



wwPDB EM Validation Summary Report ⓘ

Sep 19, 2026 – 07:37 am BST

PDB ID : 9SL1 / pdb_00009sl1
EMDB ID : EMD-54981
Title : GABA-A α 4 β 3d receptor in complex with GABA, Nb24 and Mb30
Authors : Nestorow, S.; Miller, P.S.
Deposited on : 2025-09-02
Resolution : 2.68 Å (reported)
Based on initial model : 7QN7

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:

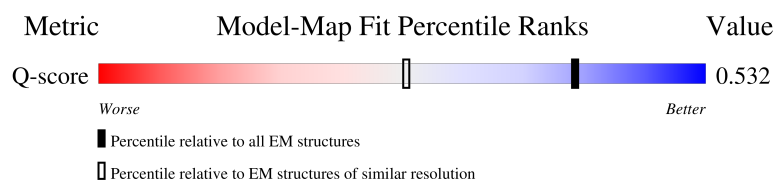
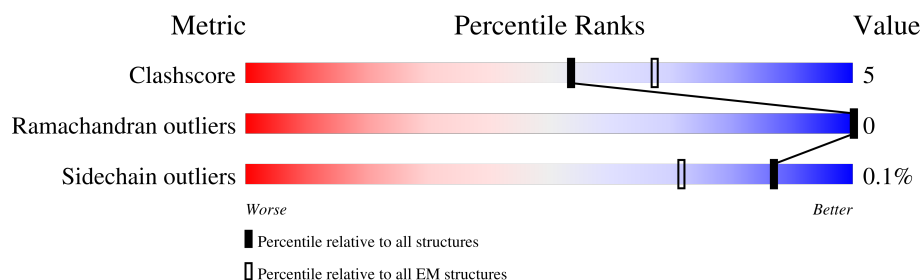
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.68 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	9255 (2.18 - 3.18)

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	364	 85% 7% 8%
1	C	364	 84% 8% 8%
2	B	451	 66% 8% 26%
2	D	451	 63% 10% 27%

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Mol	Chain	Length	Quality of chain
3	E	430	
4	F	138	
4	H	138	
5	G	133	
5	I	133	
6	Q	3	
7	R	3	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34690 atoms, of which 17153 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 Gamma-aminobutyric acid receptor subunit alpha-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0
			5416	1762	2714	437	483	20		
1	C	335	Total	C	H	N	O	S	0	0
			5418	1762	2716	437	483	20		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P48169
A	2	ASN	-	expression tag	UNP P48169
A	3	SER	-	expression tag	UNP P48169
A	4	LYS	-	expression tag	UNP P48169
A	5	ASP	-	expression tag	UNP P48169
A	6	GLU	-	expression tag	UNP P48169
A	7	LYS	-	expression tag	UNP P48169
A	8	LEU	-	expression tag	UNP P48169
A	9	CYS	-	expression tag	UNP P48169
A	10	PRO	-	expression tag	UNP P48169
A	120	THR	MET	engineered mutation	UNP P48169
A	311	SER	-	linker	UNP P48169
A	312	GLN	-	linker	UNP P48169
A	313	PRO	-	linker	UNP P48169
A	314	ALA	-	linker	UNP P48169
A	315	ARG	-	linker	UNP P48169
A	316	ALA	-	linker	UNP P48169
A	317	ALA	-	linker	UNP P48169
A	428	GLY	-	expression tag	UNP P48169
A	429	THR	-	expression tag	UNP P48169
A	430	LYS	-	expression tag	UNP P48169
A	431	HIS	-	expression tag	UNP P48169
A	432	HIS	-	expression tag	UNP P48169
A	433	HIS	-	expression tag	UNP P48169
A	434	HIS	-	expression tag	UNP P48169
A	435	HIS	-	expression tag	UNP P48169

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Chain	Residue	Modelled	Actual	Comment	Reference
A	436	HIS	-	expression tag	UNP P48169
C	1	GLY	-	expression tag	UNP P48169
C	2	ASN	-	expression tag	UNP P48169
C	3	SER	-	expression tag	UNP P48169
C	4	LYS	-	expression tag	UNP P48169
C	5	ASP	-	expression tag	UNP P48169
C	6	GLU	-	expression tag	UNP P48169
C	7	LYS	-	expression tag	UNP P48169
C	8	LEU	-	expression tag	UNP P48169
C	9	CYS	-	expression tag	UNP P48169
C	10	PRO	-	expression tag	UNP P48169
C	120	THR	MET	engineered mutation	UNP P48169
C	311	SER	-	linker	UNP P48169
C	312	GLN	-	linker	UNP P48169
C	313	PRO	-	linker	UNP P48169
C	314	ALA	-	linker	UNP P48169
C	315	ARG	-	linker	UNP P48169
C	316	ALA	-	linker	UNP P48169
C	317	ALA	-	linker	UNP P48169
C	428	GLY	-	expression tag	UNP P48169
C	429	THR	-	expression tag	UNP P48169
C	430	LYS	-	expression tag	UNP P48169
C	431	HIS	-	expression tag	UNP P48169
C	432	HIS	-	expression tag	UNP P48169
C	433	HIS	-	expression tag	UNP P48169
C	434	HIS	-	expression tag	UNP P48169
C	435	HIS	-	expression tag	UNP P48169
C	436	HIS	-	expression tag	UNP P48169

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	332	Total	C	H	N	O	S	0	0
			5397	1780	2679	444	478	16		
2	D	331	Total	C	H	N	O	S	0	0
			5396	1778	2682	443	477	16		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	307A	SER	-	linker	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	307B	GLN	-	linker	UNP P28472
B	307C	PRO	-	linker	UNP P28472
B	307D	ALA	-	linker	UNP P28472
B	307E	GLY	-	linker	UNP P28472
B	307F	THR	-	linker	UNP P28472
B	307M	TRP	MET	engineered mutation	UNP P0ABE7
B	311D	ILE	HIS	engineered mutation	UNP P0ABE7
B	311H	LEU	ARG	engineered mutation	UNP P0ABE7
B	417	THR	-	linker	UNP P0ABE7
B	418	GLY	-	linker	UNP P0ABE7
B	419	ARG	-	linker	UNP P0ABE7
B	420	ALA	-	linker	UNP P0ABE7
B	421	ALA	-	linker	UNP P0ABE7
D	307A	SER	-	linker	UNP P28472
D	307B	GLN	-	linker	UNP P28472
D	307C	PRO	-	linker	UNP P28472
D	307D	ALA	-	linker	UNP P28472
D	307E	GLY	-	linker	UNP P28472
D	307F	THR	-	linker	UNP P28472
D	307M	TRP	MET	engineered mutation	UNP P0ABE7
D	311D	ILE	HIS	engineered mutation	UNP P0ABE7
D	311H	LEU	ARG	engineered mutation	UNP P0ABE7
D	417	THR	-	linker	UNP P0ABE7
D	418	GLY	-	linker	UNP P0ABE7
D	419	ARG	-	linker	UNP P0ABE7
D	420	ALA	-	linker	UNP P0ABE7
D	421	ALA	-	linker	UNP P0ABE7

- Molecule 3 is a protein called GABA-A receptor SBP-delta-glvi, Gamma-aminobutyric acid receptor subunit delta, Gamma-aminobutyric acid receptor subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	328	Total	C	H	N	O	S	0	0
			5183	1698	2564	434	474	13		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	ASP	-	linker	PDB ?
E	-15	TYR	-	linker	PDB ?
E	-14	ASP	-	linker	PDB ?
E	-13	ILE	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	PRO	-	linker	PDB ?
E	-11	THR	-	linker	PDB ?
E	-10	THR	-	linker	PDB ?
E	-9	GLU	-	linker	PDB ?
E	-8	ASN	-	linker	PDB ?
E	-7	LEU	-	linker	PDB ?
E	-6	TYR	-	linker	PDB ?
E	-5	PHE	-	linker	PDB ?
E	-4	GLN	-	linker	PDB ?
E	-3	GLY	-	linker	PDB ?
E	-2	THR	-	linker	PDB ?
E	-1	GLY	-	linker	PDB ?
E	313	SER	-	linker	UNP O14764
E	314	GLN	-	linker	UNP O14764
E	315	PRO	-	linker	UNP O14764
E	316	ALA	-	linker	UNP O14764
E	317	ARG	-	linker	UNP O14764
E	318	ALA	-	linker	UNP O14764
E	319	ALA	-	linker	UNP O14764

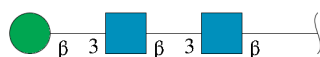
- | Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------|--------|---------|-------|
| 4 | F | 122 | Total
1873 | C
601 | H
914 | N
170 | O
184 | S
4 | 0 | 0 |
| 4 | H | 122 | Total
1873 | C
601 | H
914 | N
170 | O
184 | S
4 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------|--------|---------|-------|
| 5 | G | 123 | Total
1840 | C
583 | H
896 | N
171 | O
186 | S
4 | 0 | 0 |
| 5 | I | 123 | Total
1840 | C
583 | H
896 | N
171 | O
186 | S
4 | 0 | 0 |

-

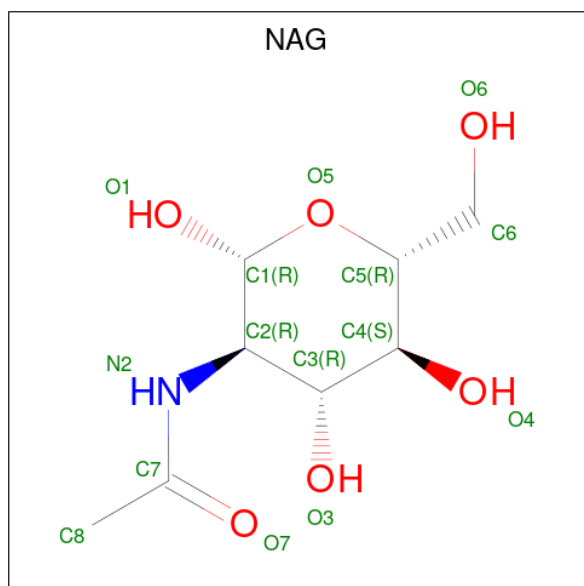
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	3	Total	C	H	N	O	0	0
			71	22	32	2	15		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	3	Total	C	H	N	O	0	0
			71	22	32	2	15		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



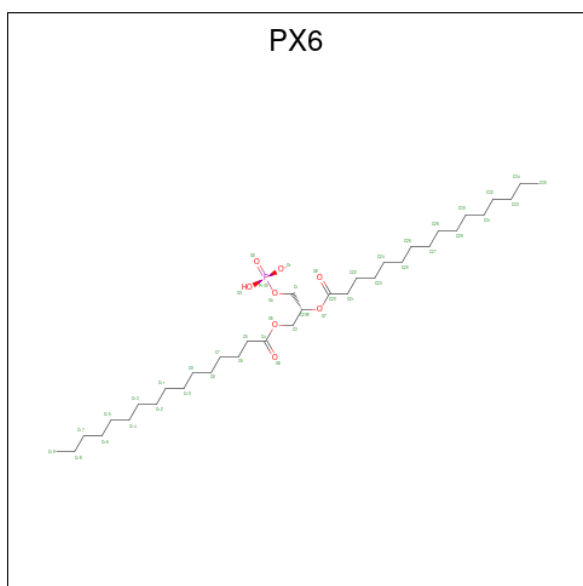
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

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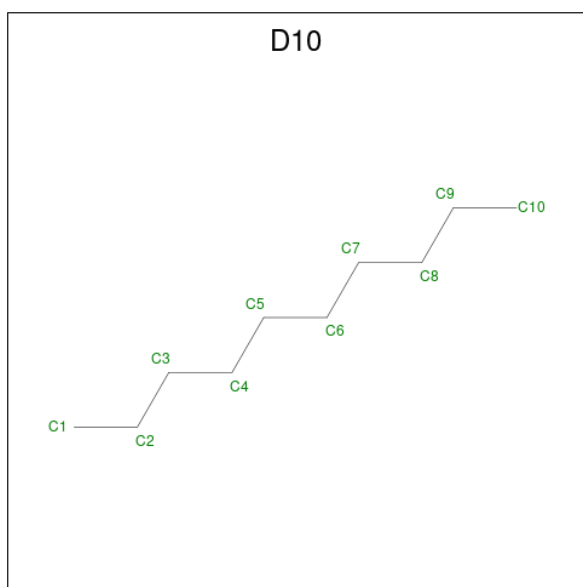
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	E	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 9 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX6) (formula: C₃₅H₆₈O₈P).



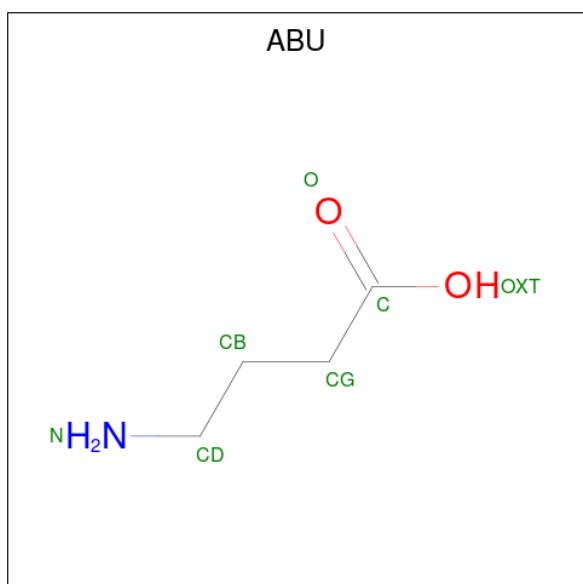
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 10 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 10 10	0
10	B	1	Total C 10 10	0
10	D	1	Total C 10 10	0
10	E	1	Total C 10 10	0

- Molecule 11 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	H	N	O	0
			15	4	8	1	2	
11	D	1	Total	C	H	N	O	0
			15	4	8	1	2	

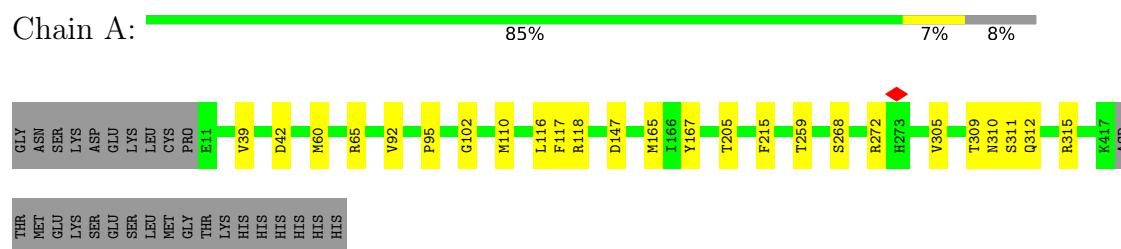
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	O	0
			1	1	
12	C	1	Total	O	0
			1	1	

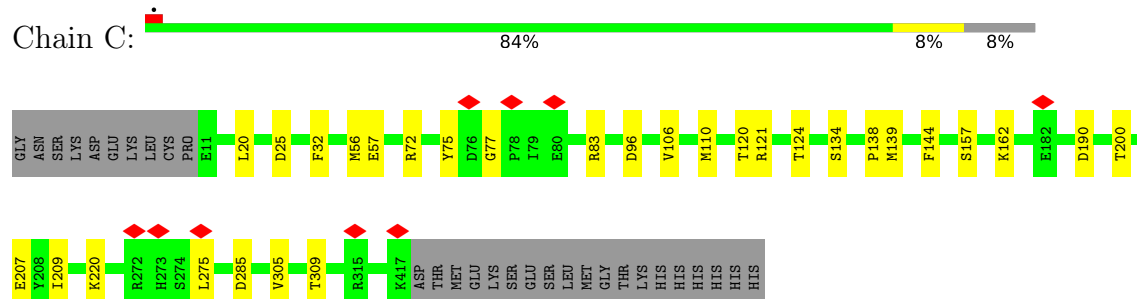
3 Residue-property plots [i](#)

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

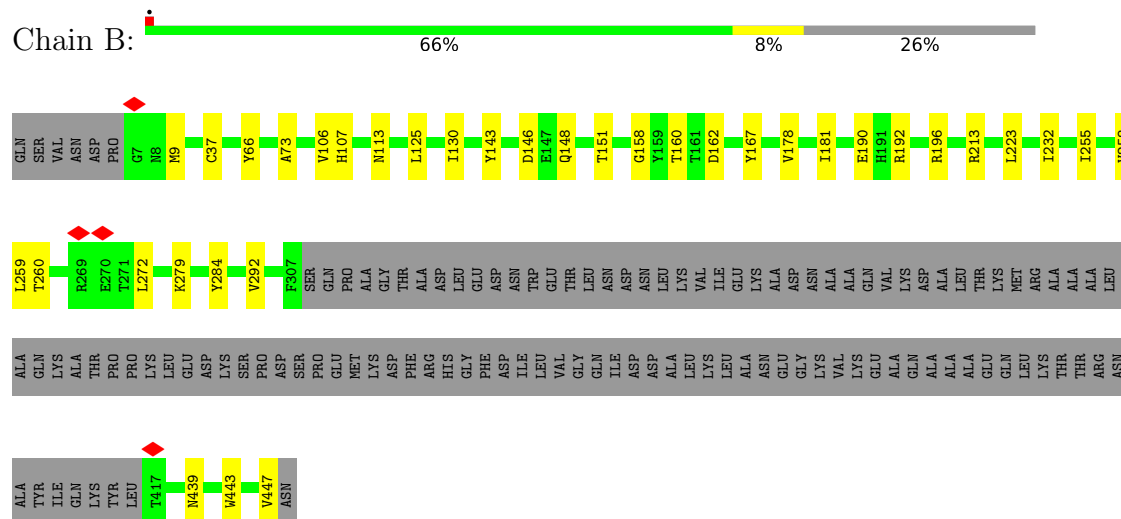
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-4



- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-4



- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3, Soluble cytochrome b562

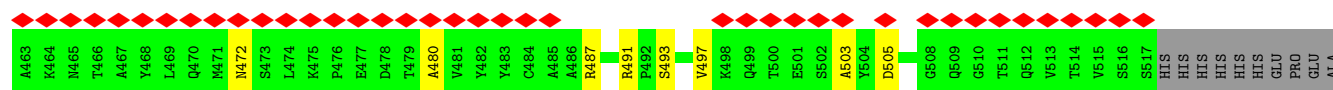


- Chain D: 

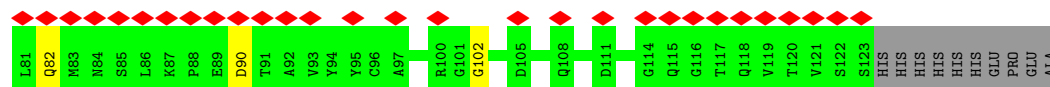
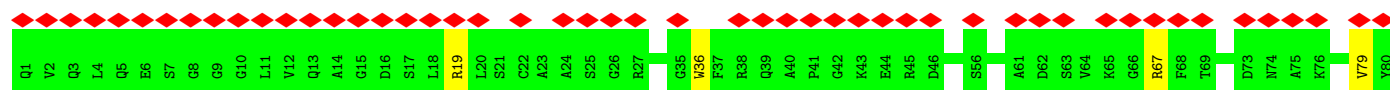
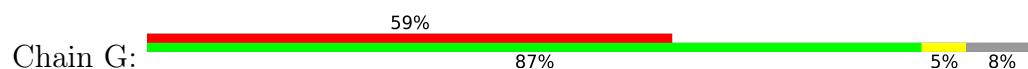
- Chain E:
-

- Chain F: 

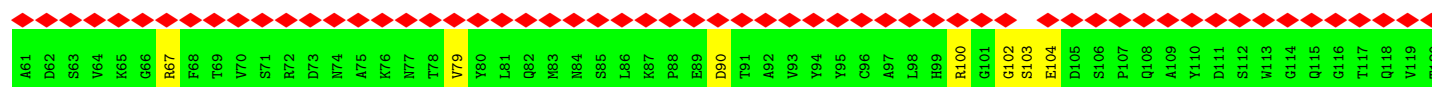
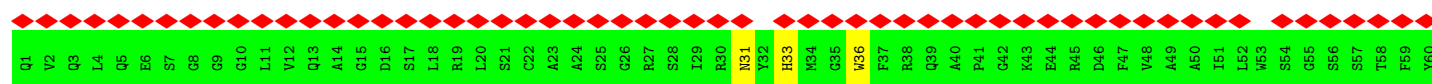
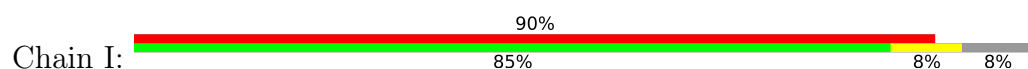
- Chain H:
-
- Sequence logo for Chain H. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists positions Q1 to R46. A bar chart at the top shows the percentage of conserved positions: 64% (red), 76% (green), 12% (yellow), and 12% (grey).
- | Position | Conservation Level |
|----------|--------------------|
| Q1 | High |
| V2 | High |
| Q3 | High |
| L4 | High |
| Q5 | High |
| E6 | High |
| S7 | High |
| C8 | High |
| GLY | High |
| GLY | High |
| LEU | High |
| VAL | High |
| GLN | High |
| GLY | High |
| S404 | High |
| L405 | High |
| R406 | High |
| L407 | High |
| S408 | High |
| C409 | High |
| T410 | High |
| A411 | High |
| S412 | High |
| Q413 | High |
| L414 | High |
| T415 | High |
| F416 | High |
| S417 | High |
| N418 | High |
| F424 | High |
| R425 | High |
| Q426 | High |
| L427 | High |
| P428 | High |
| Q429 | High |
| K430 | High |
| E431 | High |
| R432 | High |
| E433 | High |
| F434 | High |
| V435 | High |
| A436 | High |
| A447 | High |
| Y448 | High |
| G449 | High |
| T450 | High |
| S451 | High |
| I452 | High |
| R453 | High |
| G454 | High |
| R455 | High |
| F456 | High |
| T457 | High |
| I458 | High |
| S459 | High |
| R460 | High |
| D461 | High |
| V462 | High |



• Molecule 5: Nanobody Nb24



• Molecule 5: Nanobody Nb24



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117418	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 ($e^-/\text{\AA}^2$)	51.12	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.432	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0754	Depositor
Map size (Å)	349.91998, 349.91998, 349.91998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABU, NAG, PX6, D10, BMA

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	0.31	0/2775	0.55	0/3768
1	C	0.30	0/2775	0.54	0/3768
2	B	0.30	0/2790	0.56	0/3795
2	D	0.30	0/2786	0.57	0/3790
3	E	0.31	0/2692	0.53	0/3672
4	F	0.27	0/981	0.57	0/1329
4	H	0.31	0/981	0.56	0/1329
5	G	0.32	0/964	0.60	0/1303
5	I	0.32	0/964	0.60	0/1303
All	All	0.30	0/17708	0.56	0/24057

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

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	2702	2714	2710	35	0
1	C	2702	2716	2711	24	0
2	B	2718	2679	2711	44	0
2	D	2714	2682	2709	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2619	2564	2563	32	0
4	F	959	914	912	2	0
4	H	959	914	912	10	0
5	G	944	896	894	4	0
5	I	944	896	894	16	0
6	Q	39	32	34	5	0
7	R	39	32	34	3	0
8	A	28	28	26	0	0
8	B	28	28	26	0	0
8	C	14	14	13	1	0
8	D	14	14	13	0	0
8	E	14	14	13	0	0
9	A	44	0	68	13	0
10	A	10	0	22	0	0
10	B	10	0	22	0	0
10	D	10	0	22	0	0
10	E	10	0	22	1	0
11	B	7	8	0	0	0
11	D	7	8	0	0	0
12	A	1	0	0	0	0
12	C	1	0	0	0	0
All	All	17537	17153	17331	182	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 182 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)
3:E:197:PHE:CE1	3:E:215:LEU:HD13	1.53	1.43
2:B:66:TYR:CE2	2:B:125:LEU:HD13	1.63	1.32
2:B:66:TYR:CZ	2:B:125:LEU:HD13	1.78	1.18
3:E:197:PHE:CD1	3:E:215:LEU:HD13	1.83	1.12
3:E:197:PHE:CE1	3:E:215:LEU:CD1	2.31	1.12

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	333/364 (92%)	326 (98%)	7 (2%)	0	100	100
1	C	333/364 (92%)	327 (98%)	6 (2%)	0	100	100
2	B	328/451 (73%)	321 (98%)	7 (2%)	0	100	100
2	D	327/451 (72%)	318 (97%)	9 (3%)	0	100	100
3	E	326/430 (76%)	313 (96%)	13 (4%)	0	100	100
4	F	118/138 (86%)	115 (98%)	3 (2%)	0	100	100
4	H	118/138 (86%)	110 (93%)	8 (7%)	0	100	100
5	G	121/133 (91%)	114 (94%)	7 (6%)	0	100	100
5	I	121/133 (91%)	114 (94%)	7 (6%)	0	100	100
All	All	2125/2602 (82%)	2058 (97%)	67 (3%)	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	301/328 (92%)	301 (100%)	0	100	100
1	C	301/328 (92%)	301 (100%)	0	100	100
2	B	296/393 (75%)	296 (100%)	0	100	100
2	D	296/393 (75%)	294 (99%)	2 (1%)	76	89
3	E	279/363 (77%)	279 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	99/111 (89%)	99 (100%)	0	100	100
4	H	99/111 (89%)	99 (100%)	0	100	100
5	G	99/108 (92%)	99 (100%)	0	100	100
5	I	99/108 (92%)	99 (100%)	0	100	100
All	All	1869/2243 (83%)	1867 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	111	VAL
2	D	220	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	39	GLN
5	I	33	HIS
5	I	39	GLN
2	D	41	ASN
2	D	85	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](#)

6 monosaccharides 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	$\# Z > 2$
6	NAG	Q	1	2,6	14,14,15	0.41	0	17,19,21	0.52	0
6	NAG	Q	2	6	14,14,15	0.39	0	17,19,21	1.73	3 (17%)
6	BMA	Q	3	6	11,11,12	0.22	0	15,15,17	0.64	0
7	NAG	R	1	2,7	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
7	NAG	R	2	7	14,14,15	0.63	0	17,19,21	1.80	3 (17%)
7	BMA	R	3	7	11,11,12	0.24	0	15,15,17	0.62	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
6	NAG	Q	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
7	NAG	R	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	4/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2	NAG	O5-C1-C2	-5.23	103.02	111.29
6	Q	2	NAG	O5-C1-C2	-4.78	103.74	111.29
7	R	2	NAG	O3-C3-C2	3.41	116.53	109.47
7	R	1	NAG	O3-C3-C2	2.99	115.66	109.47
6	Q	2	NAG	C1-O5-C5	2.80	115.98	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2

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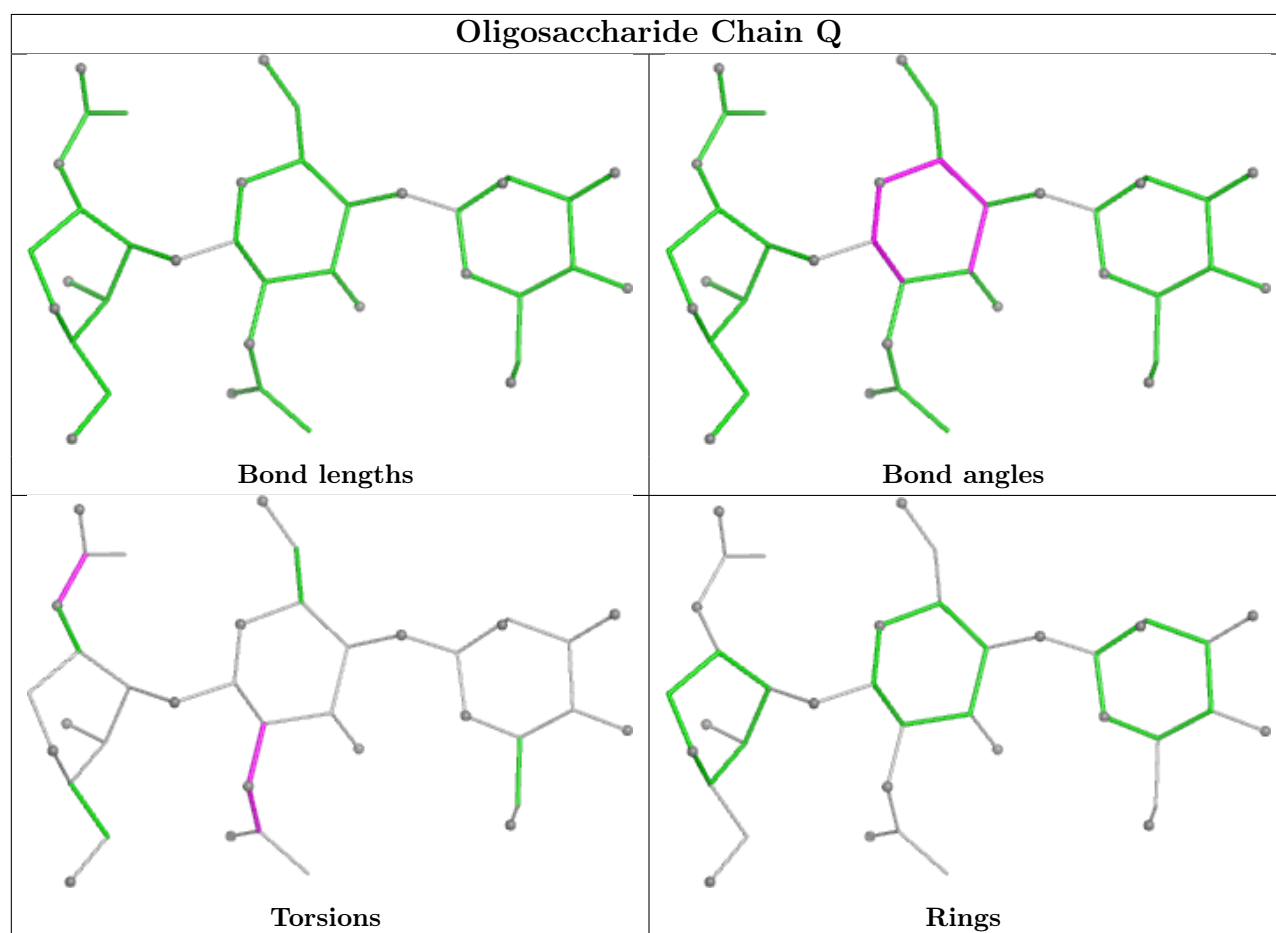
Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	O7-C7-N2-C2
7	R	2	NAG	C8-C7-N2-C2

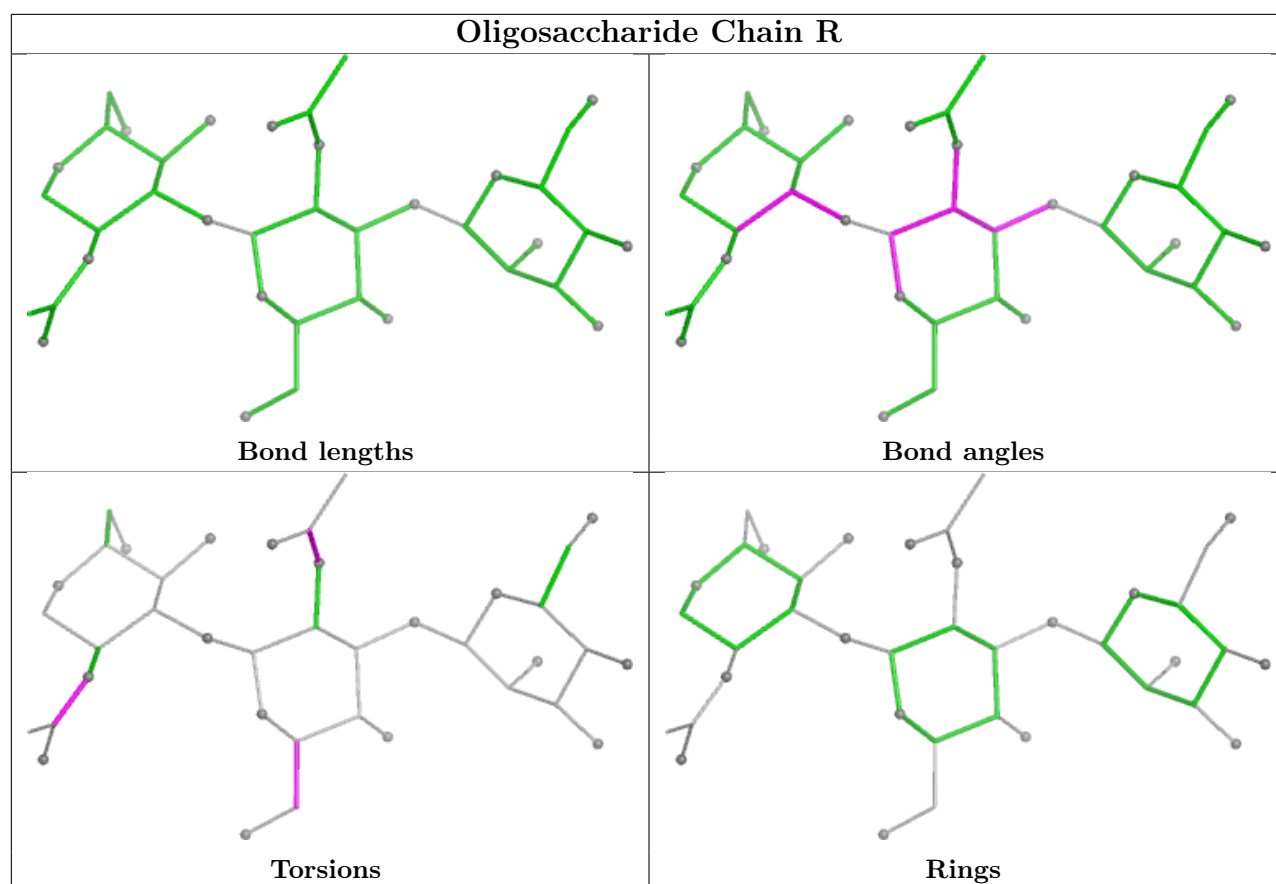
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	2	NAG	2	0
7	R	3	BMA	2	0
6	Q	1	NAG	3	0
7	R	2	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
8	NAG	E	501	3	14,14,15	0.22	0	17,19,21	0.45	0
10	D10	B	504	-	9,9,9	0.18	0	8,8,8	0.10	0
8	NAG	B	503	2	14,14,15	0.22	0	17,19,21	0.49	0
8	NAG	C	501	1	14,14,15	0.28	0	17,19,21	1.26	1 (5%)
9	PX6	A	503	-	43,43,43	0.28	0	47,48,48	0.32	0
11	ABU	B	501	-	6,6,6	0.76	0	6,6,6	1.69	2 (33%)
11	ABU	D	501	-	6,6,6	0.76	0	6,6,6	1.66	2 (33%)
8	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	502	1	14,14,15	0.22	0	17,19,21	0.50	0
10	D10	E	502	-	9,9,9	0.17	0	8,8,8	0.10	0
10	D10	A	504	-	9,9,9	0.17	0	8,8,8	0.10	0
8	NAG	B	502	2	14,14,15	0.23	0	17,19,21	0.52	0
10	D10	D	503	-	9,9,9	0.17	0	8,8,8	0.11	0
8	NAG	D	502	2	14,14,15	0.21	0	17,19,21	0.49	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
8	NAG	E	501	3	-	0/6/23/26	0/1/1/1
10	D10	B	504	-	-	0/7/7/7	-
8	NAG	B	503	2	-	0/6/23/26	0/1/1/1
8	NAG	C	501	1	-	1/6/23/26	0/1/1/1
9	PX6	A	503	-	-	7/45/45/45	-
11	ABU	B	501	-	-	0/4/4/4	-
11	ABU	D	501	-	-	0/4/4/4	-
8	NAG	A	501	1	-	0/6/23/26	0/1/1/1
8	NAG	A	502	1	-	0/6/23/26	0/1/1/1
10	D10	E	502	-	-	0/7/7/7	-
10	D10	A	504	-	-	0/7/7/7	-
8	NAG	B	502	2	-	0/6/23/26	0/1/1/1
10	D10	D	503	-	-	0/7/7/7	-
8	NAG	D	502	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	NAG	C1-O5-C5	4.90	118.83	112.19
11	B	501	ABU	O-C-CG	-2.99	113.47	123.08
11	D	501	ABU	O-C-CG	-2.96	113.57	123.08
11	B	501	ABU	OXT-C-CG	2.82	123.09	114.03
11	D	501	ABU	OXT-C-CG	2.78	122.96	114.03

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

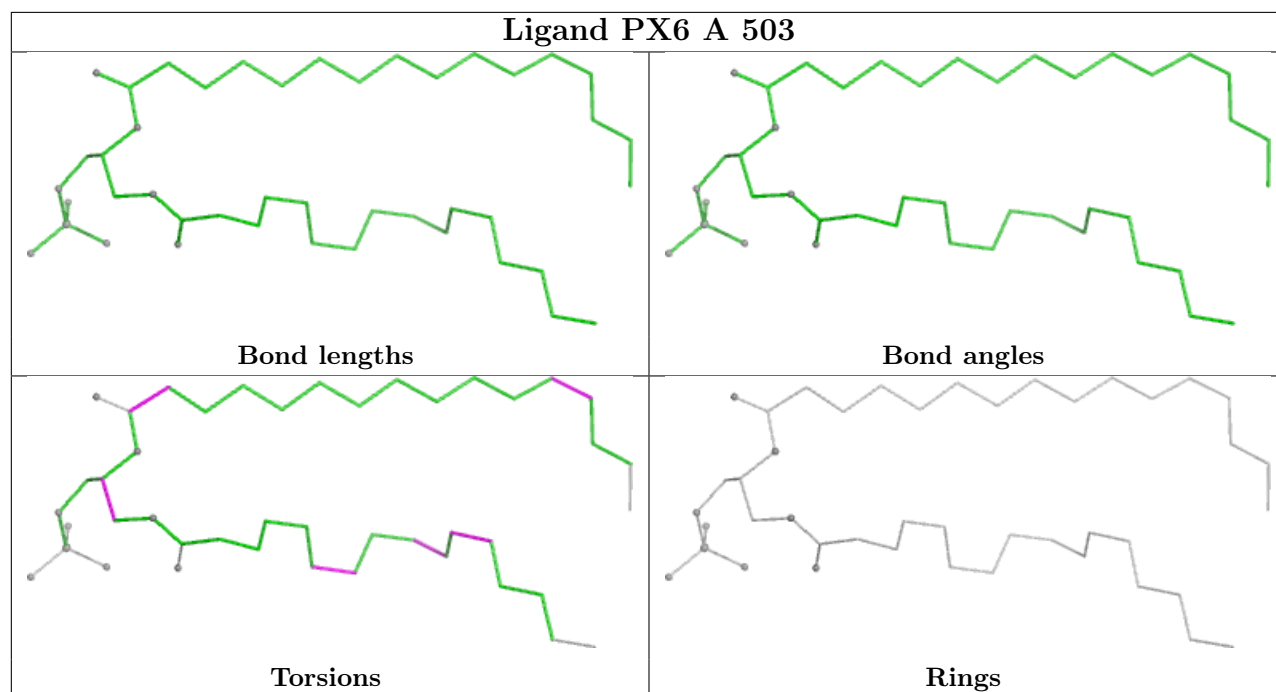
Mol	Chain	Res	Type	Atoms
8	C	501	NAG	O5-C5-C6-O6
9	A	503	PX6	C11-C10-C9-C8
9	A	503	PX6	O7-C2-C3-O5
9	A	503	PX6	C1-C2-C3-O5
9	A	503	PX6	C13-C14-C15-C16

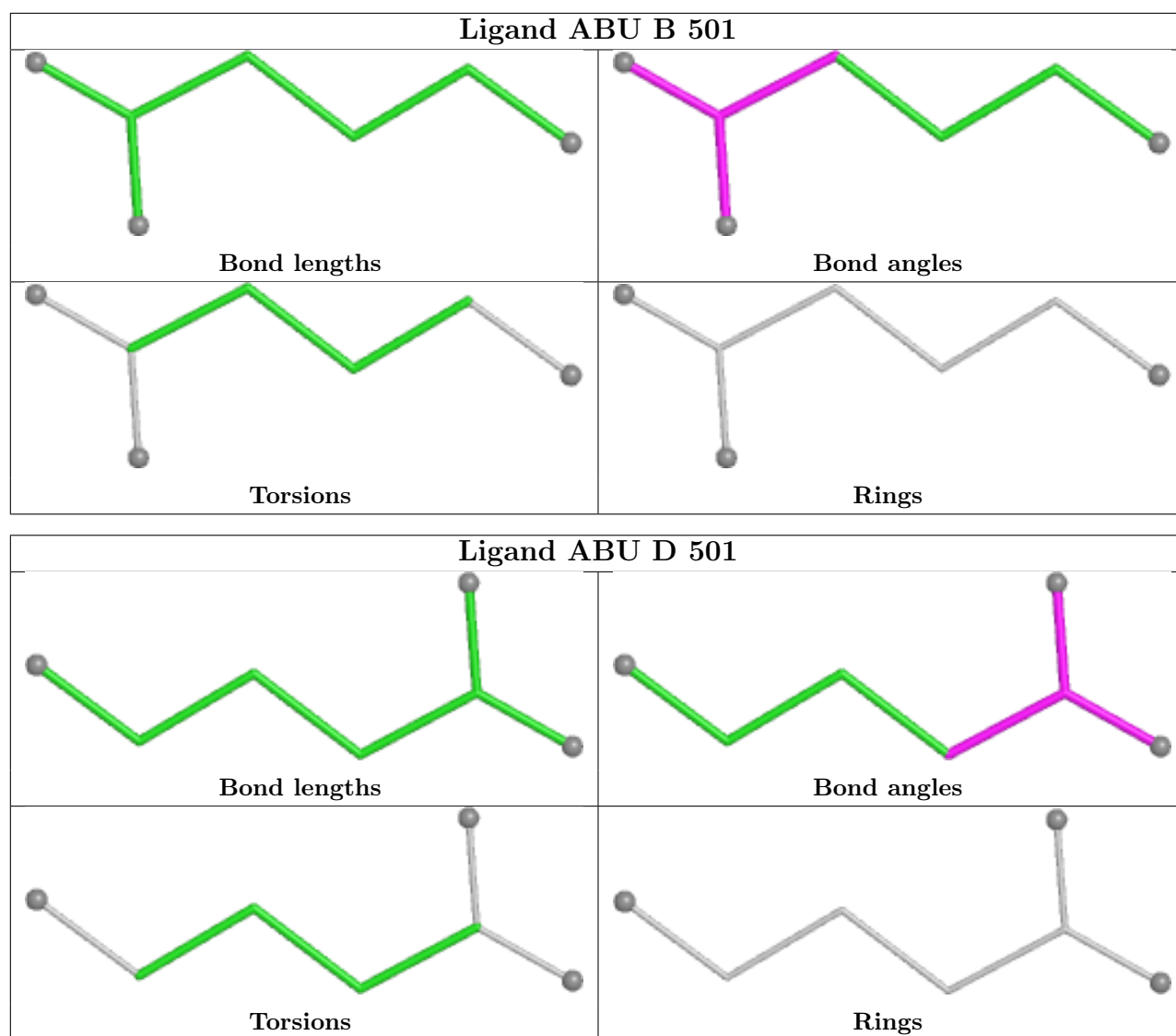
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	501	NAG	1	0
9	A	503	PX6	13	0
10	E	502	D10	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.

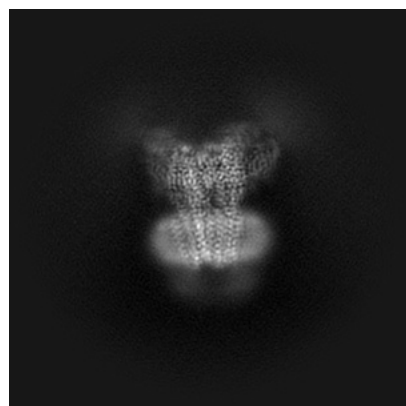
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54981. These allow visual inspection of the internal detail of the map and identification of artifacts.

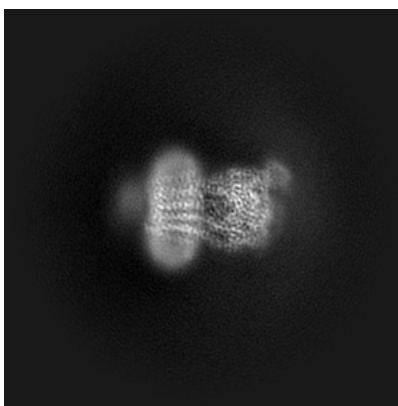
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

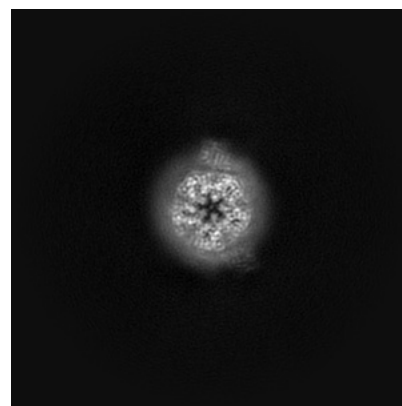
6.1.1 Primary map



X

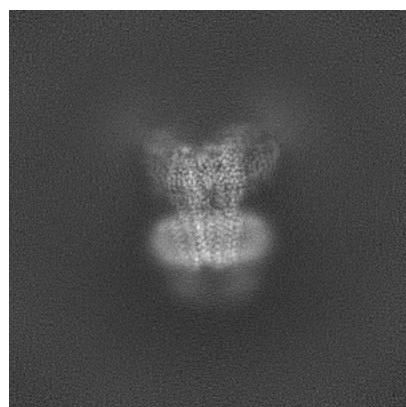


Y

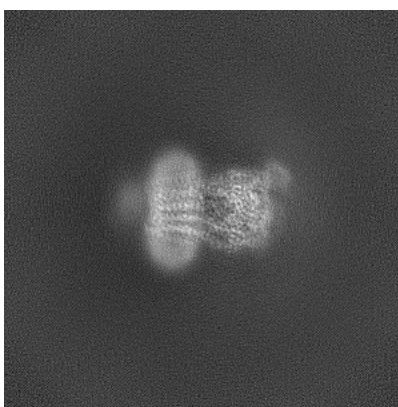


Z

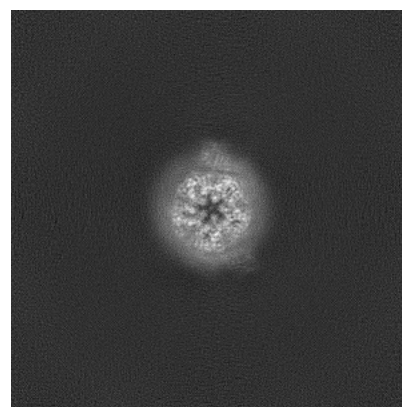
6.1.2 Raw map



X



Y

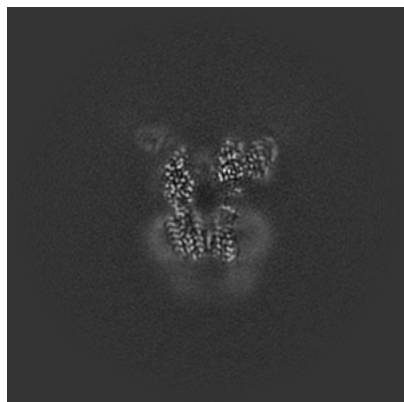


Z

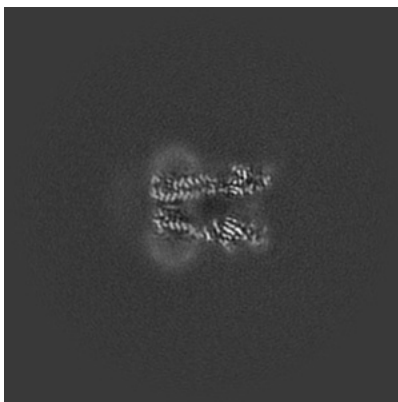
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

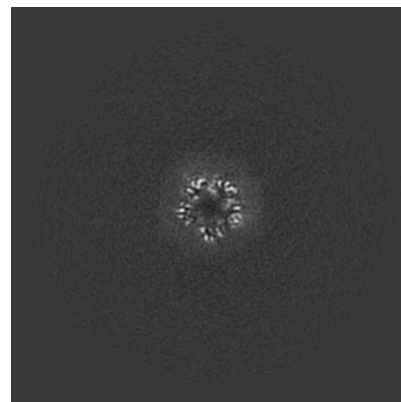
6.2.1 Primary map



X Index: 240

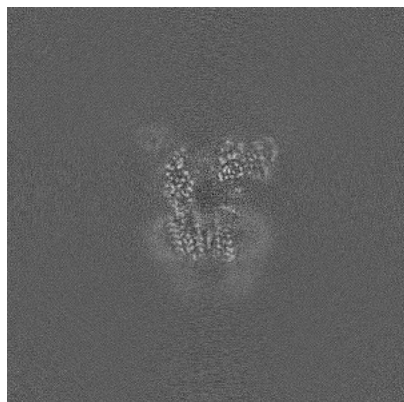


Y Index: 240



Z Index: 240

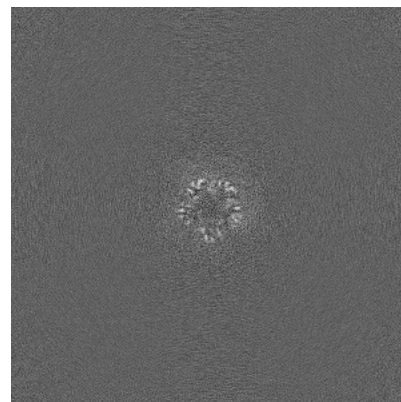
6.2.2 Raw map



X Index: 240



Y Index: 240

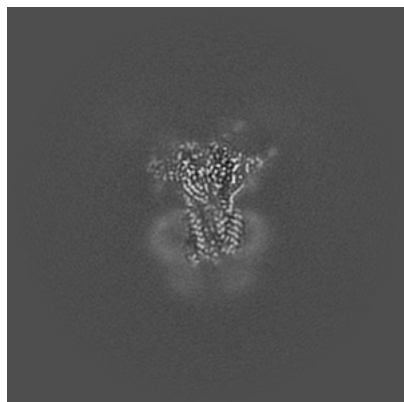


Z Index: 240

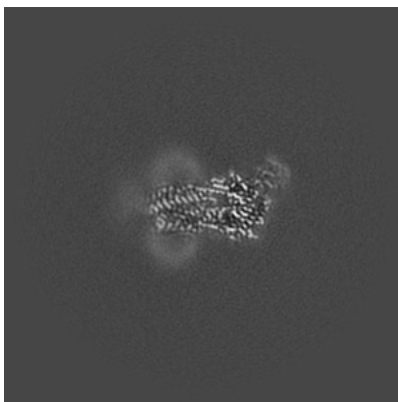
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

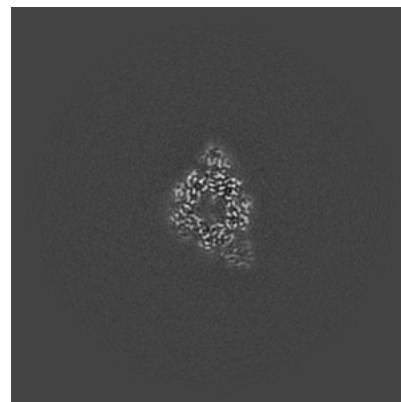
6.3.1 Primary map



X Index: 260

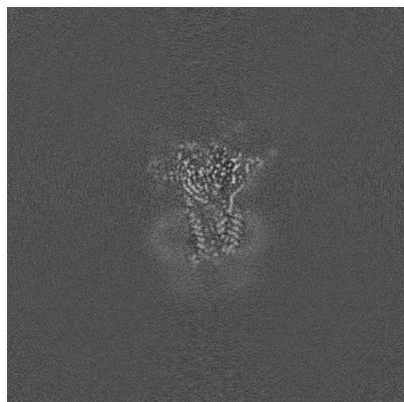


Y Index: 268

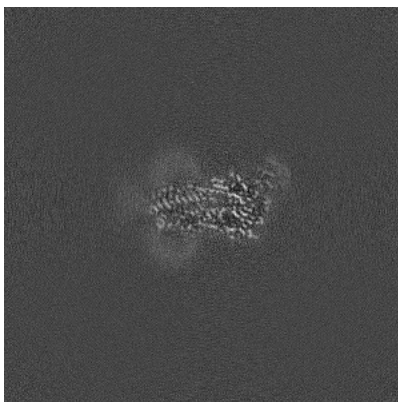


Z Index: 282

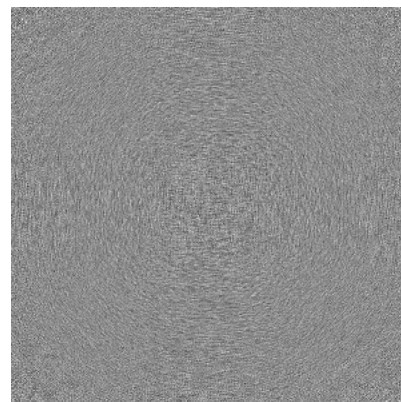
6.3.2 Raw map



X Index: 260



Y Index: 268

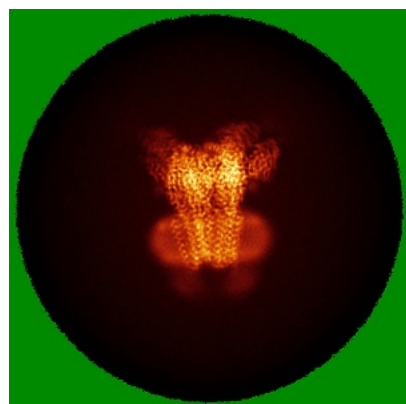


Z Index: 0

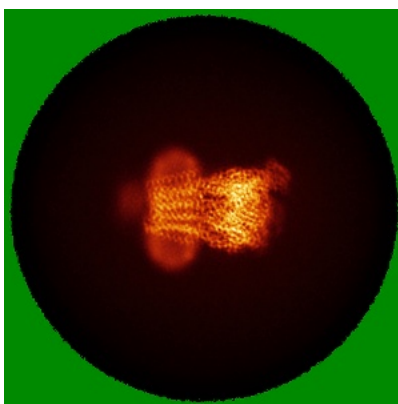
The images above show the largest variance slices of the map in three orthogonal directions.

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

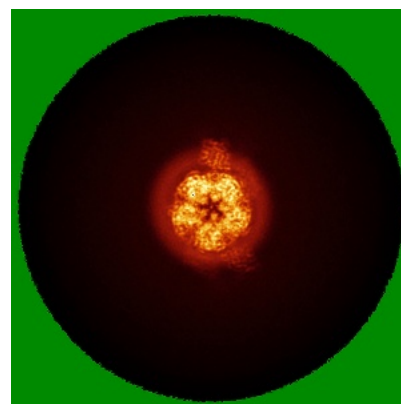
6.4.1 Primary map



X

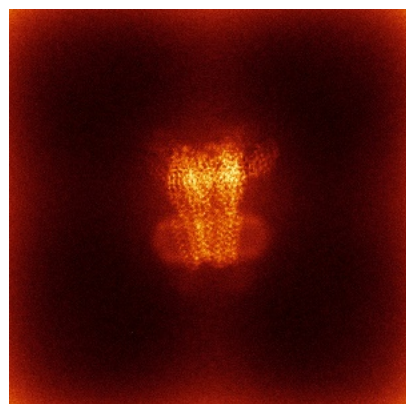


Y

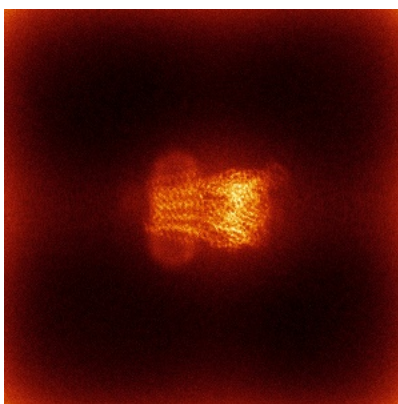


Z

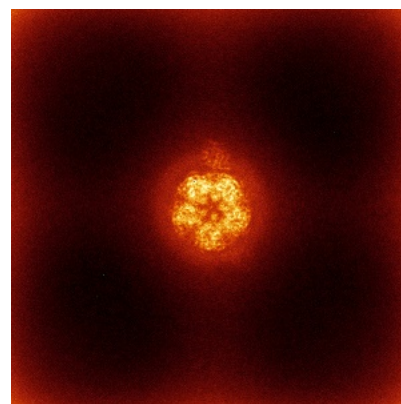
6.4.2 Raw map



X



Y

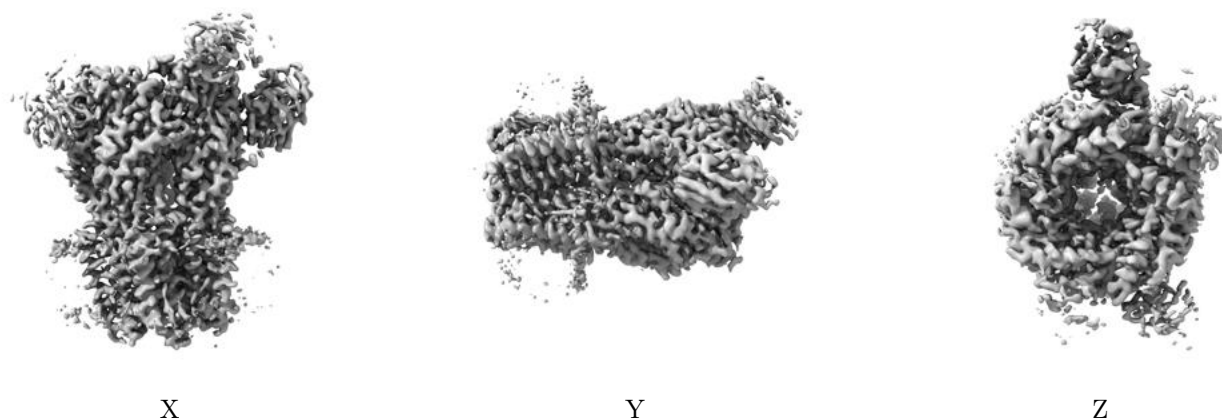


Z

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

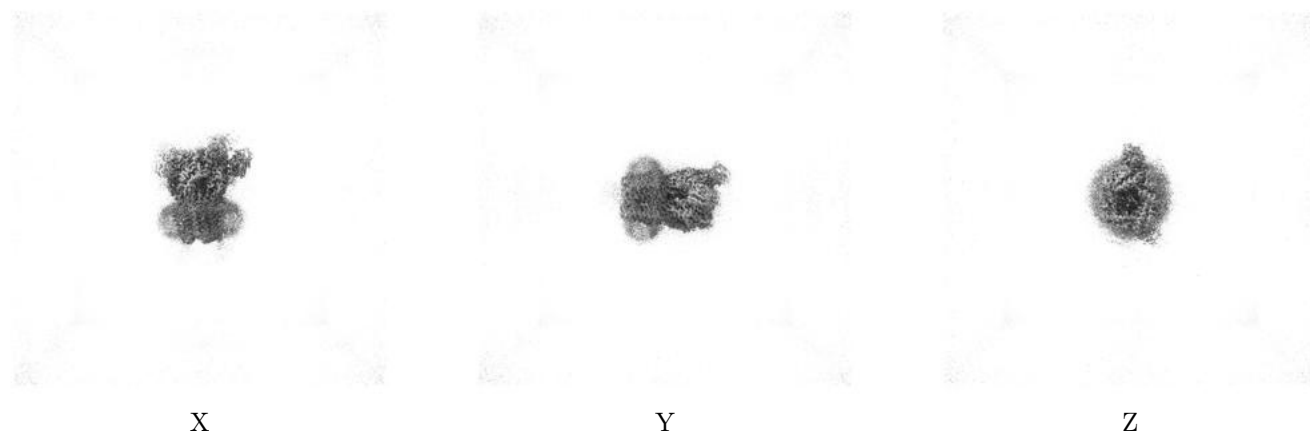
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0754. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

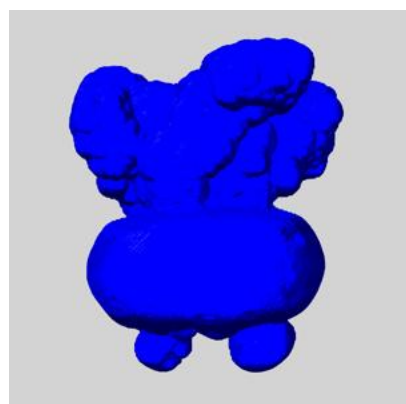
6.6 Mask visualisation [i](#)

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

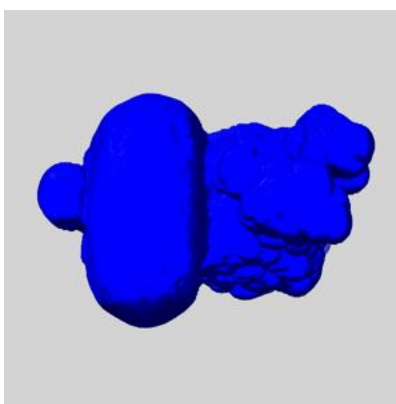
A mask typically either:

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

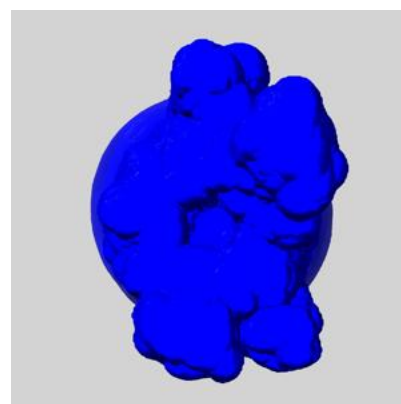
6.6.1 emd_54981_msk_1.map [i](#)



X



Y

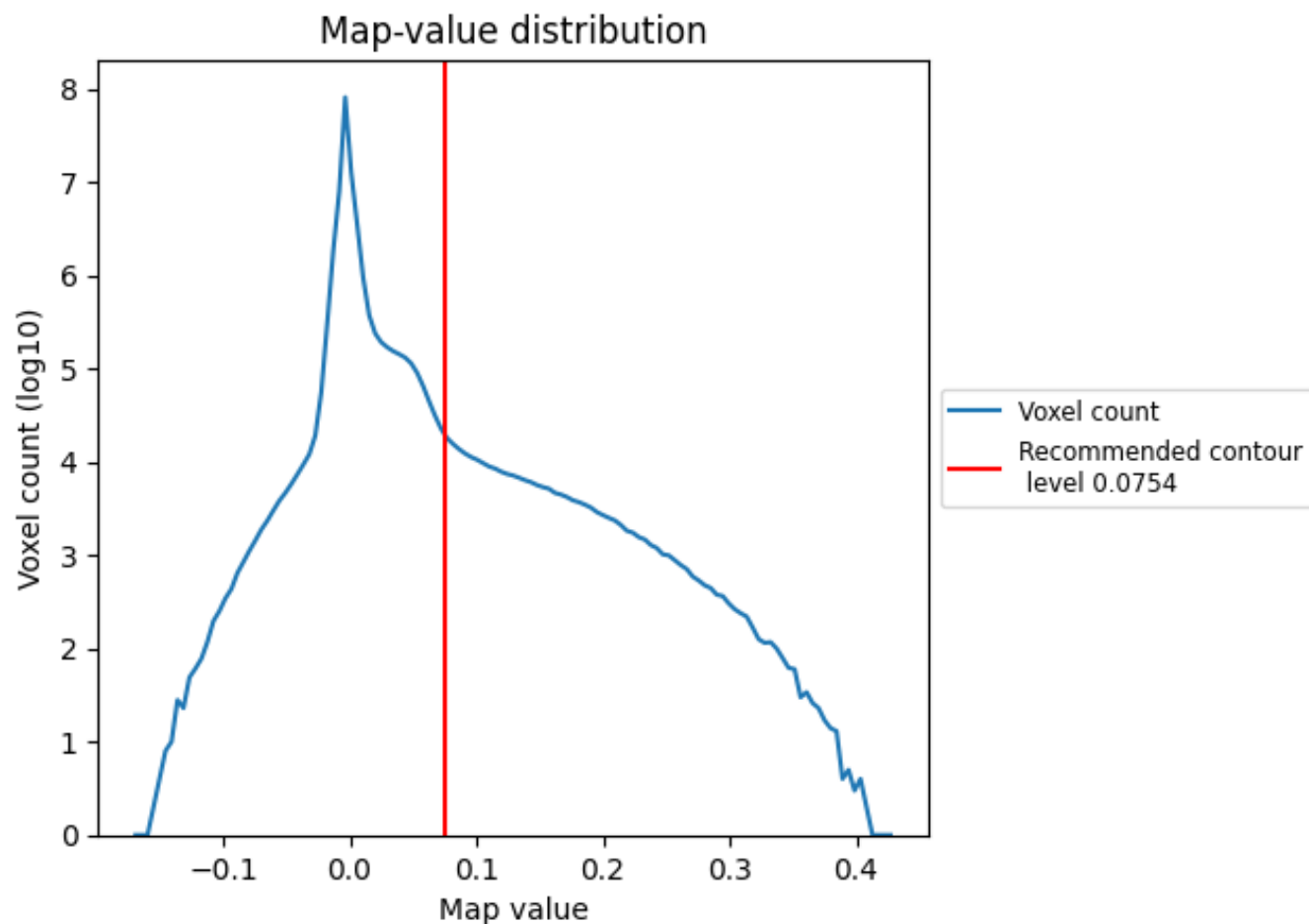


Z

7 Map analysis [i](#)

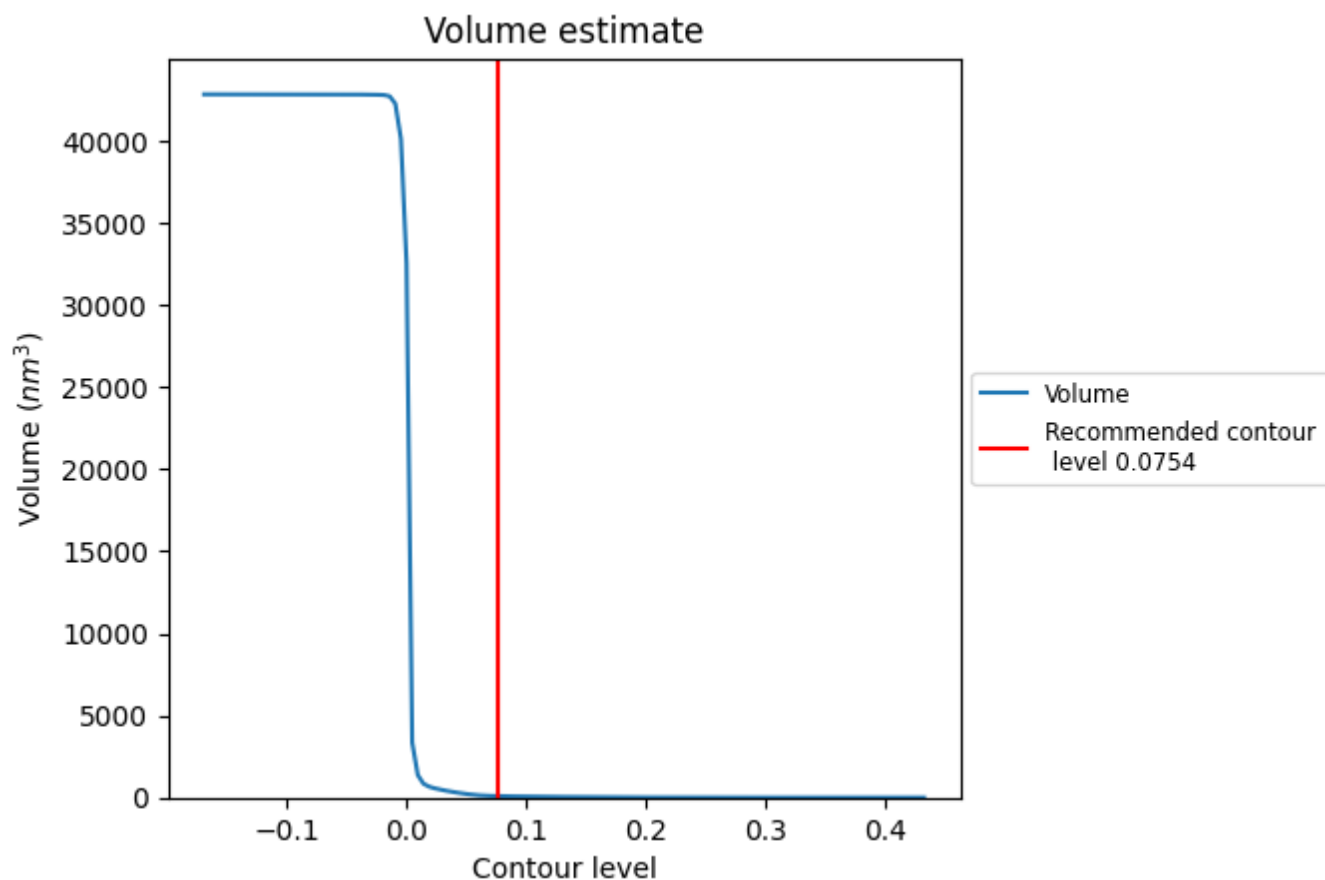
This section contains the results of statistical analysis of the map.

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.

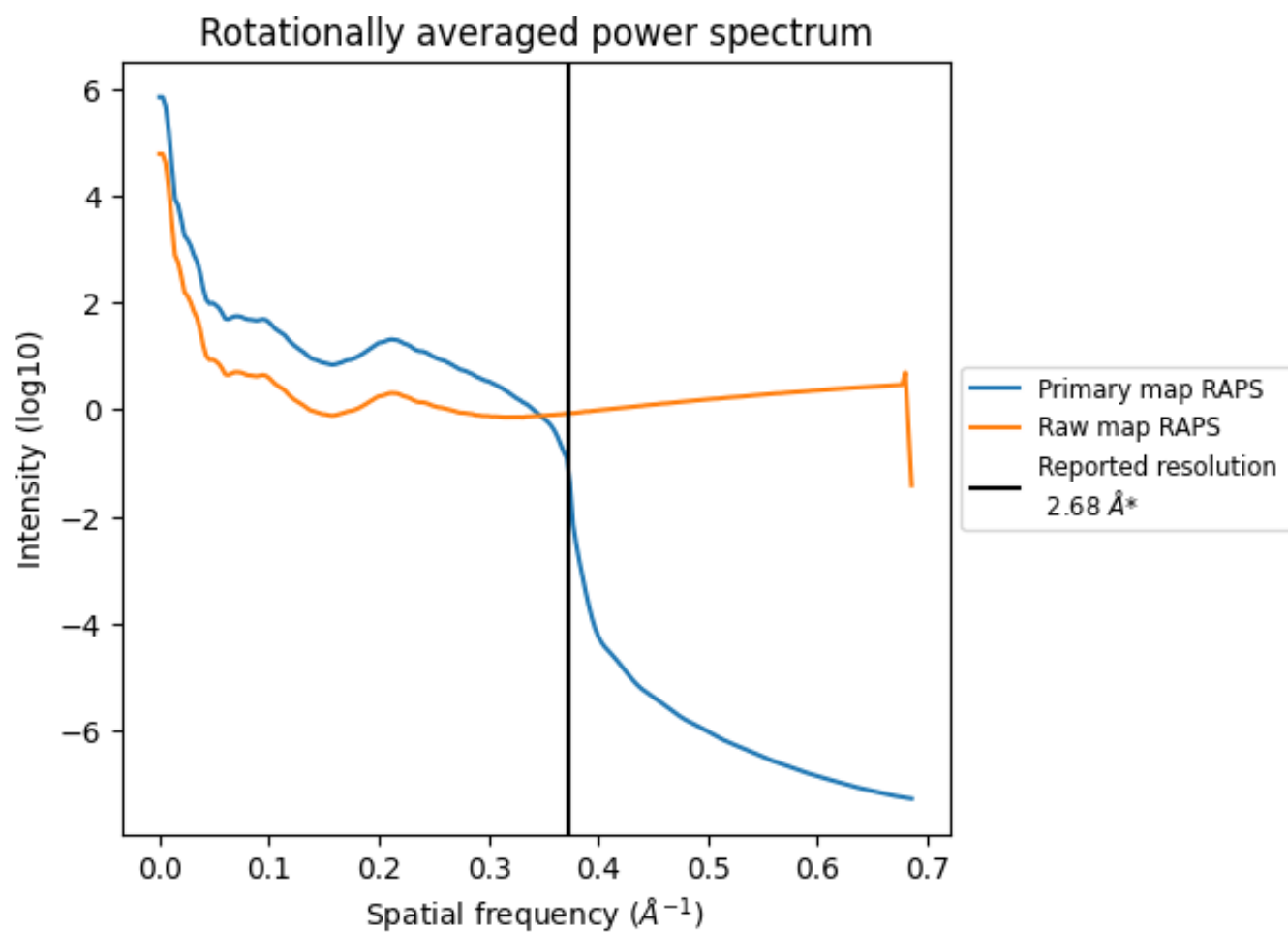
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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 ⓘ

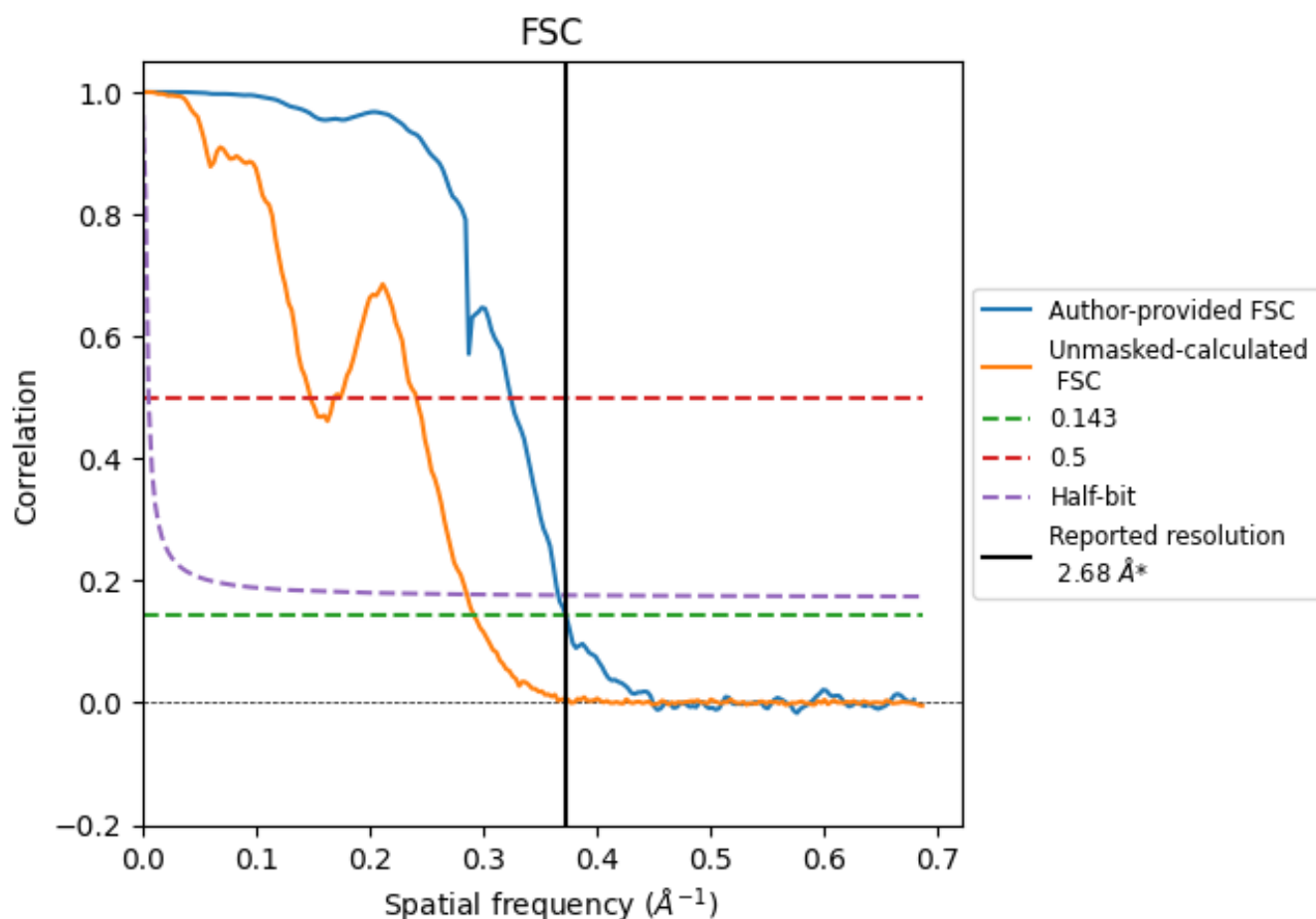


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

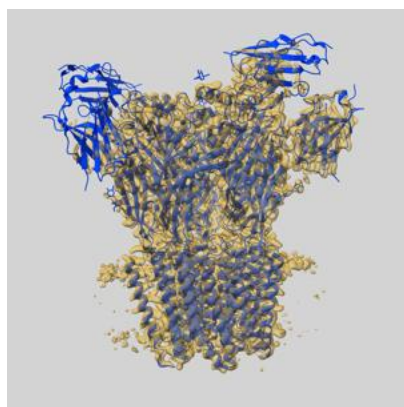
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.09	2.73
Unmasked-calculated*	3.43	6.76	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.68 by more than 10 %

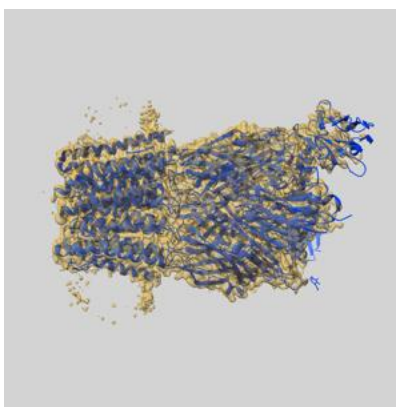
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54981 and PDB model 9SL1. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

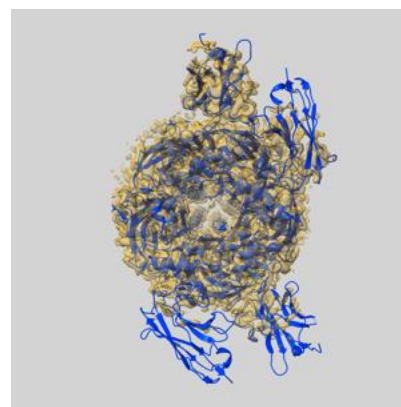
9.1 Map-model overlay [i](#)



X



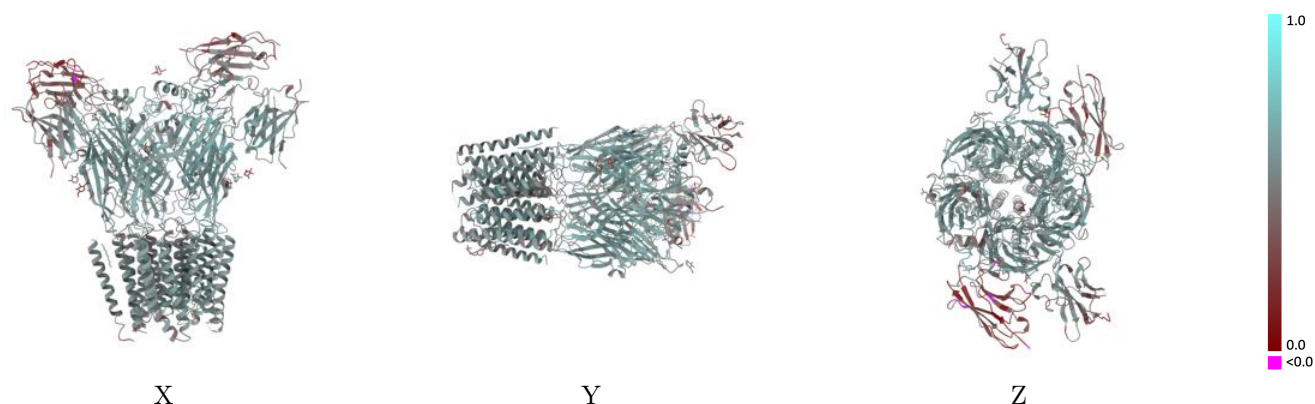
Y



Z

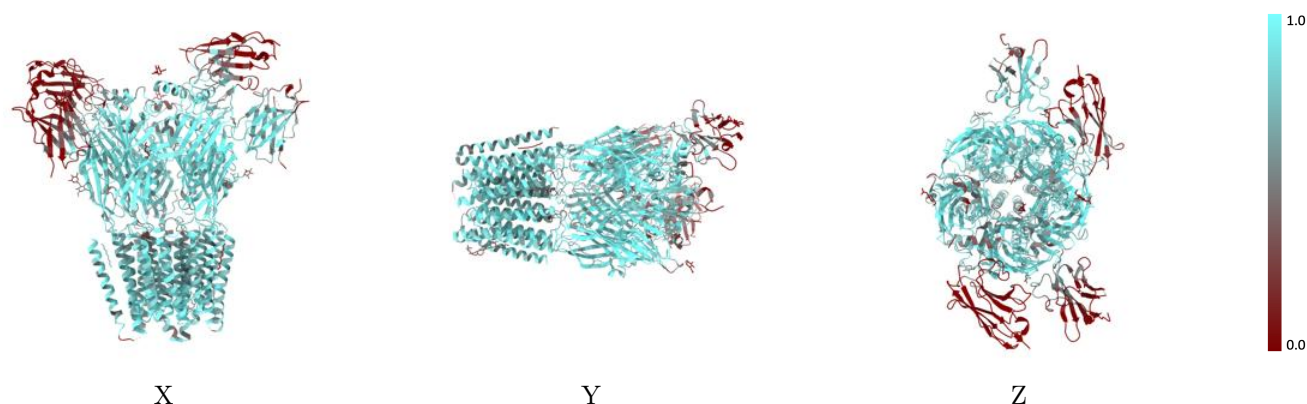
The images above show the 3D surface view of the map at the recommended contour level 0.0754 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



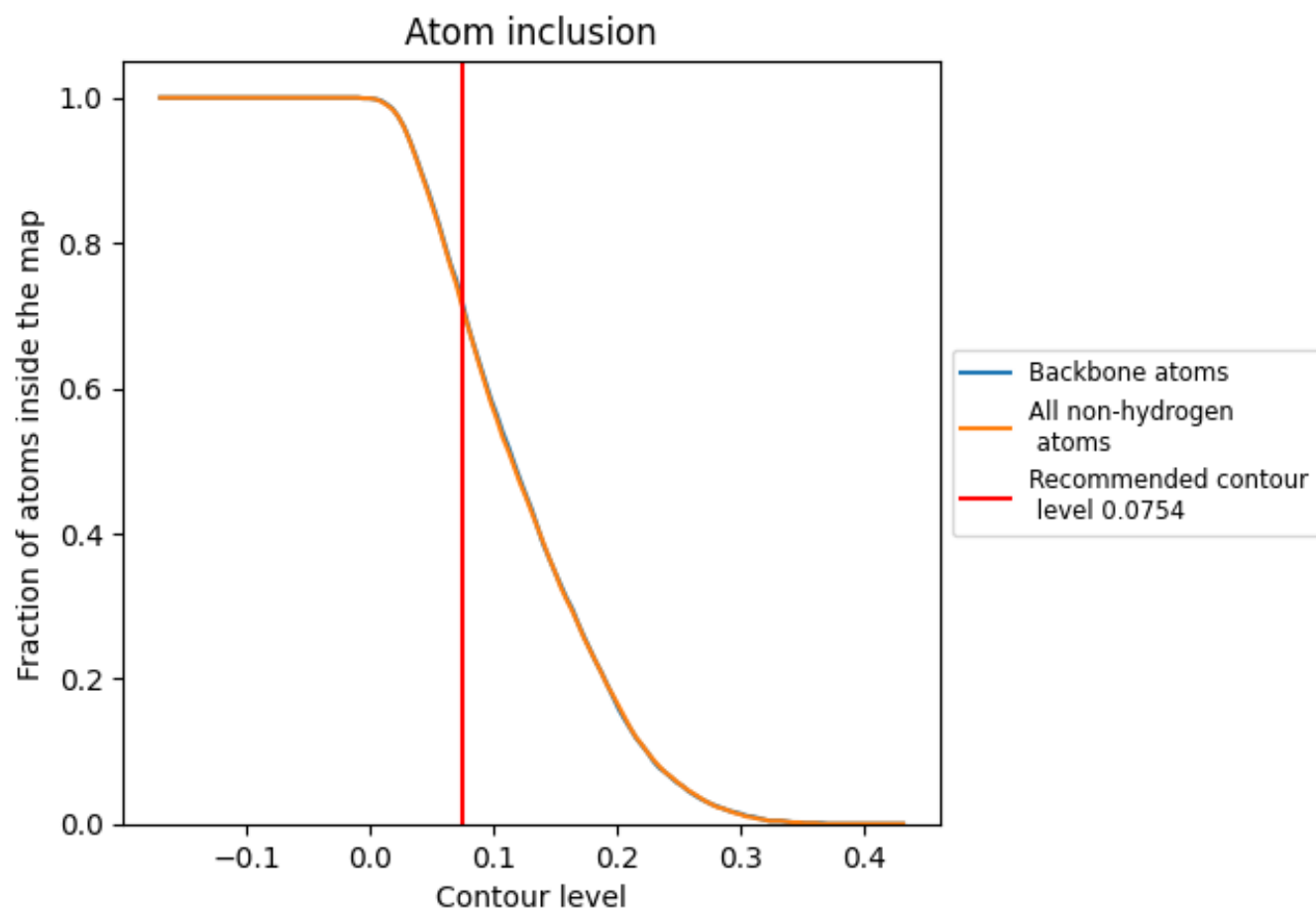
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0754).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.0754) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.5320
A	0.8650	0.5710
B	0.8590	0.5780
C	0.8240	0.5610
D	0.8160	0.5530
E	0.8160	0.5470
F	0.6660	0.5350
G	0.3250	0.4290
H	0.2490	0.4690
I	0.0500	0.2810
Q	0.5640	0.2800
R	0.4870	0.2860

1.0
0.0
<0.0