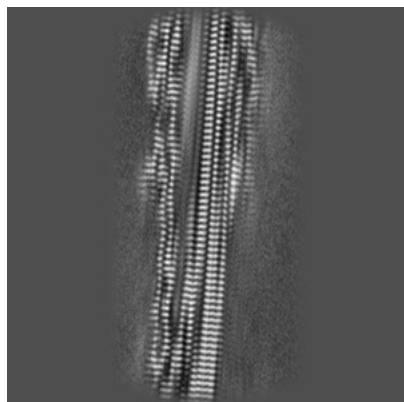


Y Index: 152

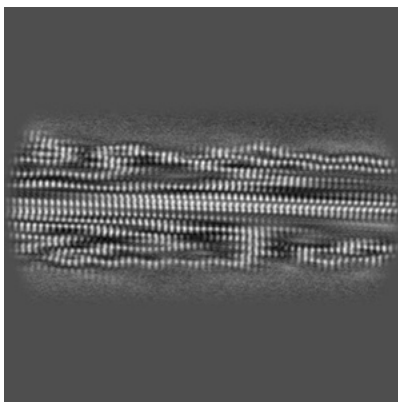


Z Index: 180

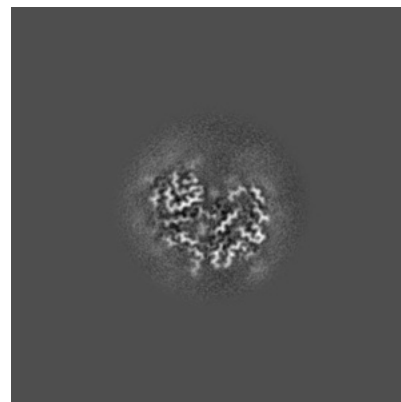
6.3.2 Raw map



X Index: 146



Y Index: 152

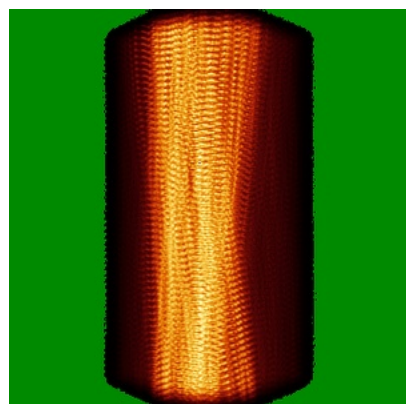


Z Index: 177

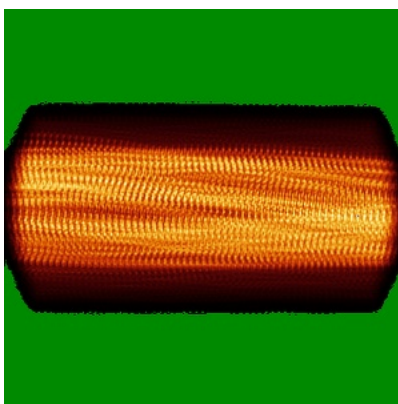
The images above show the largest variance slices of the map in three orthogonal directions.

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

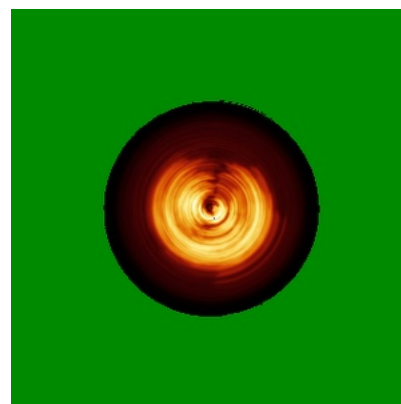
6.4.1 Primary map



X

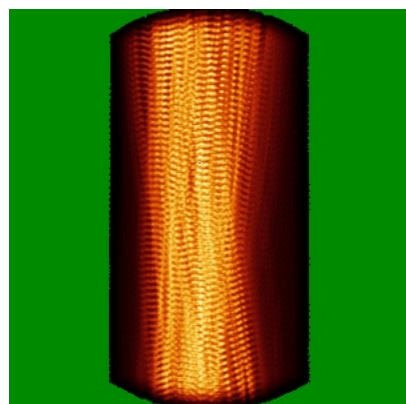


Y

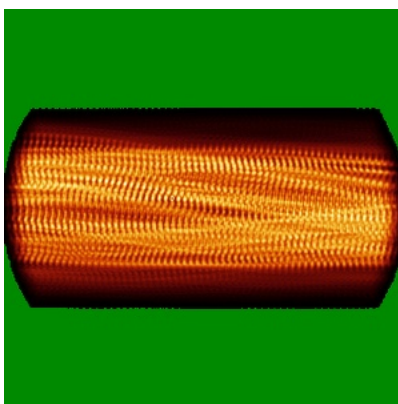


Z

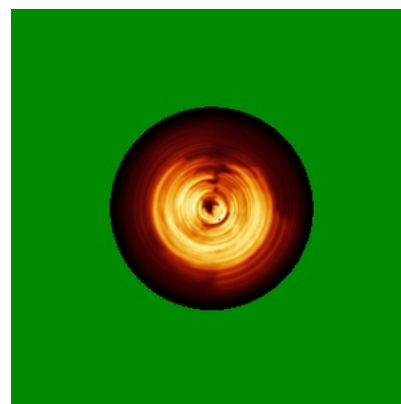
6.4.2 Raw map



X



Y

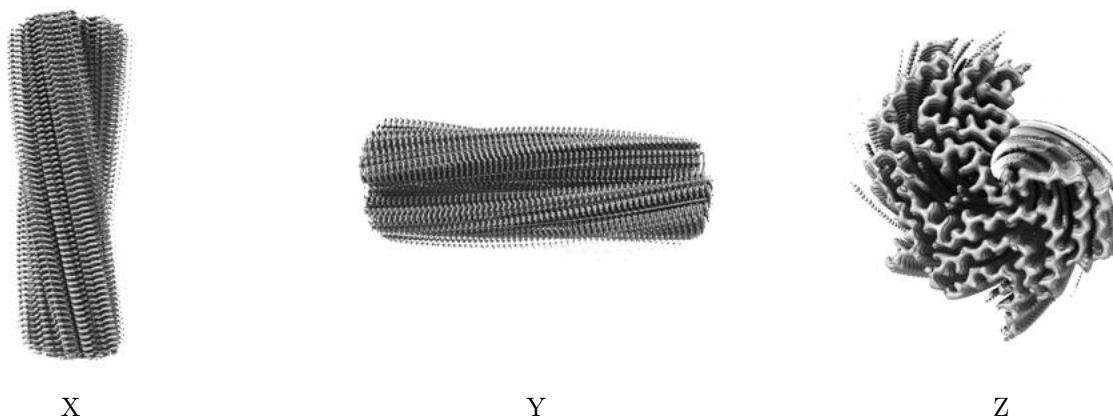


Z

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.

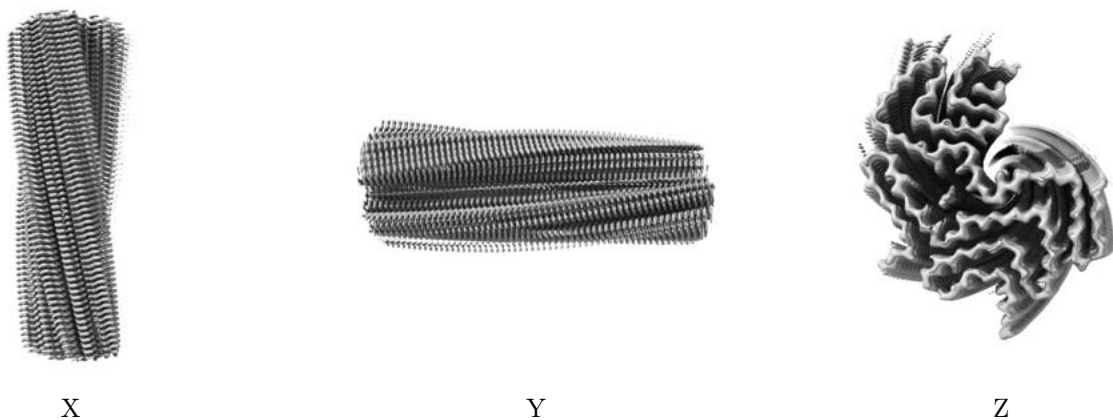
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.06. 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.

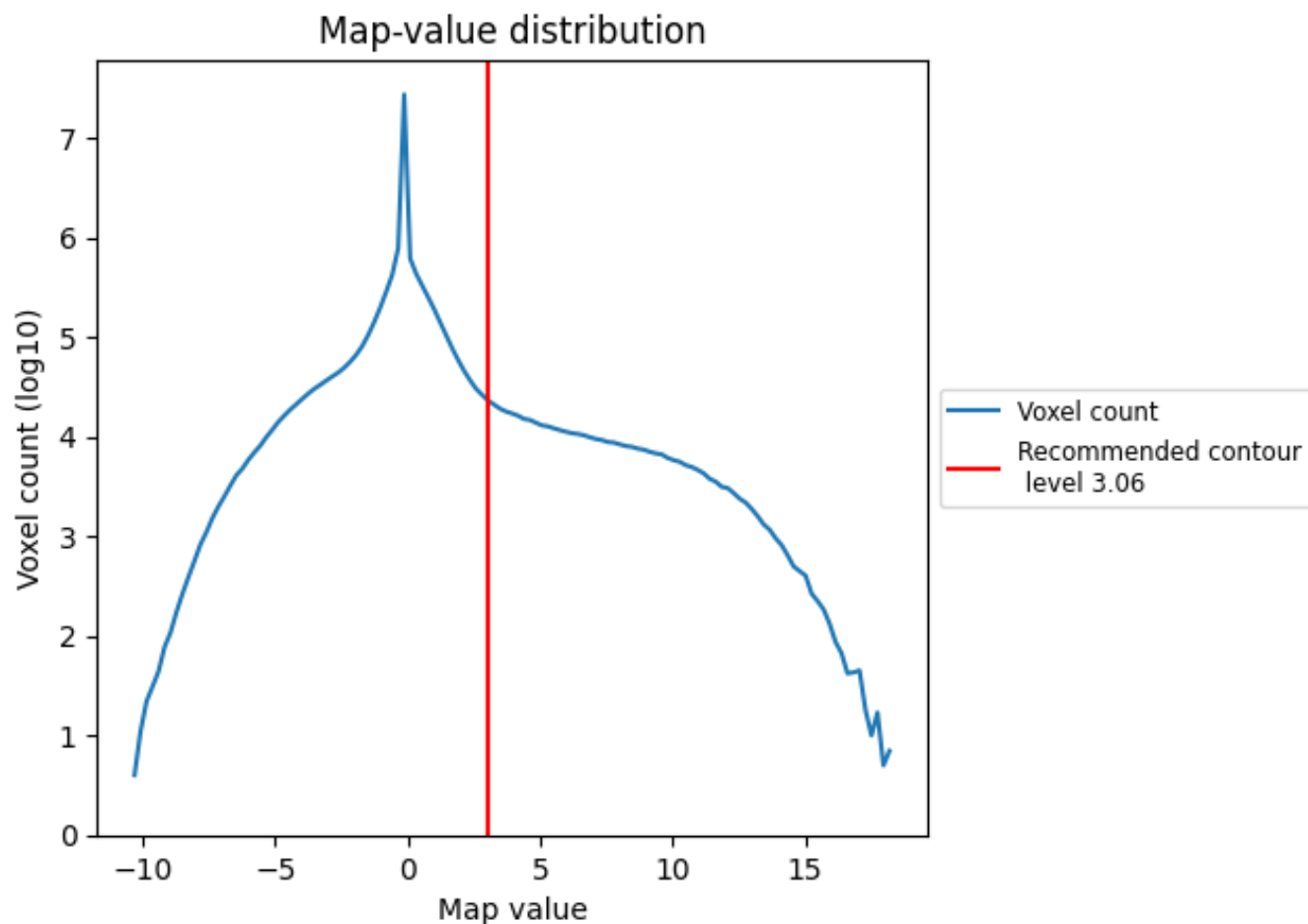
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

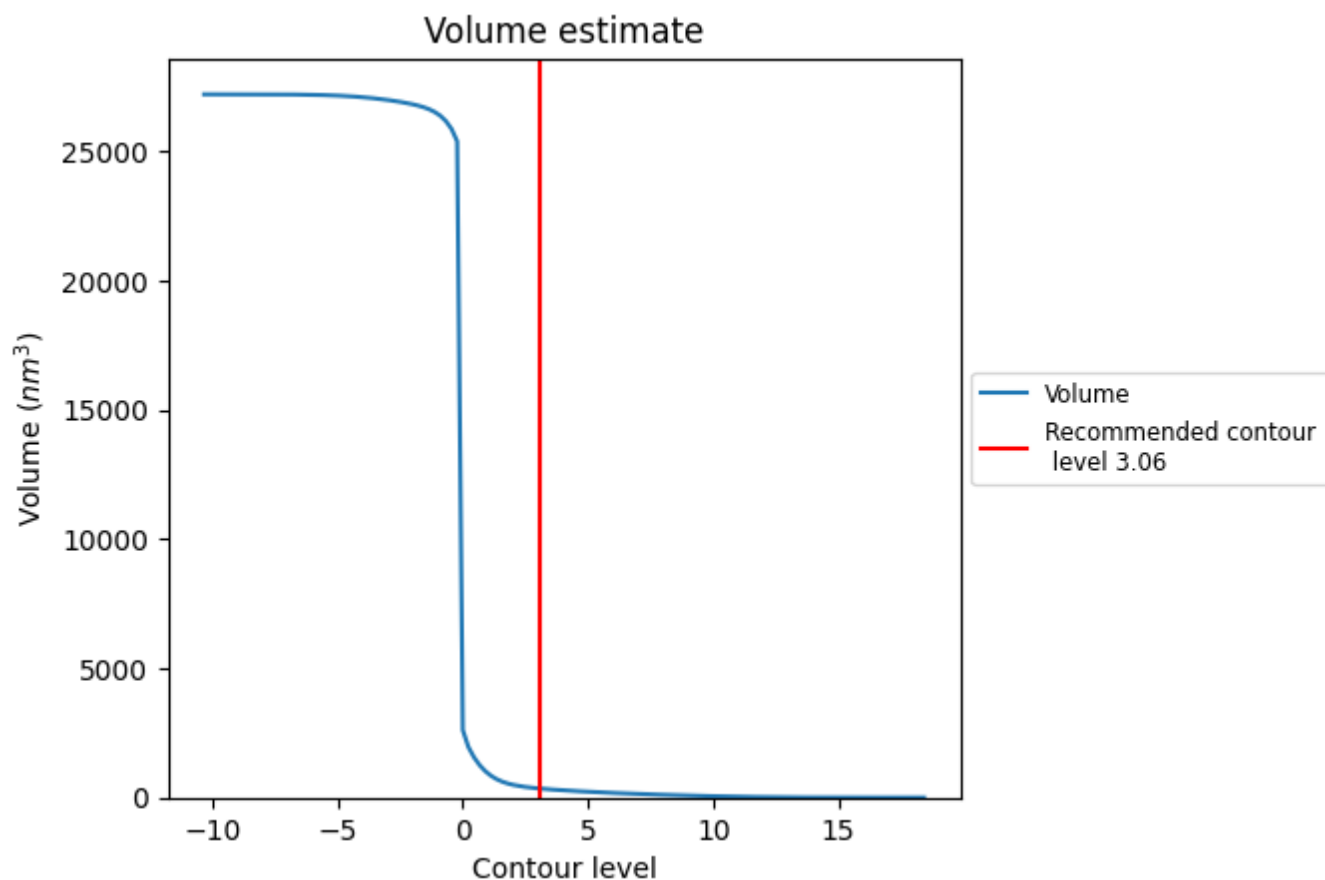
This section contains the results of statistical analysis of the map.

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.

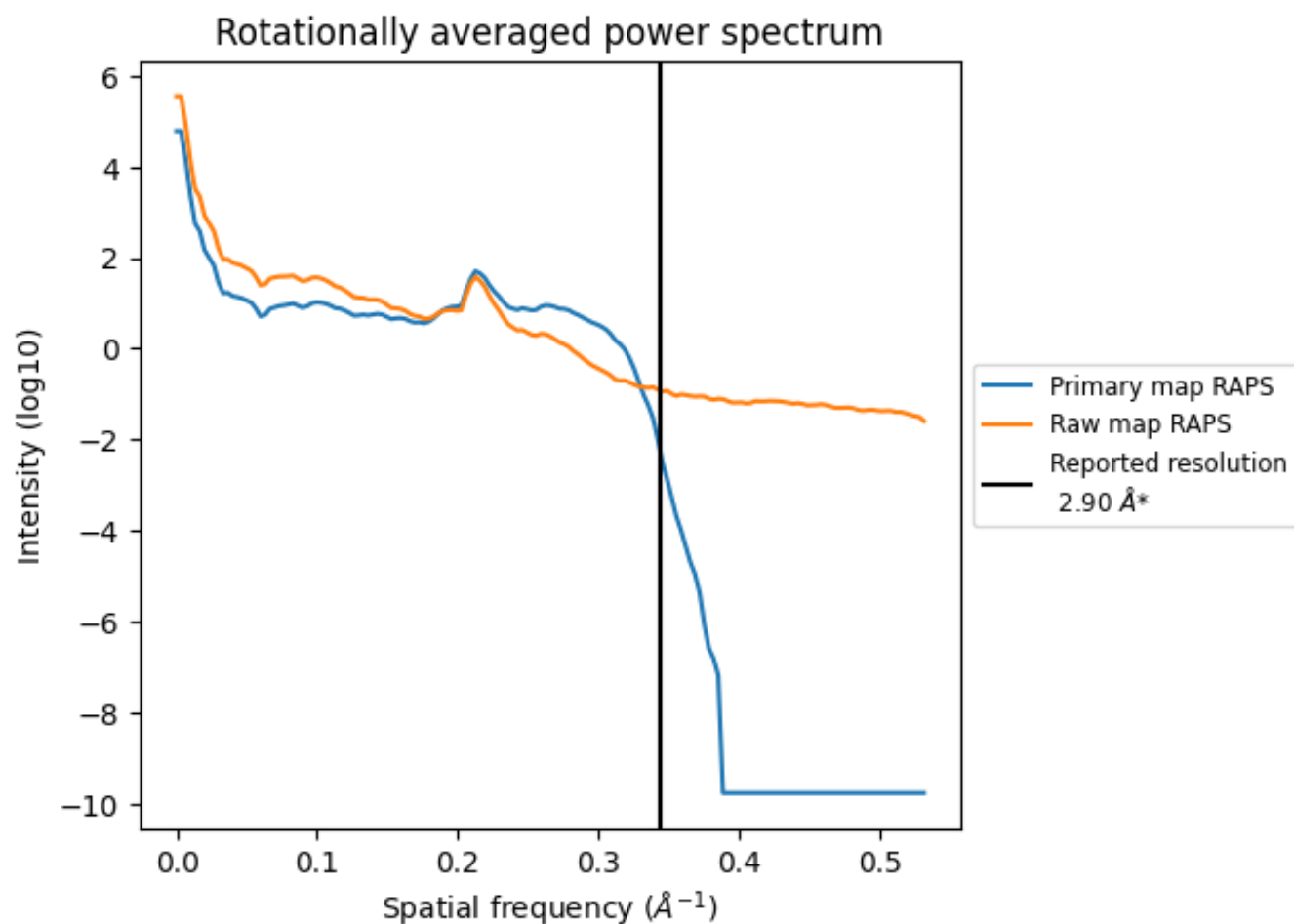
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351 nm³; this corresponds to an approximate mass of 317 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 ⓘ

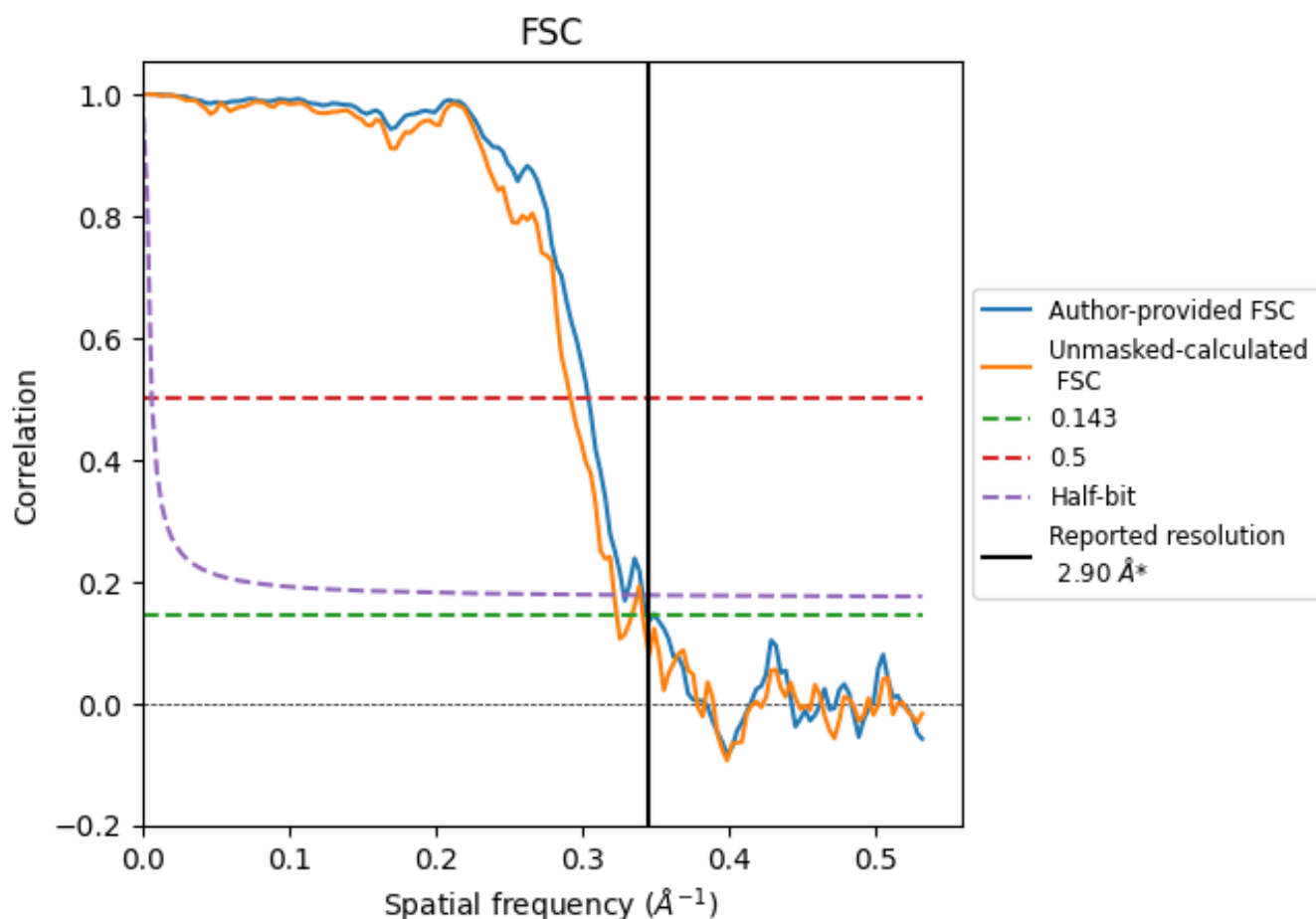


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

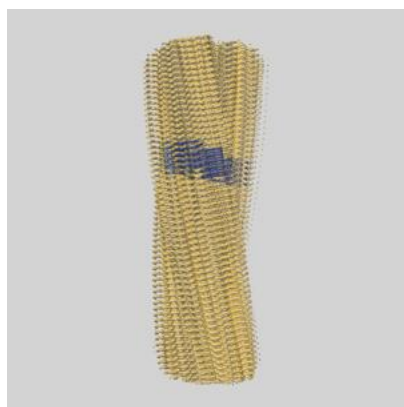
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.29	3.04
Unmasked-calculated*	3.09	3.42	3.11

*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-47735 and PDB model 9E8Y. Per-residue inclusion information can be found in section [3](#) on page [6](#).

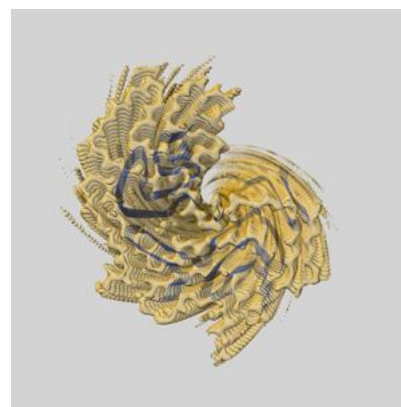
9.1 Map-model overlay [i](#)



X



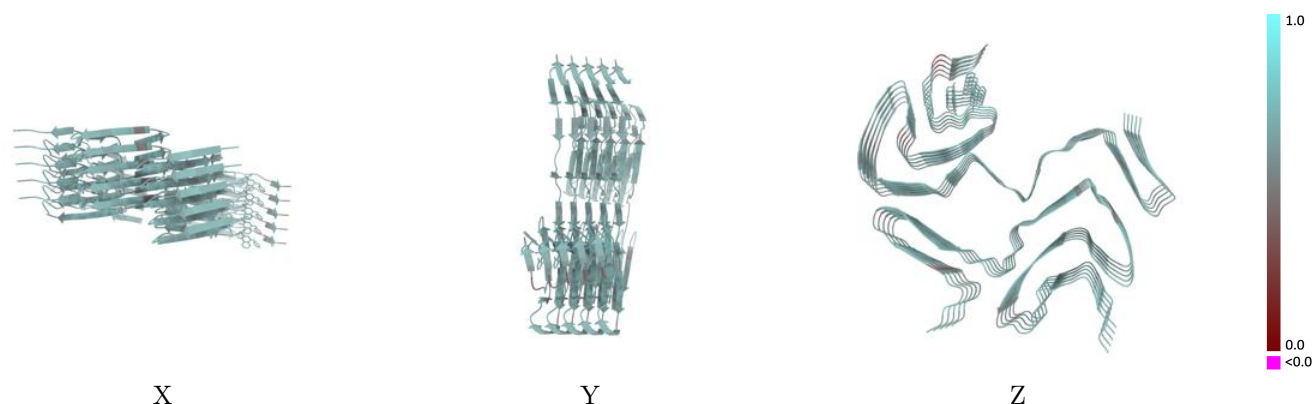
Y



Z

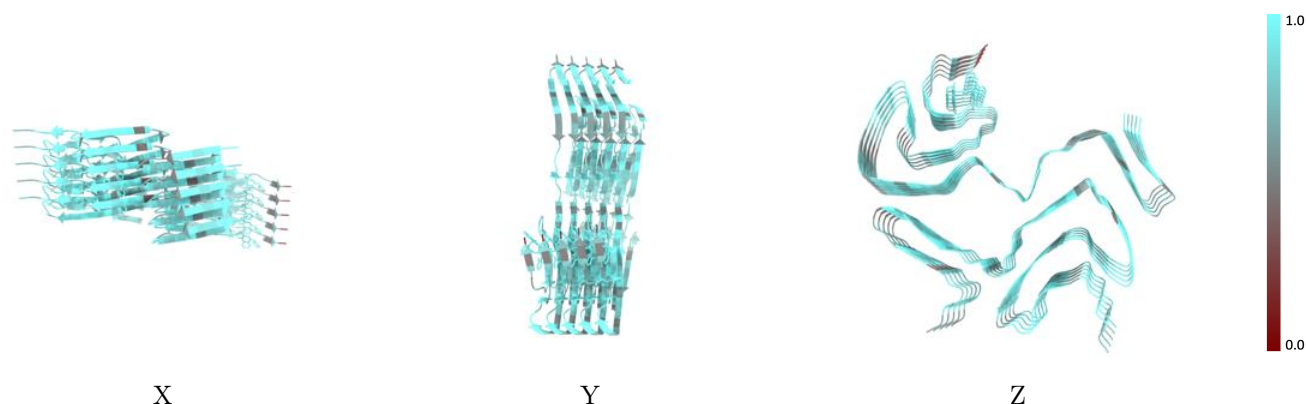
The images above show the 3D surface view of the map at the recommended contour level 3.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



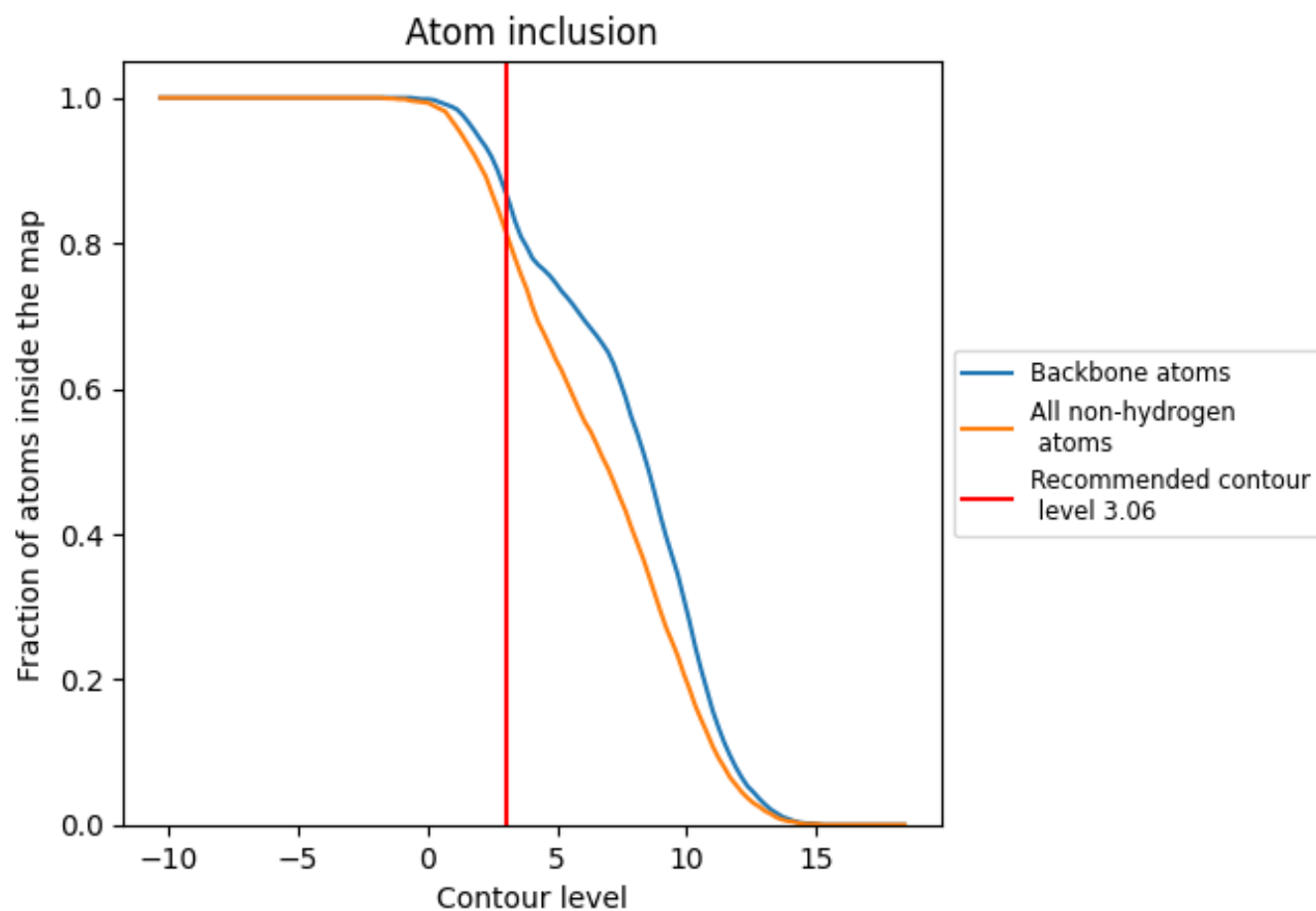
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (3.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8120	<div><div></div></div> 0.5980
A	<div><div></div></div> 0.8000	<div><div></div></div> 0.5950
B	<div><div></div></div> 0.8290	<div><div></div></div> 0.6050
C	<div><div></div></div> 0.7900	<div><div></div></div> 0.5920
D	<div><div></div></div> 0.8300	<div><div></div></div> 0.6040
E	<div><div></div></div> 0.8020	<div><div></div></div> 0.5920
F	<div><div></div></div> 0.8340	<div><div></div></div> 0.6050
G	<div><div></div></div> 0.7870	<div><div></div></div> 0.5890
H	<div><div></div></div> 0.8380	<div><div></div></div> 0.6050
I	<div><div></div></div> 0.7940	<div><div></div></div> 0.5910
J	<div><div></div></div> 0.8300	<div><div></div></div> 0.6050

1.0

0.0

<0.0