



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 10:11 PM EDT

PDB ID : 7TVI
EMDB ID : EMD-26141
Title : Alpha1/BetaB Heteromeric Glycine Receptor in Glycine-Bound State
Authors : Gibbs, E.; Chakrapani, S.; Kumar, A.
Deposited on : 2022-02-04
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

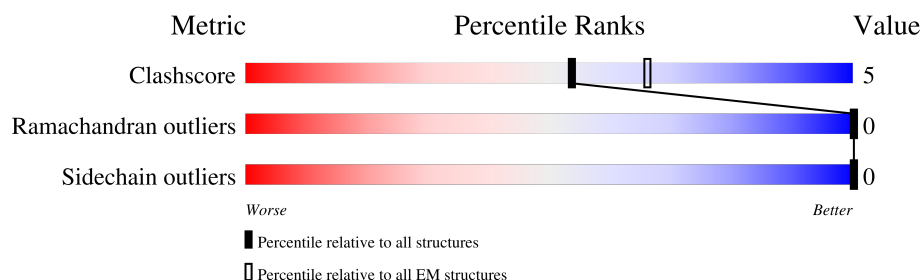
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	458	
1	B	458	
1	C	458	
1	D	458	
2	E	591	

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
3	GLY	A	501	-	X	-	-
3	GLY	B	501	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13746 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 Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	339	Total	C	N	O	S	0	0
			2749	1795	448	488	18		
1	D	338	Total	C	N	O	S	0	0
			2738	1789	444	487	18		
1	C	336	Total	C	N	O	S	0	0
			2723	1777	443	485	18		
1	B	337	Total	C	N	O	S	0	0
			2731	1783	444	486	18		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	LEU	-	expression tag	UNP O93430
A	446	VAL	-	expression tag	UNP O93430
A	447	PRO	-	expression tag	UNP O93430
A	448	ARG	-	expression tag	UNP O93430
A	449	GLY	-	expression tag	UNP O93430
A	450	SER	-	expression tag	UNP O93430
A	451	HIS	-	expression tag	UNP O93430
A	452	HIS	-	expression tag	UNP O93430
A	453	HIS	-	expression tag	UNP O93430
A	454	HIS	-	expression tag	UNP O93430
A	455	HIS	-	expression tag	UNP O93430
A	456	HIS	-	expression tag	UNP O93430
A	457	HIS	-	expression tag	UNP O93430
A	458	HIS	-	expression tag	UNP O93430
D	445	LEU	-	expression tag	UNP O93430
D	446	VAL	-	expression tag	UNP O93430
D	447	PRO	-	expression tag	UNP O93430
D	448	ARG	-	expression tag	UNP O93430
D	449	GLY	-	expression tag	UNP O93430
D	450	SER	-	expression tag	UNP O93430
D	451	HIS	-	expression tag	UNP O93430
D	452	HIS	-	expression tag	UNP O93430

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Chain	Residue	Modelled	Actual	Comment	Reference
D	453	HIS	-	expression tag	UNP O93430
D	454	HIS	-	expression tag	UNP O93430
D	455	HIS	-	expression tag	UNP O93430
D	456	HIS	-	expression tag	UNP O93430
D	457	HIS	-	expression tag	UNP O93430
D	458	HIS	-	expression tag	UNP O93430
C	445	LEU	-	expression tag	UNP O93430
C	446	VAL	-	expression tag	UNP O93430
C	447	PRO	-	expression tag	UNP O93430
C	448	ARG	-	expression tag	UNP O93430
C	449	GLY	-	expression tag	UNP O93430
C	450	SER	-	expression tag	UNP O93430
C	451	HIS	-	expression tag	UNP O93430
C	452	HIS	-	expression tag	UNP O93430
C	453	HIS	-	expression tag	UNP O93430
C	454	HIS	-	expression tag	UNP O93430
C	455	HIS	-	expression tag	UNP O93430
C	456	HIS	-	expression tag	UNP O93430
C	457	HIS	-	expression tag	UNP O93430
C	458	HIS	-	expression tag	UNP O93430
B	445	LEU	-	expression tag	UNP O93430
B	446	VAL	-	expression tag	UNP O93430
B	447	PRO	-	expression tag	UNP O93430
B	448	ARG	-	expression tag	UNP O93430
B	449	GLY	-	expression tag	UNP O93430
B	450	SER	-	expression tag	UNP O93430
B	451	HIS	-	expression tag	UNP O93430
B	452	HIS	-	expression tag	UNP O93430
B	453	HIS	-	expression tag	UNP O93430
B	454	HIS	-	expression tag	UNP O93430
B	455	HIS	-	expression tag	UNP O93430
B	456	HIS	-	expression tag	UNP O93430
B	457	HIS	-	expression tag	UNP O93430
B	458	HIS	-	expression tag	UNP O93430

- Molecule 2 is a protein called Glycine receptor beta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	332	Total	C	N	O	S	0	0
			2696	1763	431	485	17		

There are 97 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-51	TRP	-	insertion	UNP Q6DC22
E	-50	SER	-	insertion	UNP Q6DC22
E	-49	HIS	-	insertion	UNP Q6DC22
E	-48	PRO	-	insertion	UNP Q6DC22
E	-47	GLN	-	insertion	UNP Q6DC22
E	-46	PHE	-	insertion	UNP Q6DC22
E	-45	GLU	-	insertion	UNP Q6DC22
E	-44	LYS	-	insertion	UNP Q6DC22
E	-43	GLY	-	insertion	UNP Q6DC22
E	-42	GLY	-	insertion	UNP Q6DC22
E	-41	GLY	-	insertion	UNP Q6DC22
E	-40	SER	-	insertion	UNP Q6DC22
E	-39	GLY	-	insertion	UNP Q6DC22
E	-38	GLY	-	insertion	UNP Q6DC22
E	-37	GLY	-	insertion	UNP Q6DC22
E	-36	SER	-	insertion	UNP Q6DC22
E	-35	GLY	-	insertion	UNP Q6DC22
E	-34	GLY	-	insertion	UNP Q6DC22
E	-33	GLY	-	insertion	UNP Q6DC22
E	-32	SER	-	insertion	UNP Q6DC22
E	-31	TRP	-	insertion	UNP Q6DC22
E	-30	SER	-	insertion	UNP Q6DC22
E	-29	HIS	-	insertion	UNP Q6DC22
E	-28	PRO	-	insertion	UNP Q6DC22
E	-27	GLN	-	insertion	UNP Q6DC22
E	-26	PHE	-	insertion	UNP Q6DC22
E	-25	GLU	-	insertion	UNP Q6DC22
E	-24	LYS	-	insertion	UNP Q6DC22
E	-23	GLY	-	insertion	UNP Q6DC22
E	-22	GLY	-	insertion	UNP Q6DC22
E	-21	GLY	-	insertion	UNP Q6DC22
E	-20	SER	-	insertion	UNP Q6DC22
E	-19	GLY	-	insertion	UNP Q6DC22
E	-18	GLY	-	insertion	UNP Q6DC22
E	-17	GLY	-	insertion	UNP Q6DC22
E	-16	SER	-	insertion	UNP Q6DC22
E	-15	GLY	-	insertion	UNP Q6DC22
E	-14	GLY	-	insertion	UNP Q6DC22
E	-13	GLY	-	insertion	UNP Q6DC22
E	-12	SER	-	insertion	UNP Q6DC22
E	-11	TRP	-	insertion	UNP Q6DC22
E	-10	SER	-	insertion	UNP Q6DC22
E	-9	HIS	-	insertion	UNP Q6DC22

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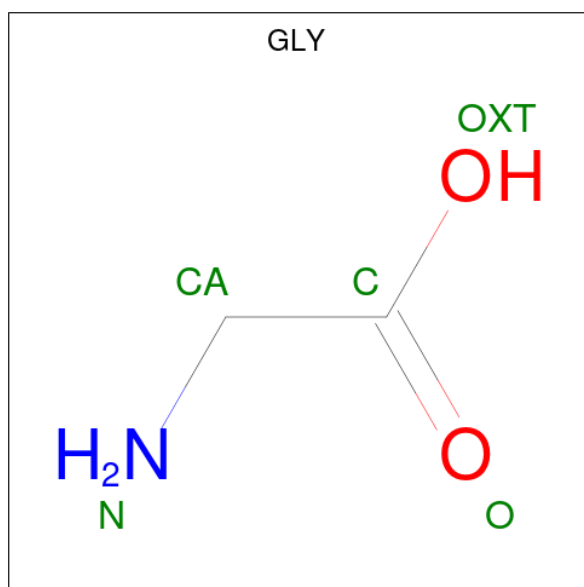
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	PRO	-	insertion	UNP Q6DC22
E	-7	GLN	-	insertion	UNP Q6DC22
E	-6	PHE	-	insertion	UNP Q6DC22
E	-5	GLU	-	insertion	UNP Q6DC22
E	-4	LYS	-	insertion	UNP Q6DC22
E	-3	GLY	-	insertion	UNP Q6DC22
E	-2	GLY	-	insertion	UNP Q6DC22
E	-1	GLY	-	insertion	UNP Q6DC22
E	0	SER	-	insertion	UNP Q6DC22
E	1	GLY	-	insertion	UNP Q6DC22
E	2	GLY	-	insertion	UNP Q6DC22
E	3	GLY	-	insertion	UNP Q6DC22
E	4	SER	-	insertion	UNP Q6DC22
E	5	GLY	-	insertion	UNP Q6DC22
E	6	GLY	-	insertion	UNP Q6DC22
E	7	GLY	-	insertion	UNP Q6DC22
E	8	SER	-	insertion	UNP Q6DC22
E	9	TRP	-	insertion	UNP Q6DC22
E	10	SER	-	insertion	UNP Q6DC22
E	11	HIS	-	insertion	UNP Q6DC22
E	12	PRO	-	insertion	UNP Q6DC22
E	13	GLN	-	insertion	UNP Q6DC22
E	14	PHE	-	insertion	UNP Q6DC22
E	15	GLU	-	insertion	UNP Q6DC22
E	16	LYS	-	insertion	UNP Q6DC22
E	17	GLU	-	insertion	UNP Q6DC22
E	18	ASN	-	insertion	UNP Q6DC22
E	19	LEU	-	insertion	UNP Q6DC22
E	20	TYR	-	insertion	UNP Q6DC22
E	21	PHE	-	insertion	UNP Q6DC22
E	22	GLN	-	insertion	UNP Q6DC22
E	23	GLY	-	insertion	UNP Q6DC22
E	24	GLU	-	insertion	UNP Q6DC22
E	25	LYS	-	insertion	UNP Q6DC22
E	26	SER	-	insertion	UNP Q6DC22
E	27	ALA	-	insertion	UNP Q6DC22
E	28	LYS	-	insertion	UNP Q6DC22
E	29	LYS	-	insertion	UNP Q6DC22
E	495	GLU	-	expression tag	UNP Q6DC22
E	496	ASN	-	expression tag	UNP Q6DC22
E	497	LEU	-	expression tag	UNP Q6DC22
E	498	TYR	-	expression tag	UNP Q6DC22

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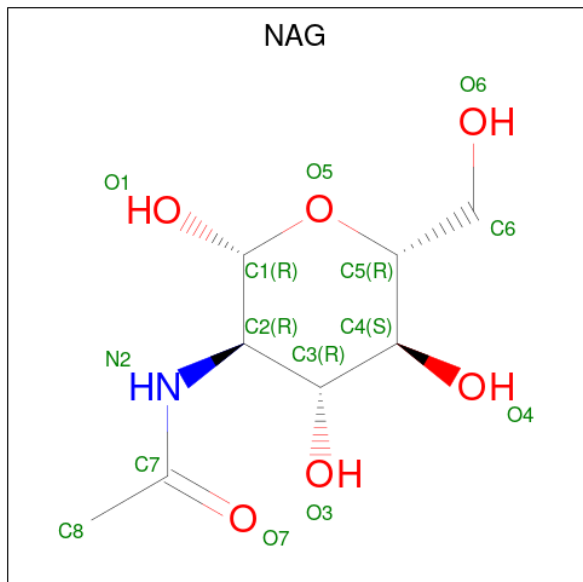
Chain	Residue	Modelled	Actual	Comment	Reference
E	499	PHE	-	expression tag	UNP Q6DC22
E	500	GLN	-	expression tag	UNP Q6DC22
E	501	GLY	-	expression tag	UNP Q6DC22
E	502	THR	-	expression tag	UNP Q6DC22
E	503	GLU	-	expression tag	UNP Q6DC22
E	504	THR	-	expression tag	UNP Q6DC22
E	505	SER	-	expression tag	UNP Q6DC22
E	506	GLN	-	expression tag	UNP Q6DC22
E	507	VAL	-	expression tag	UNP Q6DC22
E	508	ALA	-	expression tag	UNP Q6DC22
E	509	PRO	-	expression tag	UNP Q6DC22
E	510	ALA	-	expression tag	UNP Q6DC22

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	D	1	Total	C	N	O	0
			5	2	1	2	
3	D	1	Total	C	N	O	0
			5	2	1	2	
3	B	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

Chain C:

65% 9% 27%

MET PHE ALA LEU GLY ILE TYR LEU TRP GLU THR ILE VAL PHE PHE SER LEU ALA ALA SER GLN ALA ALA ARG LYS P33 L38 D39 L39 R40 L41 M42 K57 P60 F68 F67 L88 R89 S100 D104 D105 D121 E127 K128

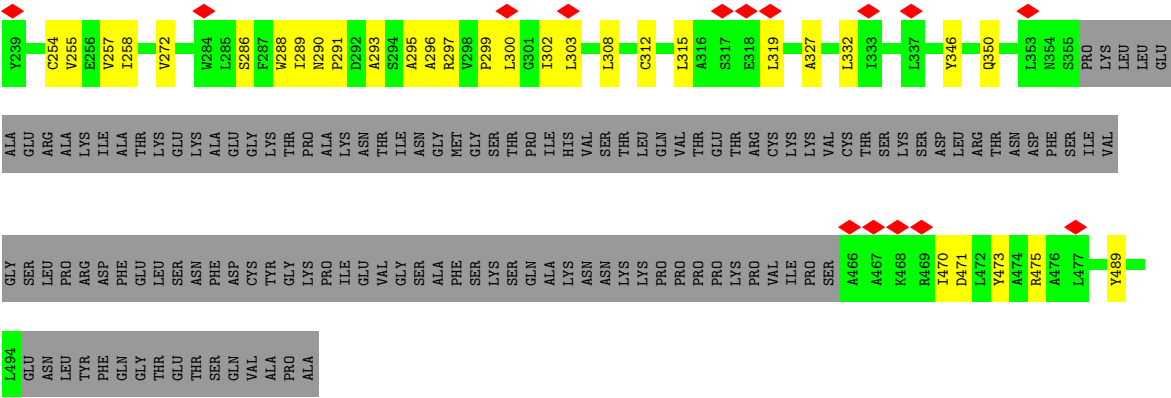
L141 R155 A161 L166 P170 M171 D172 I177 E181 G194 E215 E216 C233 R237 Q243 Y246 S252 S265 W267 A273 L279 T282 T283 L298 A306 Y325 N329 F330 R333 Q334 H335 LYS GLU LEU LEU ARG LYS

Chain B:

5% 62% 11% 26%

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 100. The logo displays the conservation of amino acids at each position. A bar chart at the top indicates the percentage of positions with conservation: 5% (red), 62% (green), 11% (yellow), and 26% (grey).

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 40	Depositor
Minimum defocus (nm)	700, 700	Depositor
Maximum defocus (nm)	1800, 1800	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.304	Depositor
Minimum map value	-1.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.33	Depositor
Map size (\AA)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: NAG

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	0.28	0/2819	0.54	0/3824
1	B	0.29	0/2801	0.55	0/3802
1	C	0.28	0/2793	0.54	0/3791
1	D	0.29	0/2807	0.53	0/3809
2	E	0.31	0/2765	0.62	0/3759
All	All	0.29	0/13985	0.56	0/18985

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	2749	0	2764	29	0
1	B	2731	0	2738	36	0
1	C	2723	0	2727	27	0
1	D	2738	0	2755	29	0
2	E	2696	0	2683	34	0
3	A	10	0	4	1	0
3	B	5	0	2	0	0
3	D	10	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	1	0
4	D	14	0	13	0	0
4	E	28	0	26	0	0
All	All	13746	0	13755	136	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 5.

The worst 5 of 136 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)
2:E:293:ALA:HB1	2:E:296:ALA:HB3	1.65	0.78
1:A:265:SER:HB2	1:A:279:LEU:HD11	1.70	0.74
1:D:124:PHE:HB2	1:D:127:GLU:HB2	1.71	0.71
1:B:68:PHE:HB3	1:B:87:PHE:HB2	1.75	0.68
1:D:94:ASP:HB3	1:D:97:LEU:HD12	1.78	0.65

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	335/458 (73%)	327 (98%)	8 (2%)	0	100	100
1	B	333/458 (73%)	327 (98%)	6 (2%)	0	100	100
1	C	332/458 (72%)	319 (96%)	13 (4%)	0	100	100
1	D	334/458 (73%)	329 (98%)	5 (2%)	0	100	100
2	E	328/591 (56%)	317 (97%)	11 (3%)	0	100	100
All	All	1662/2423 (69%)	1619 (97%)	43 (3%)	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	304/400 (76%)	304 (100%)	0	100	100
1	B	302/400 (76%)	302 (100%)	0	100	100
1	C	301/400 (75%)	301 (100%)	0	100	100
1	D	303/400 (76%)	303 (100%)	0	100	100
2	E	302/509 (59%)	302 (100%)	0	100	100
All	All	1512/2109 (72%)	1512 (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. There are no such sidechains identified.

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](#)

11 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	$\# Z > 2$
3	GLY	D	501	-	4,4,4	1.15	1 (25%)	3,4,4	1.58	0
4	NAG	A	502	1	14,14,15	0.42	0	17,19,21	0.53	0
4	NAG	E	601	2	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
4	NAG	C	501	1	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
4	NAG	D	502	1	14,14,15	0.20	0	17,19,21	0.39	0
3	GLY	B	501	-	4,4,4	1.17	1 (25%)	3,4,4	1.63	1 (33%)
4	NAG	E	602	2	14,14,15	0.47	0	17,19,21	0.43	0
4	NAG	B	502	1	14,14,15	0.23	0	17,19,21	0.46	0
3	GLY	A	503	-	4,4,4	1.18	1 (25%)	3,4,4	1.56	0
3	GLY	D	503	-	4,4,4	1.16	1 (25%)	3,4,4	1.63	1 (33%)
3	GLY	A	501	-	4,4,4	1.15	1 (25%)	3,4,4	1.67	1 (33%)

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
3	GLY	D	501	-	-	2/2/2/2	-
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
4	NAG	E	601	2	-	2/6/23/26	0/1/1/1
4	NAG	C	501	1	-	4/6/23/26	0/1/1/1
4	NAG	D	502	1	-	3/6/23/26	0/1/1/1
3	GLY	B	501	-	-	2/2/2/2	-
4	NAG	E	602	2	-	2/6/23/26	0/1/1/1
4	NAG	B	502	1	-	2/6/23/26	0/1/1/1
3	GLY	A	503	-	-	2/2/2/2	-
3	GLY	D	503	-	-	0/2/2/2	-
3	GLY	A	501	-	-	2/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GLY	OXT-C	-2.28	1.23	1.30
3	B	501	GLY	OXT-C	-2.24	1.23	1.30
3	A	501	GLY	OXT-C	-2.23	1.23	1.30
3	D	503	GLY	OXT-C	-2.22	1.23	1.30
3	D	501	GLY	OXT-C	-2.22	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GLY	OXT-C-O	-2.16	117.79	123.33
3	B	501	GLY	OXT-C-O	-2.09	117.97	123.33
3	D	503	GLY	OXT-C-O	-2.07	118.00	123.33
4	E	601	NAG	C2-N2-C7	2.05	125.65	122.90
4	C	501	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GLY	O-C-CA-N
3	A	501	GLY	OXT-C-CA-N
3	A	503	GLY	O-C-CA-N
3	A	503	GLY	OXT-C-CA-N
3	D	501	GLY	O-C-CA-N

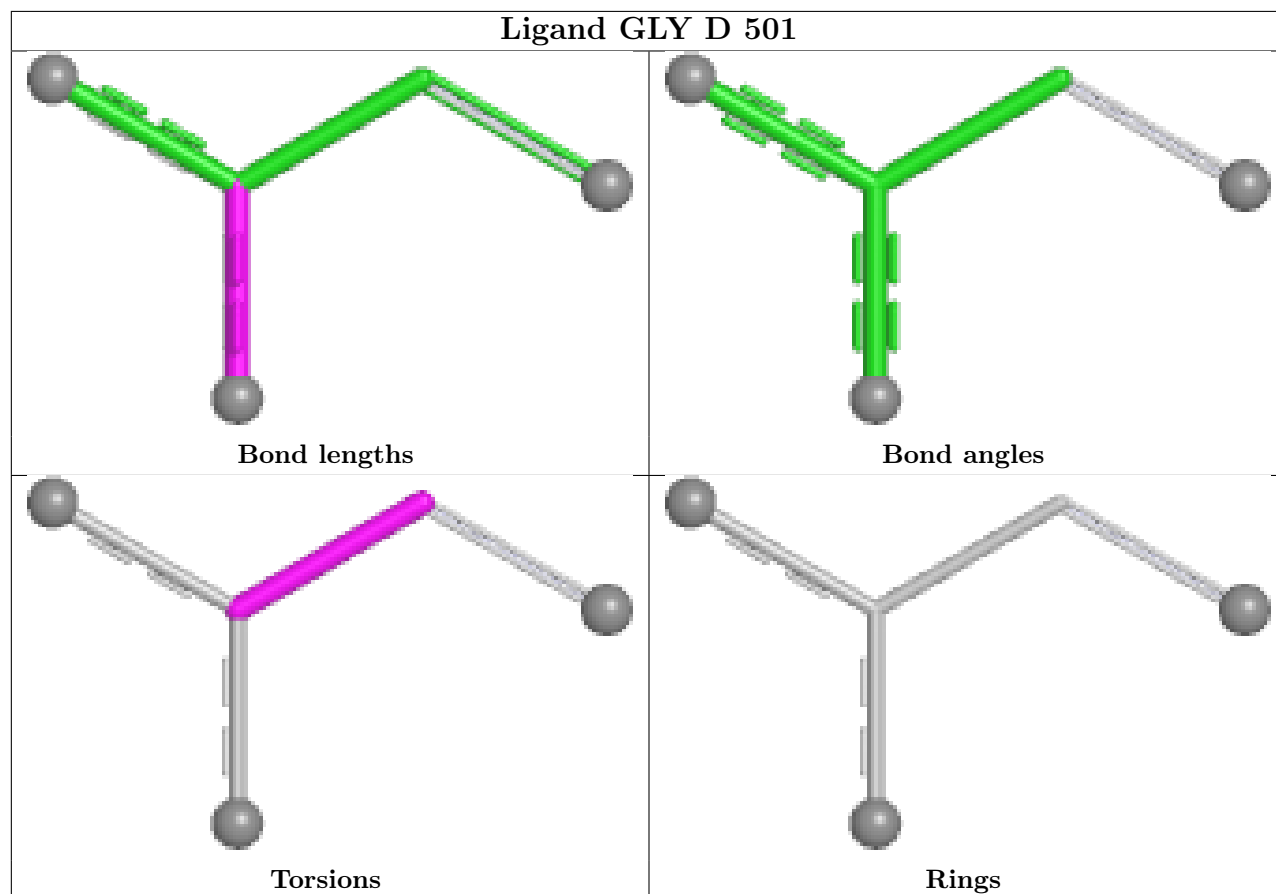
There are no ring outliers.

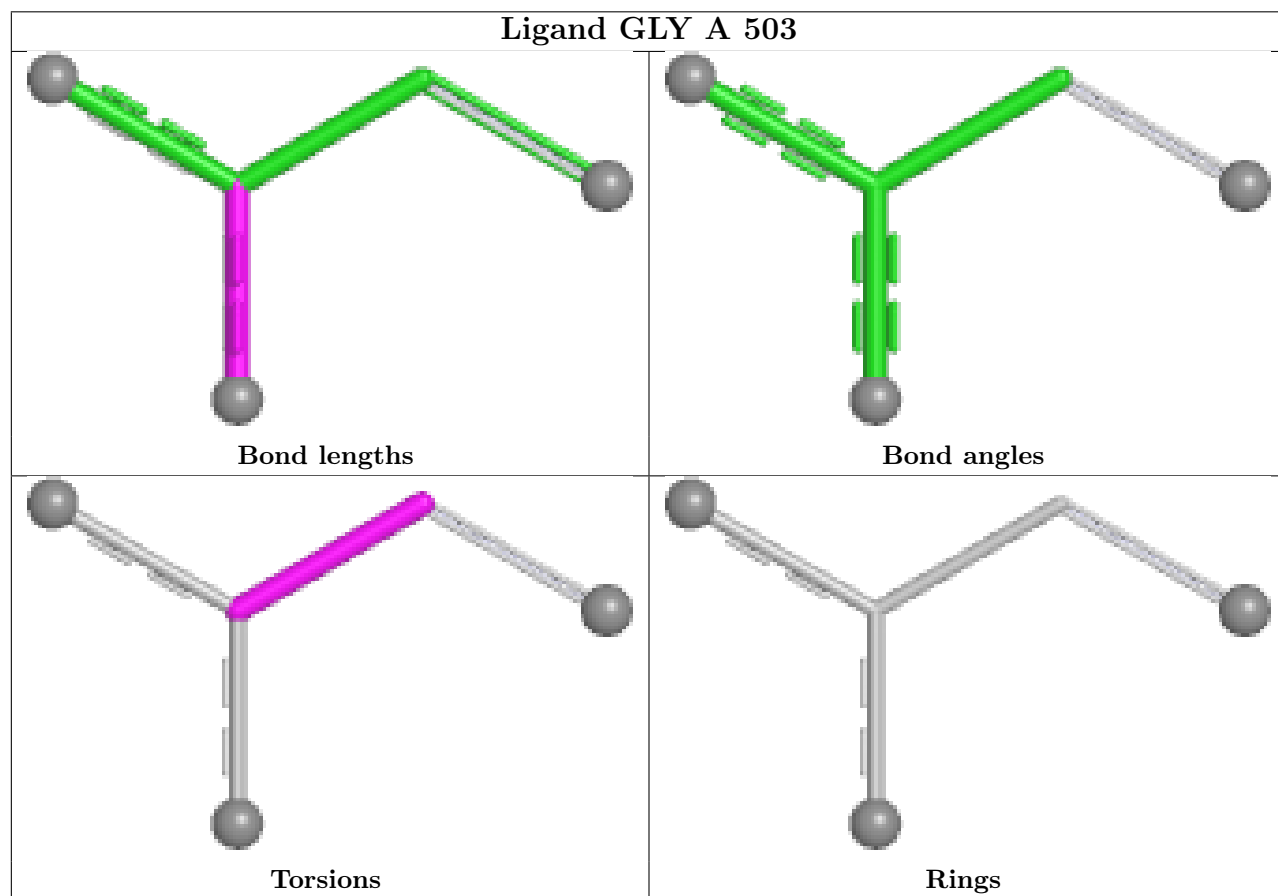
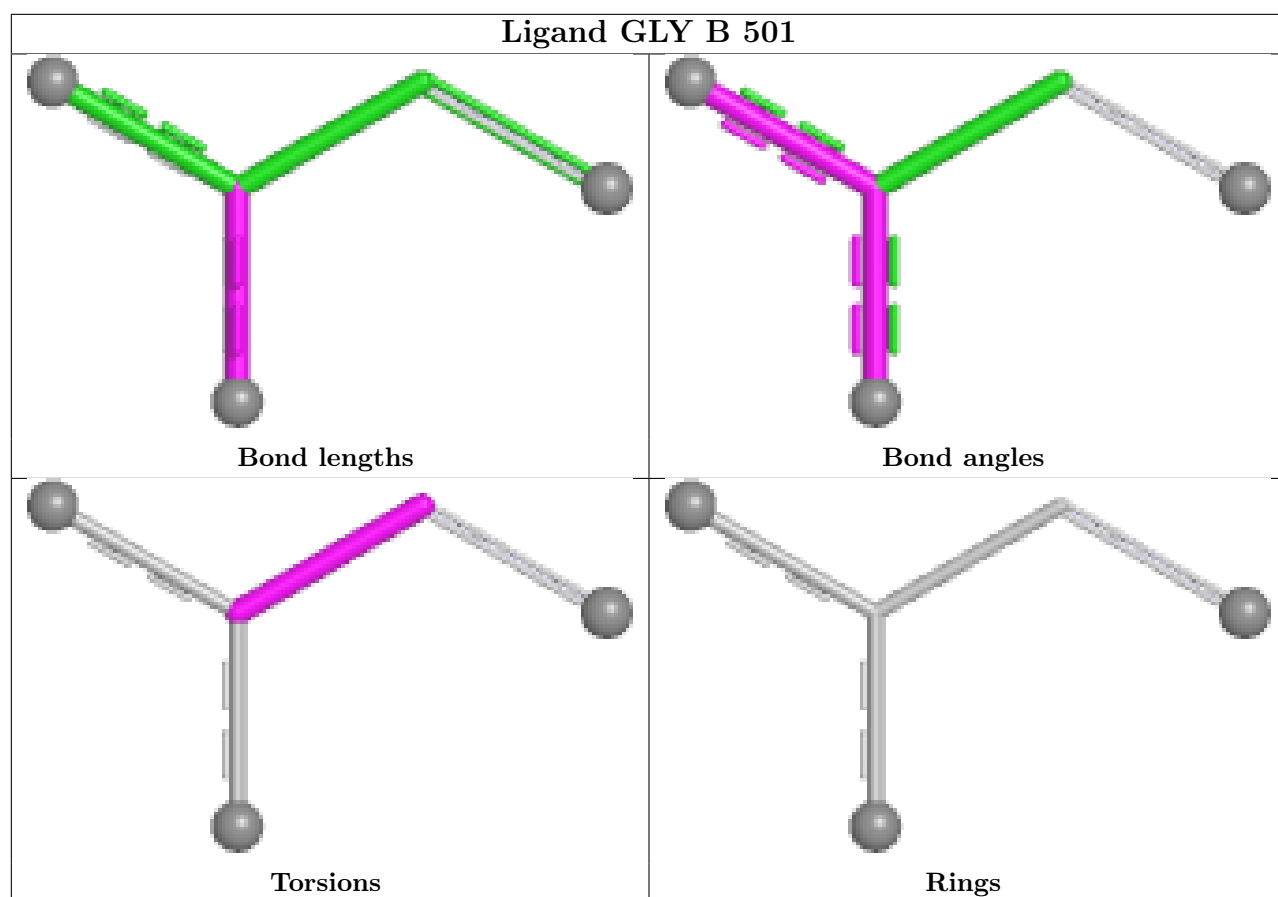
3 monomers are involved in 3 short contacts:

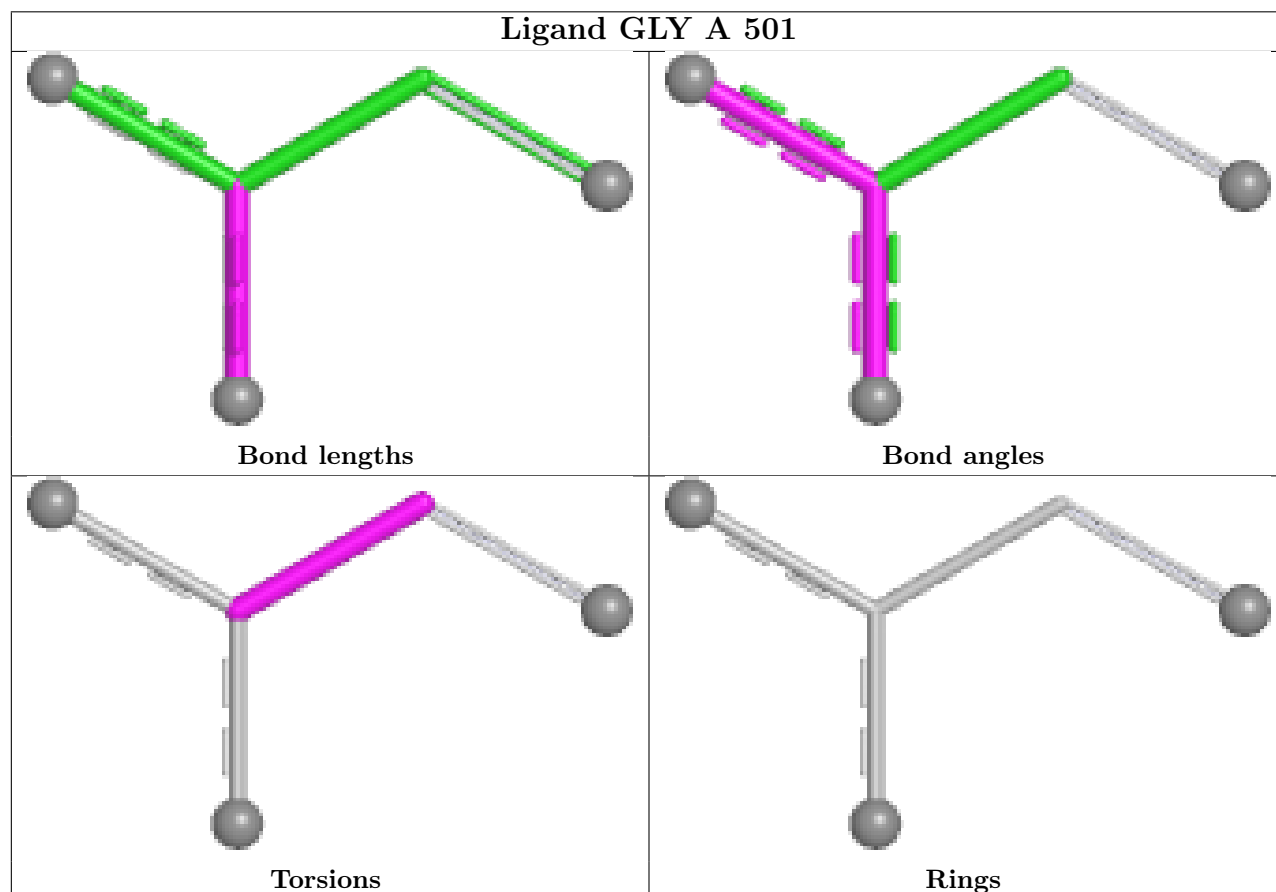
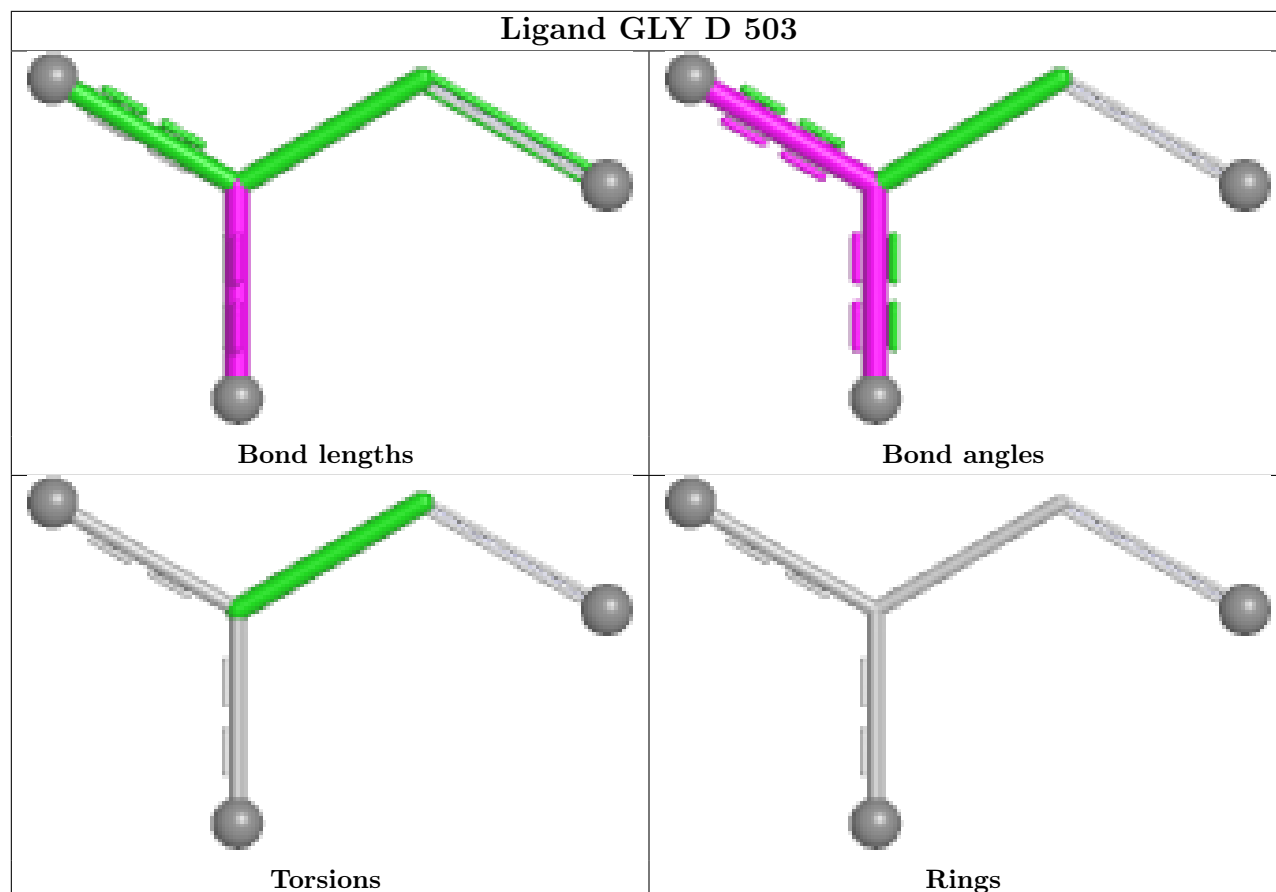
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GLY	1	0
4	C	501	NAG	1	0
3	A	501	GLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

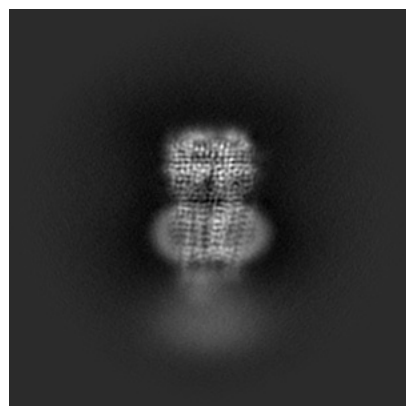
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26141. These allow visual inspection of the internal detail of the map and identification of artifacts.

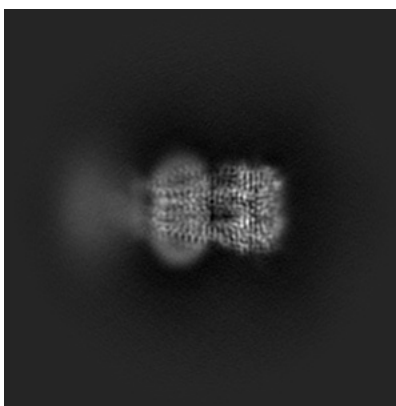
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

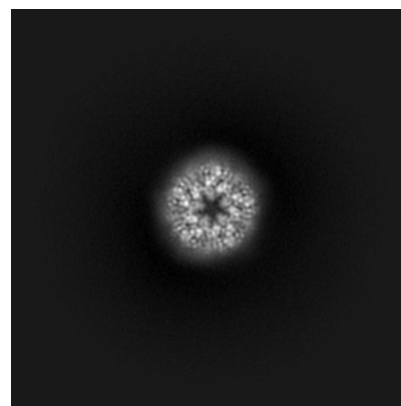
6.1.1 Primary map



X

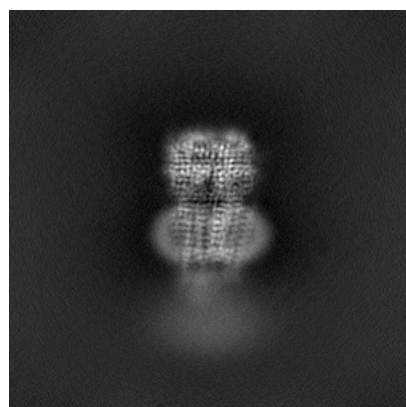


Y

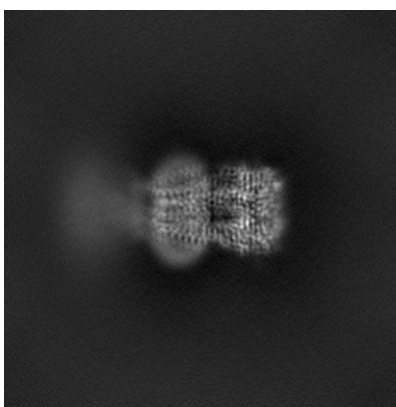


Z

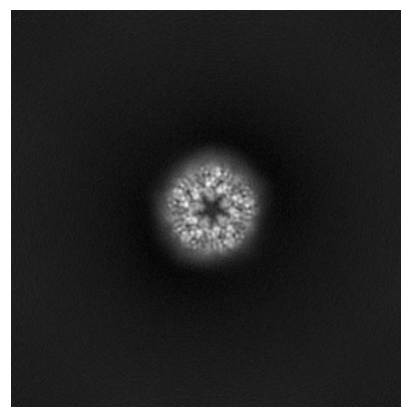
6.1.2 Raw map



X



Y

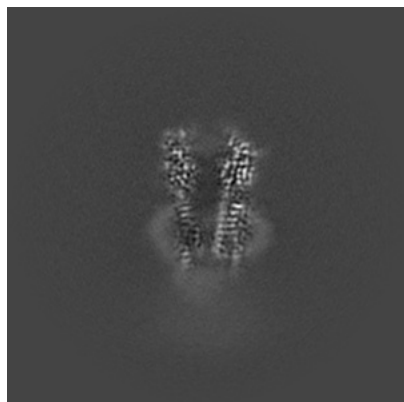


Z

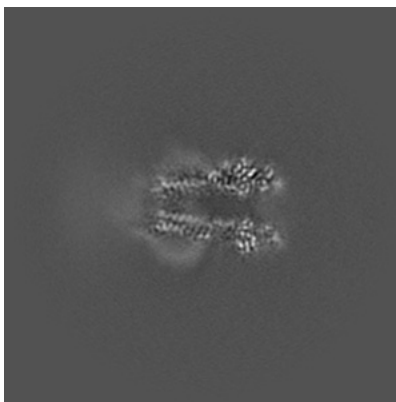
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

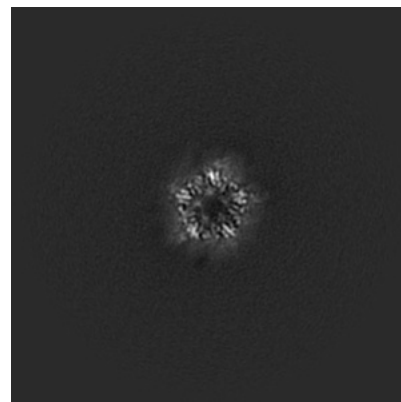
6.2.1 Primary map



X Index: 150

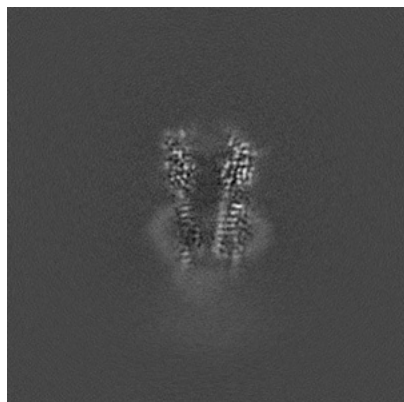


Y Index: 150

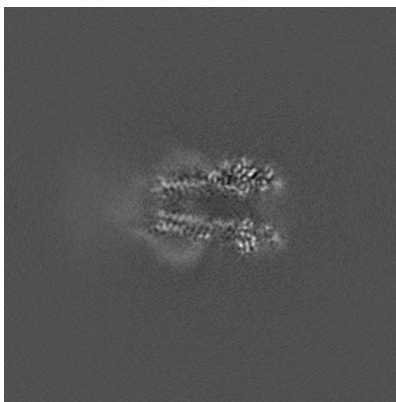


Z Index: 150

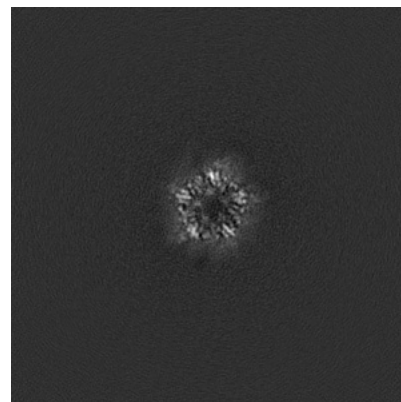
6.2.2 Raw map



X Index: 150



Y Index: 150

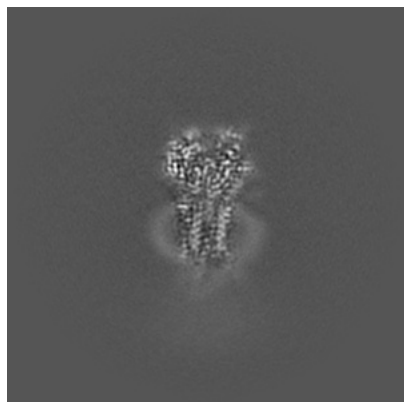


Z Index: 150

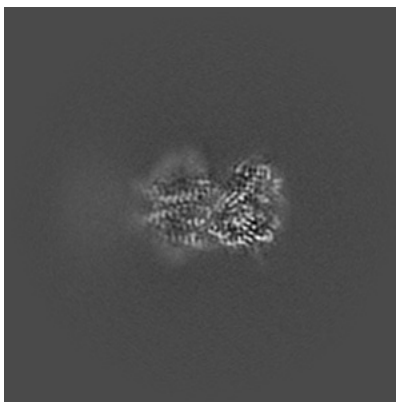
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

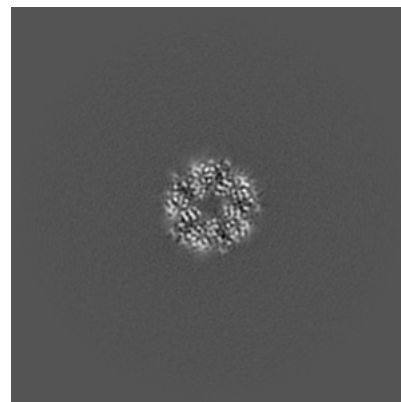
6.3.1 Primary map



X Index: 137

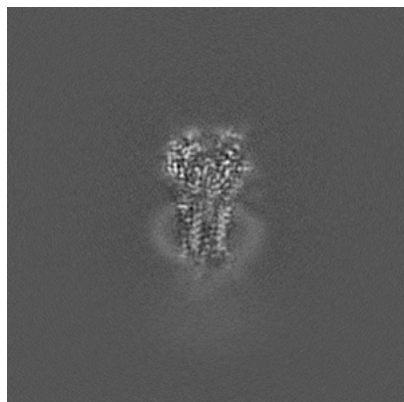


Y Index: 164

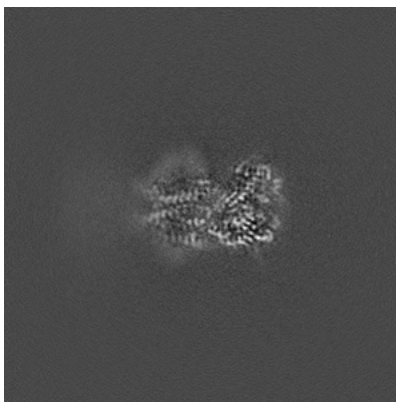


Z Index: 178

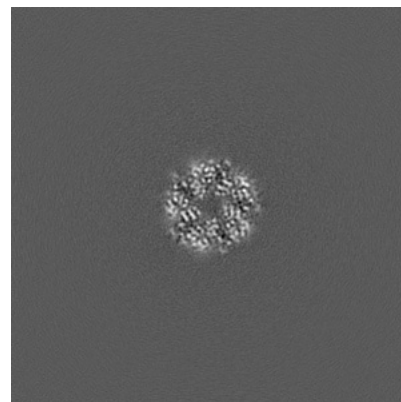
6.3.2 Raw map



X Index: 137



Y Index: 164

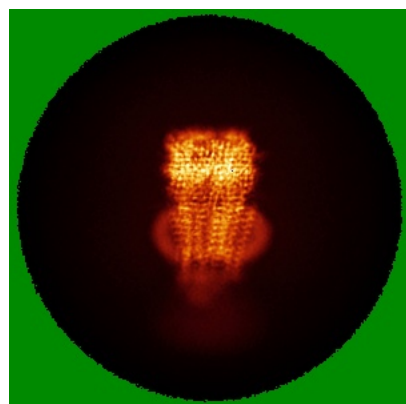


Z Index: 178

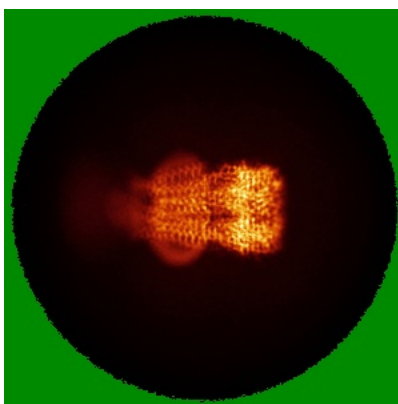
The images above show the largest variance slices of the map in three orthogonal directions.

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

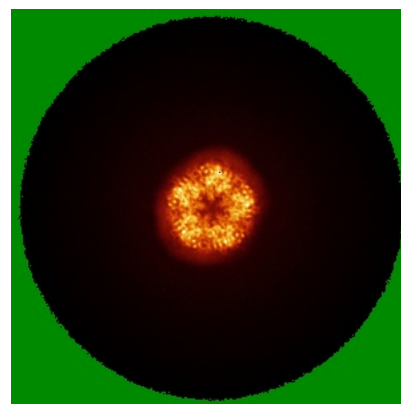
6.4.1 Primary map



X

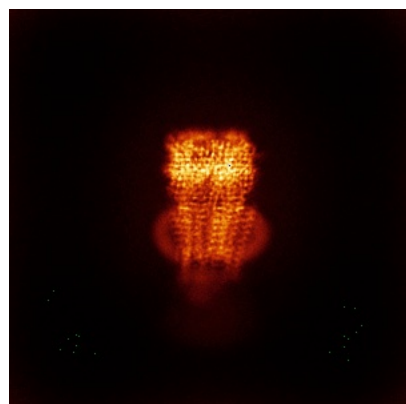


Y

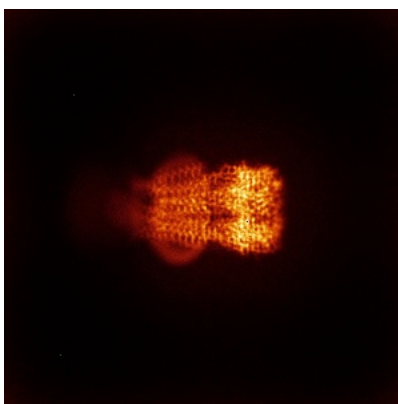


Z

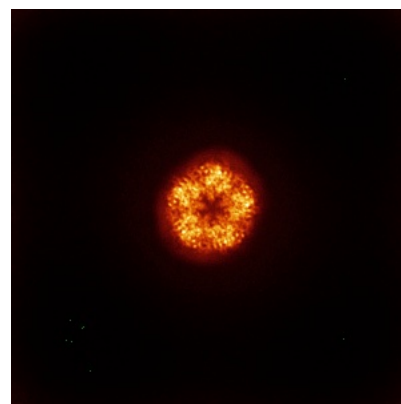
6.4.2 Raw map



X



Y

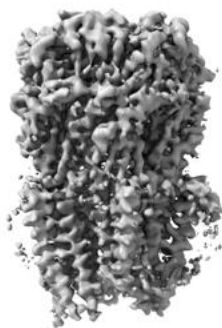


Z

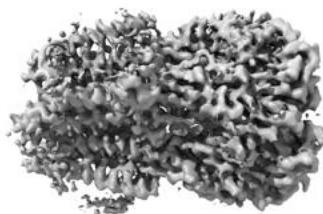
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

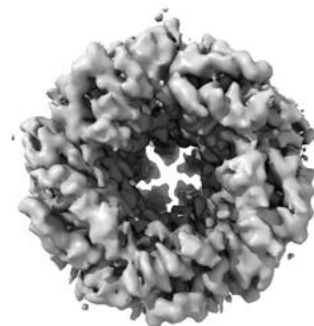
6.5.1 Primary map



X



Y



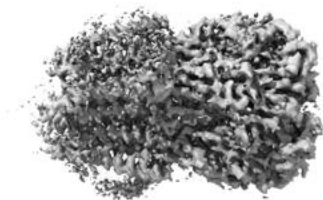
Z

The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

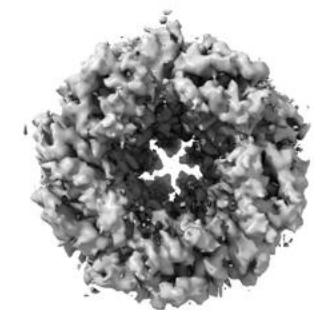
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

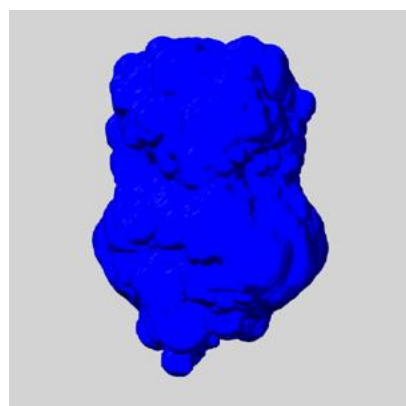
6.6 Mask visualisation [i](#)

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

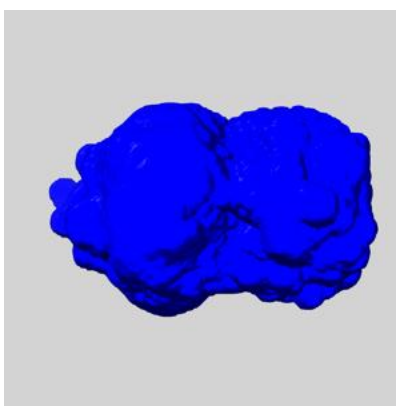
A mask typically either:

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

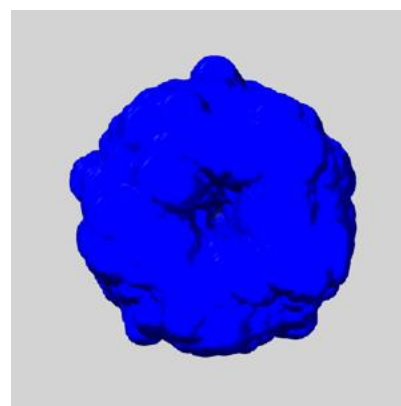
6.6.1 emd_26141_msk_1.map [i](#)



X



Y

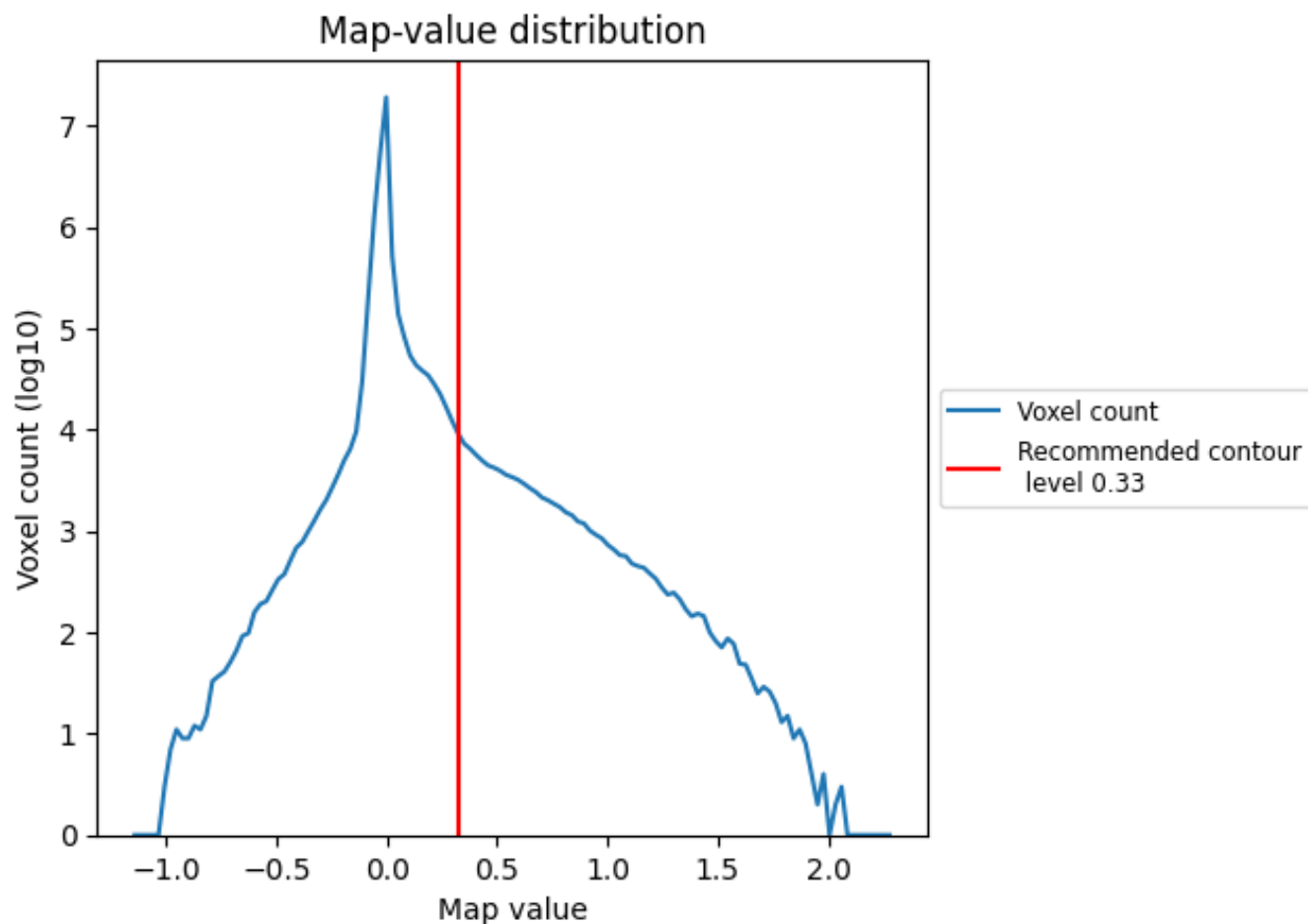


Z

7 Map analysis [i](#)

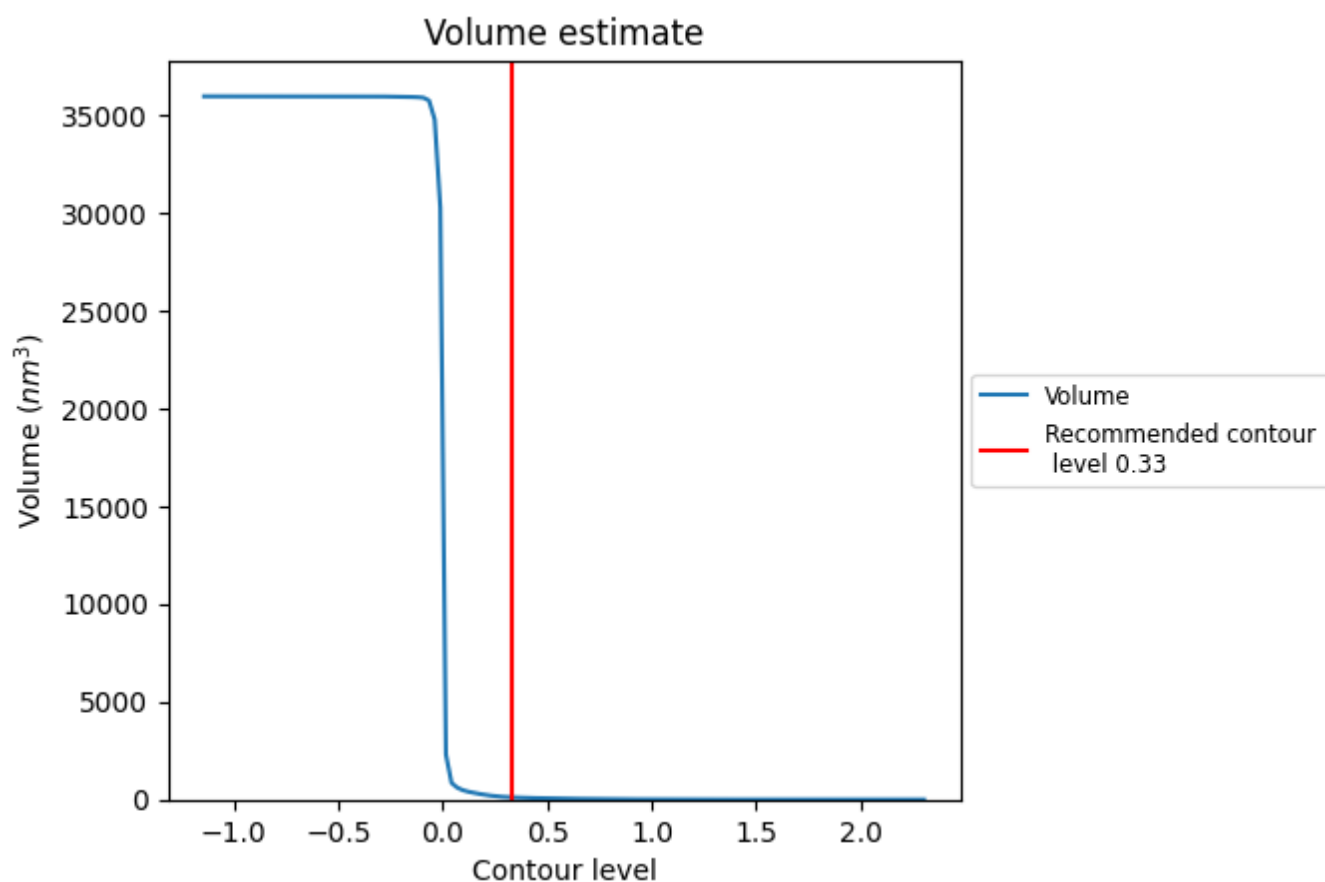
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

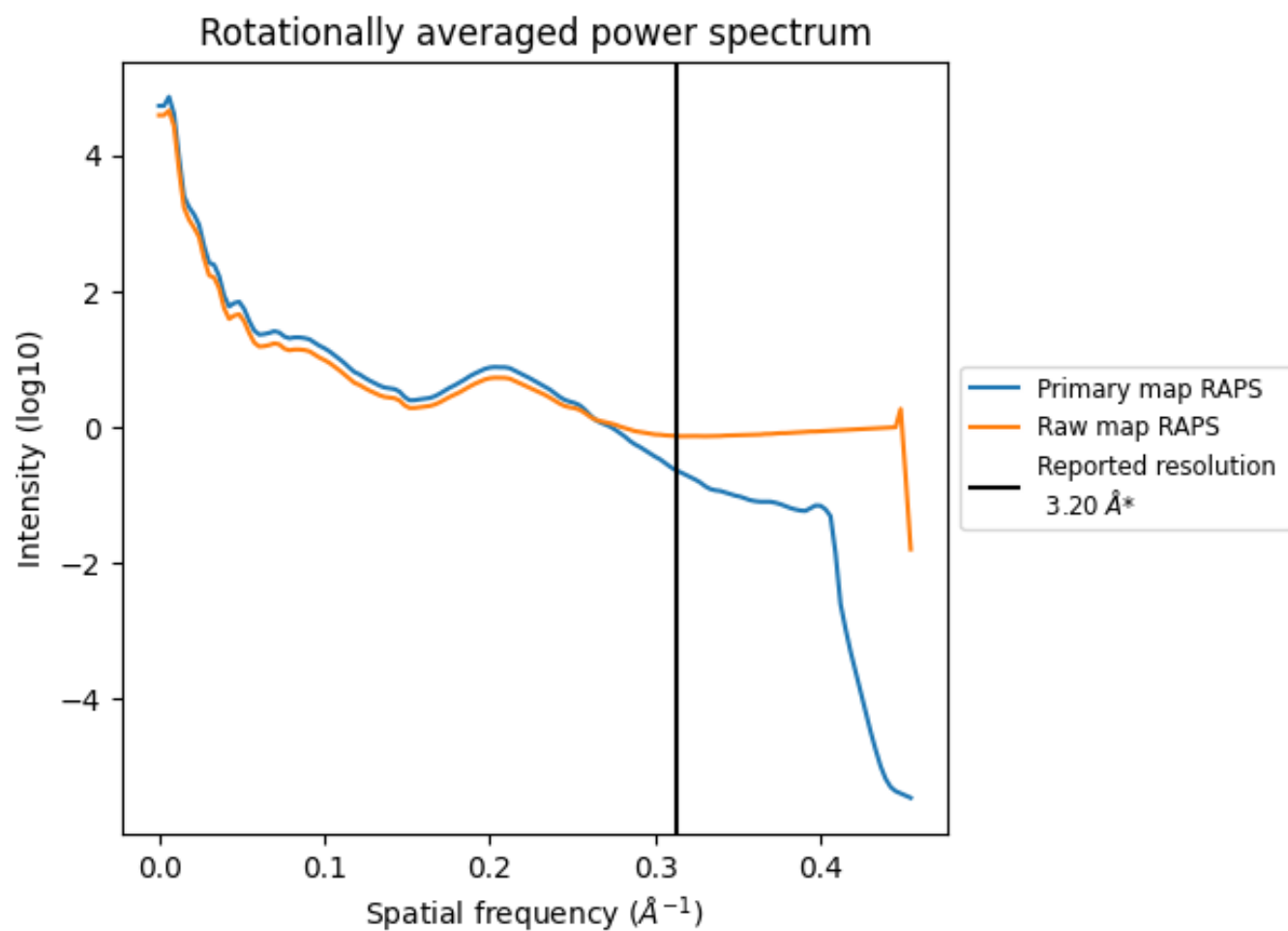
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

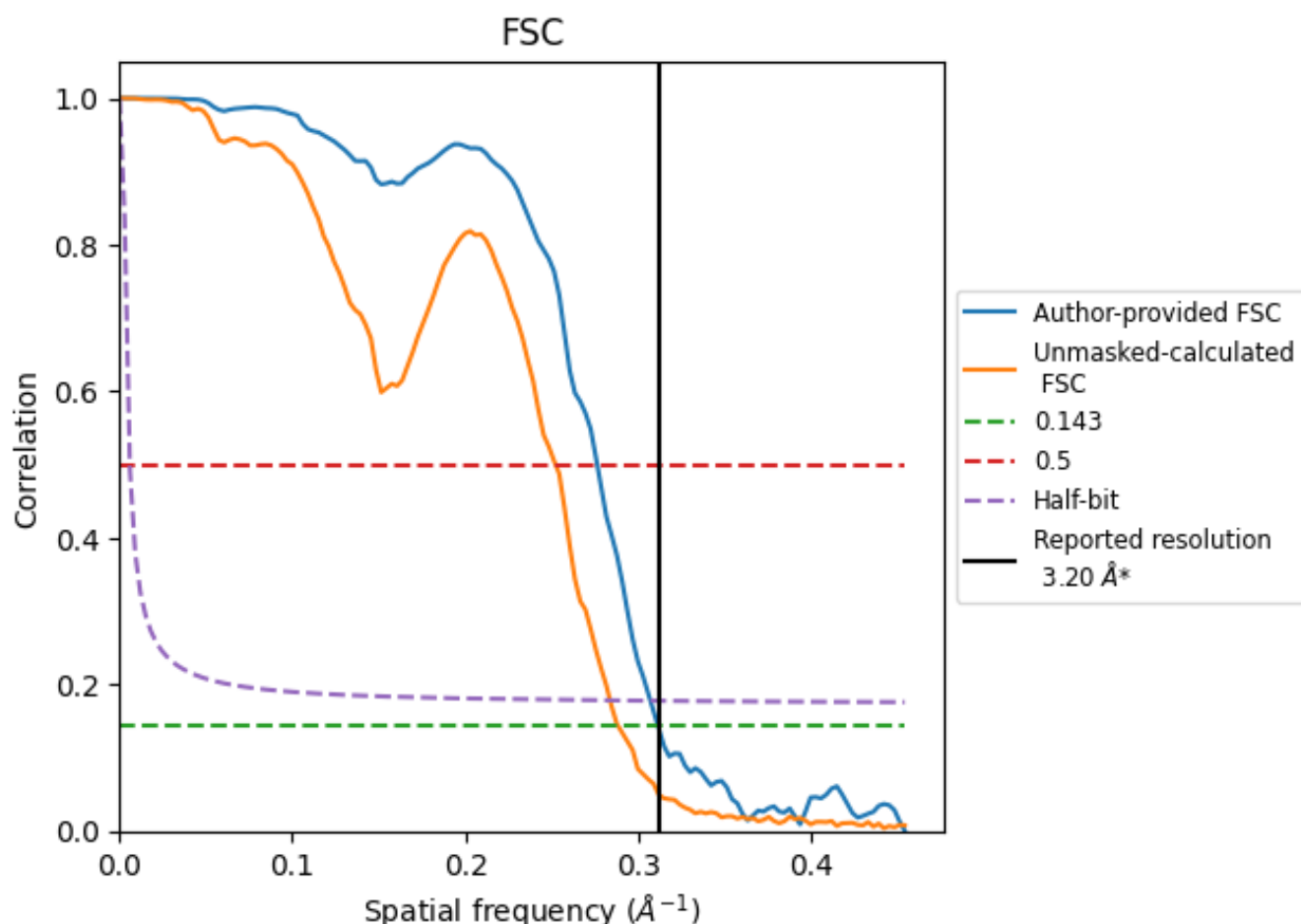


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

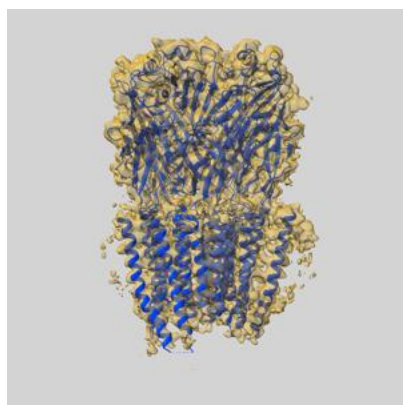
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.62	3.26
Unmasked-calculated*	3.47	3.96	3.52

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

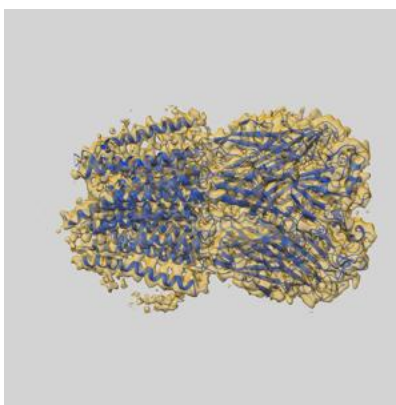
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26141 and PDB model 7TVI. Per-residue inclusion information can be found in section [3](#) on page [10](#).

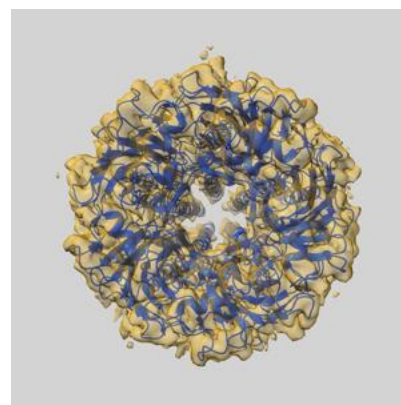
9.1 Map-model overlay [i](#)



X



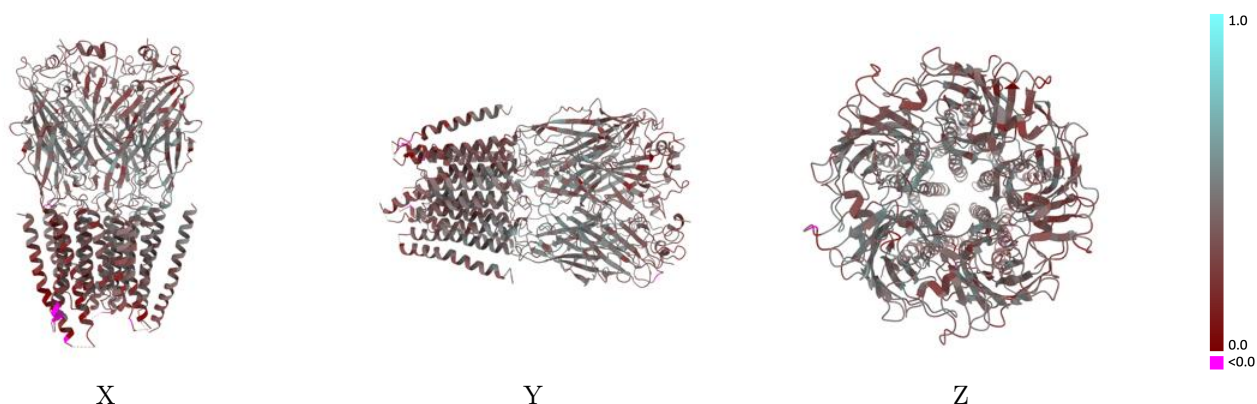
Y



Z

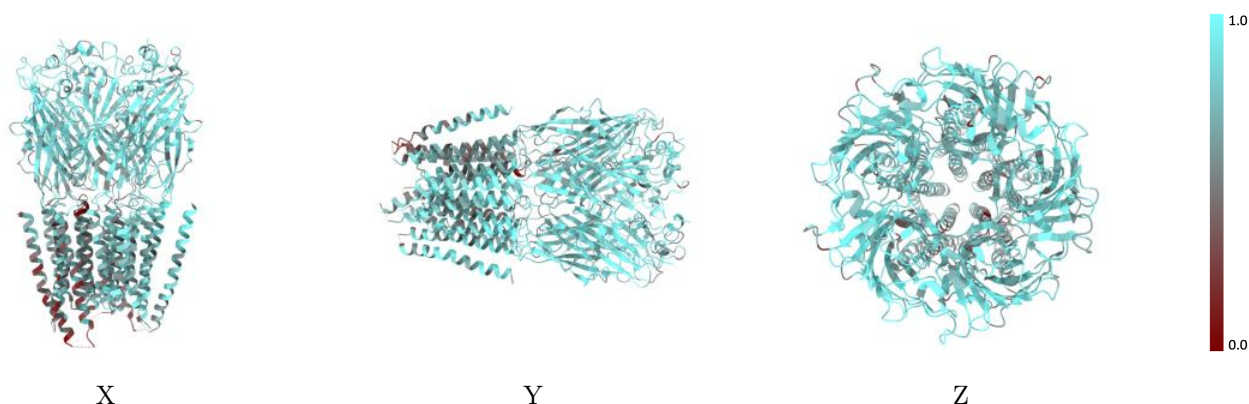
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



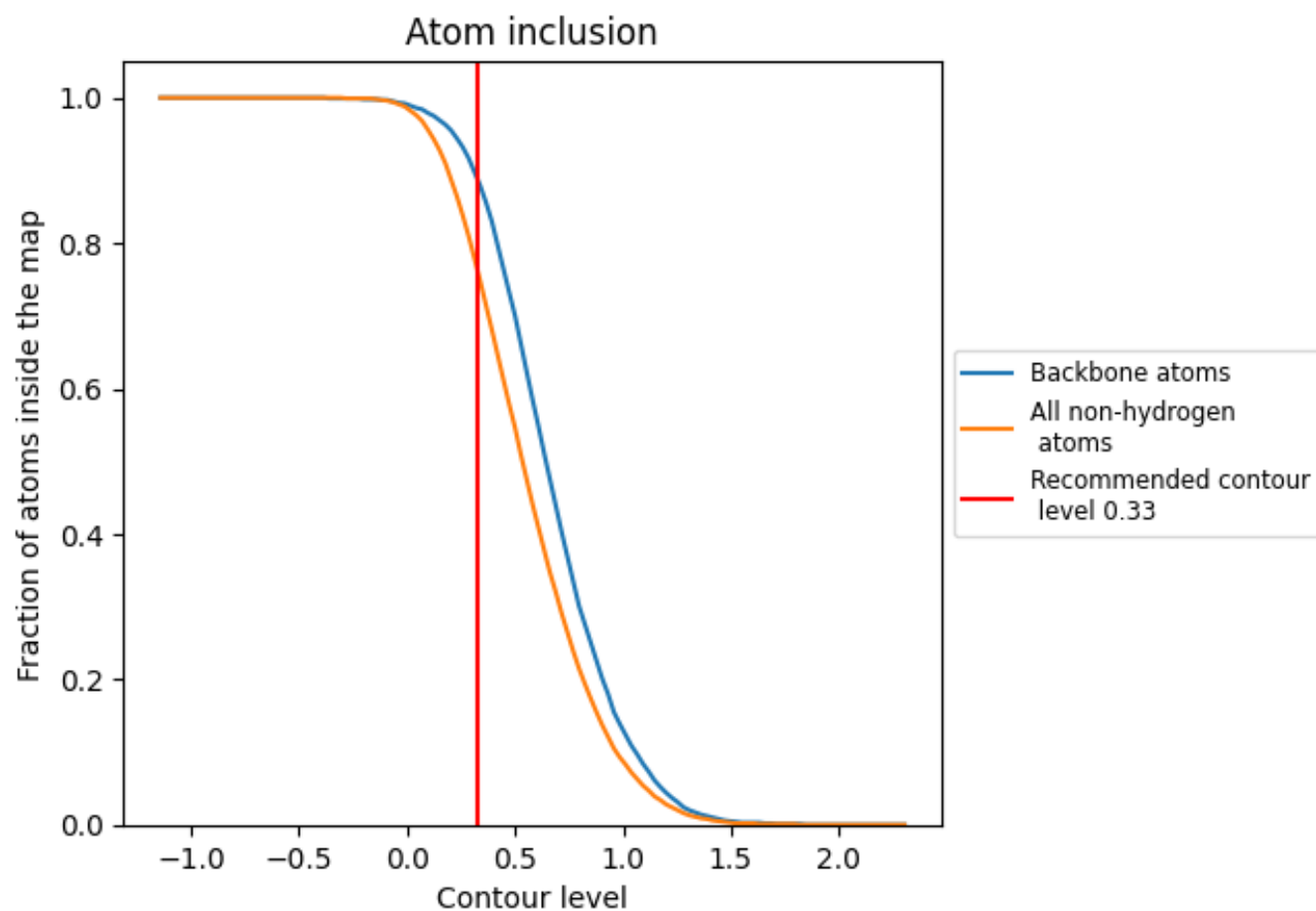
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 76% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7590	<div></div> 0.3750
A	<div></div> 0.6990	<div></div> 0.3370
B	<div></div> 0.7660	<div></div> 0.3890
C	<div></div> 0.8000	<div></div> 0.4070
D	<div></div> 0.7920	<div></div> 0.3910
E	<div></div> 0.7360	<div></div> 0.3530

