



Full wwPDB EM Validation Report ⓘ

Jun 13, 2026 – 02:18 PM EDT

PDB ID : 9OBZ / pdb_00009obz
EMDB ID : EMD-70304
Title : Ca²⁺-bound GluN1a/2B NMDAR (S2)
Authors : Steigerwald, R.; Furukawa, H.
Deposited on : 2025-04-23
Resolution : 2.81 Å(reported)

This is a Full wwPDB EM Validation 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

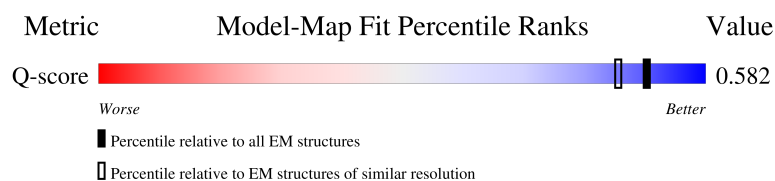
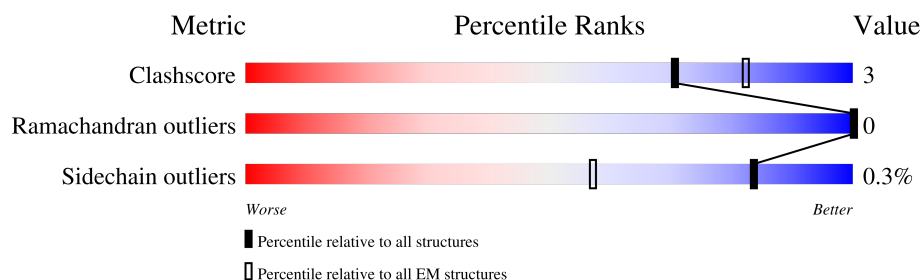
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

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	847	
1	C	847	
2	B	862	
2	D	862	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4172 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	126	Total	C	N	O	S	0	0
			930	621	143	159	7		
1	C	126	Total	C	N	O	S	0	0
			930	621	143	159	7		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	239	ASP	ASN	conflict	UNP P35439
A	350	GLN	ASN	conflict	UNP P35439
A	471	GLN	ASN	conflict	UNP P35439
A	491	GLN	ASN	conflict	UNP P35439
A	771	GLN	ASN	conflict	UNP P35439
A	844	ASN	ARG	conflict	UNP P35439
A	845	GLY	ARG	conflict	UNP P35439
A	846	ALA	LYS	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	239	ASP	ASN	conflict	UNP P35439
C	350	GLN	ASN	conflict	UNP P35439
C	471	GLN	ASN	conflict	UNP P35439
C	491	GLN	ASN	conflict	UNP P35439
C	771	GLN	ASN	conflict	UNP P35439
C	844	ASN	ARG	conflict	UNP P35439
C	845	GLY	ARG	conflict	UNP P35439
C	846	ALA	LYS	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	134	Total	C	N	O	S	0	0
			1005	674	151	171	9		
2	D	134	Total	C	N	O	S	0	0
			1005	674	151	171	9		

There are 74 discrepancies between the modelled and reference sequences:

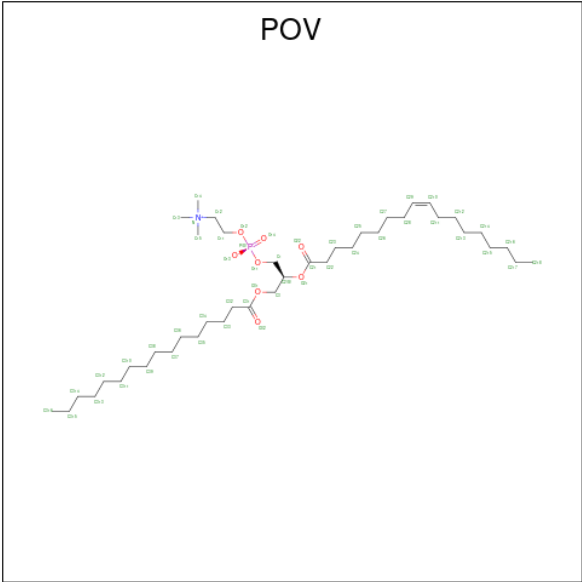
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960

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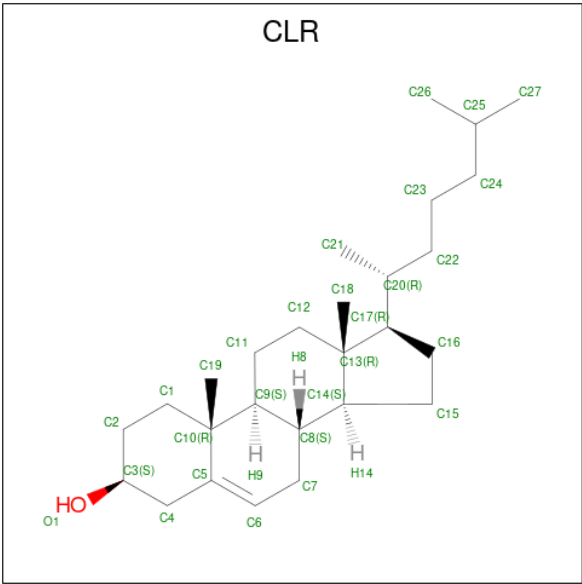
Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	

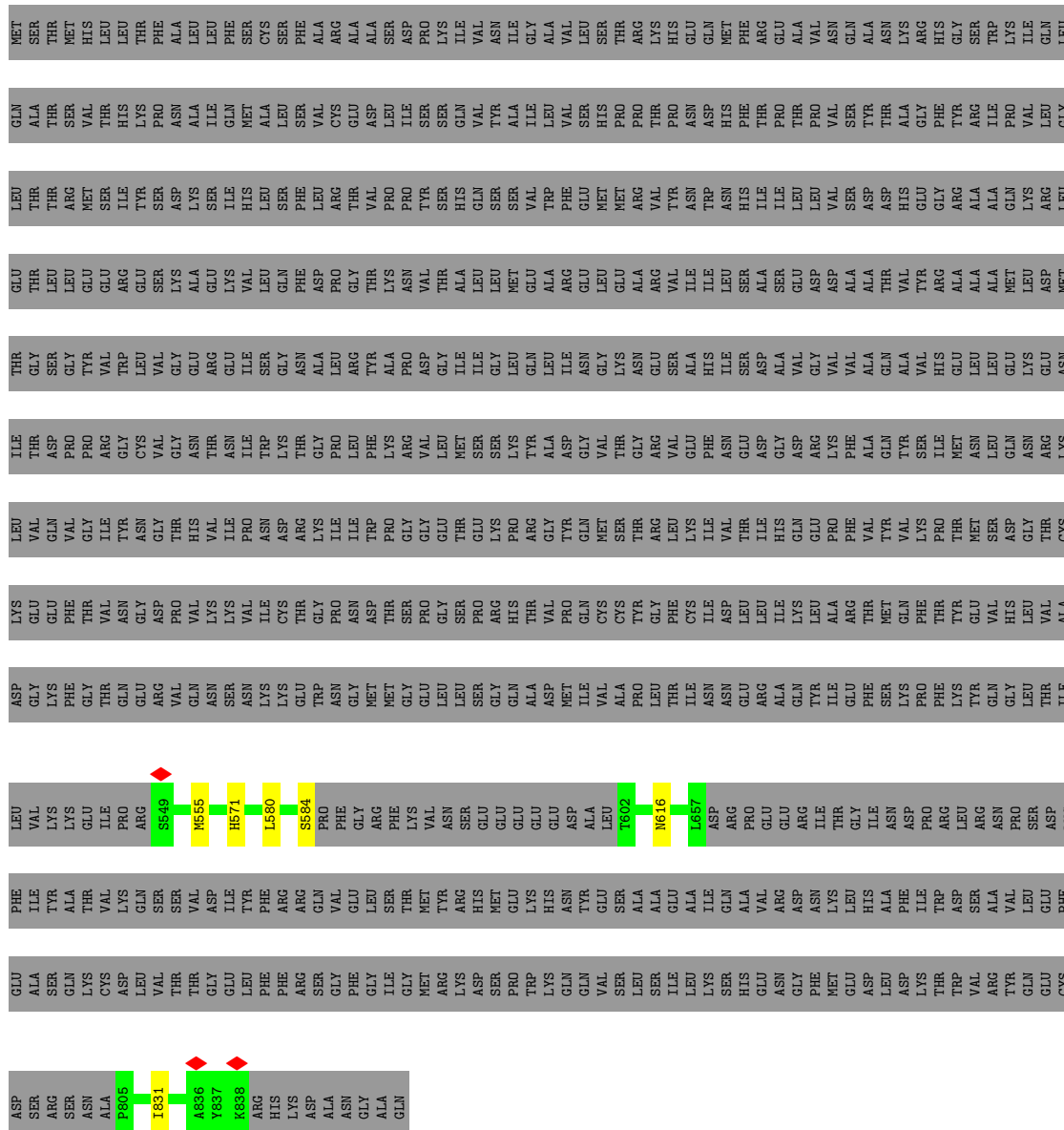
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Ca	0
			1	1	

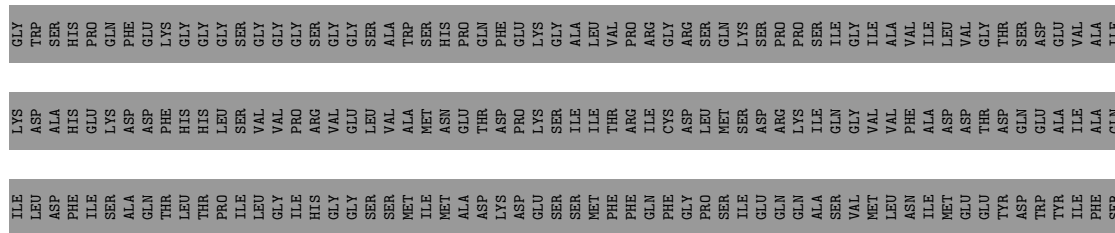
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	6	Total	O	0
			6	6	
6	B	13	Total	O	0
			13	13	
6	C	6	Total	O	0
			6	6	
6	D	12	Total	O	0
			12	12	

Chain C: 14% . 85%



Chain B: 15% . 84%





LEU	GLN	THR	LYS	ASP	SER
LEU	THR	THR	GLY	THR	VAL
PHE	GLY	ILE	SER	PHE	LYS
GLY	LEU	VAL	ASP	THR	THR
ASP	GLY	MET	VAL	ASP	LEU
GLY	ALA	ASP	SER	THR	LEU
MET	PHE	LYS	SER	TYR	THR
GLU	ILE	LYS	ARG	VAL	VAL
LEU	GLU	TYR	SER	THR	THR
LEU	ALA	ASP	GLN	GLY	ASN
ALA	ALA	PRO	ARG	GLY	GLY
VAL	VAL	ASN	ASP	VAL	LYS
LEU	LEU	ASN	PHE	HIS	LYS
THR	THR	ASN	THR	GLY	GLY
GLY	THR	SER	THR	GLY	LYS
ILE	MET	PRO	PRO	LYS	LYS
ALA	ALA	PRO	PRO	ILE	ILE
GLY	GLY	PHE	PHE	ASN	ASN
ASP	ASP	PHE	PHE	THR	THR
GLU	GLU	GLY	GLY	THR	TRP
LYS	LYS	CYS	VAL	VAL	ASN
ASN	LYS	LYS	PRO	ASN	GLY
GLU	GLU	LEU	ASN	PRO	GLY
V808	THR	VAL	GLY	THR	ILE
Y843	ILE	GLY	THR	GLY	GLY
W844	THR	THR	SER	THR	GLY
Q845	ILE	ILE	GLY	ASN	VAL
PHE	GLY	SER	GLY	ARG	VAL
ARG	GLY	GLY	LYS	ASN	MET
HIS	THR	THR	ALA	TYR	ALA
SER	SER	SER	ALA	GLY	GLY
PHE	PHE	ASP	THR	ARG	GLY
MET	MET	ASP	GLN	PHE	GLY
GLY	GLY	GLY	ASP	ASN	THR
	ILE	ALA	LYS	ALA	LEU
	ILE	ILE	GLN	MET	TYR
	LYS	GLY	LYS	GLY	VAL
	SER	SER	ASP	LYS	ASP
	THR	THR	GLY	S617	PHE
	GLY	GLY	THR	V620	SER
	ILE	ILE	ALA	PE98	GLU
	ALA	ALA	TYR	L609	ARG
	ILE	ILE	MET	L609	GLY
	GLN	GLN	GLY	GLY	ASN
	LYS	LYS	LYS	N616	THR
	ASP	ASP	PHE	S617	GLY
	SER	SER	ASN	V620	SER
	GLY	GLY	GLN	GLY	THR
	THR	THR	ARG	ARG	ILE
	LYS	LYS	VAL	VAL	VAL
	ARG	ARG	VAL	KG29	ASP
	GLN	GLN	ASP	N649	PHE
	VAL	VAL	ASP	N649	SER
	ASP	ASP	ALA	PE57	VAL
	LEU	LEU	LEU	PE57	PRO
	ALA	ALA	TYR	GLU	PHE
	ILE	ILE	VAL	VAL	ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116195	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 ($e^-/\text{\AA}^2$)	58.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.697	Depositor
Minimum map value	-0.370	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: CA, CLR, POV

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	0.23	0/951	0.32	0/1294
1	C	0.24	0/951	0.33	0/1294
2	B	0.10	0/1031	0.24	0/1405
2	D	0.10	0/1031	0.24	0/1405
All	All	0.18	0/3964	0.29	0/5398

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	930	0	933	5	0
1	C	930	0	933	6	0
2	B	1005	0	984	8	0
2	D	1005	0	984	12	0
3	A	104	0	164	3	0
3	B	52	0	82	4	0
3	C	52	0	82	1	0
4	B	28	0	46	0	0
4	D	28	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	6	0	0	0	0
6	B	13	0	0	3	0
6	C	6	0	0	0	0
6	D	12	0	0	4	0
All	All	4172	0	4254	29	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 3.

All (29) 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:B:616:ASN:HB2	6:B:1008:HOH:O	1.71	0.90
2:D:620:VAL:HG21	6:D:1011:HOH:O	1.80	0.82
2:B:620:VAL:HG21	6:B:1013:HOH:O	1.79	0.81
2:B:617:SER:HA	6:B:1004:HOH:O	1.84	0.77
2:D:617:SER:HA	6:D:1004:HOH:O	1.87	0.75
1:A:655:LEU:HD13	2:D:649:ASN:HD22	1.54	0.73
2:D:616:ASN:HB2	6:D:1008:HOH:O	1.93	0.68
2:D:620:VAL:CG2	6:D:1011:HOH:O	2.41	0.66
1:C:616:ASN:ND2	2:D:617:SER:OG	2.32	0.61
1:A:616:ASN:ND2	2:B:617:SER:OG	2.33	0.60
1:A:831:ILE:HD12	2:D:576:VAL:HG13	1.84	0.58
1:C:580:LEU:O	1:C:584:SER:OG	2.28	0.52
1:A:819:LEU:HD23	3:A:901:POV:H36A	1.92	0.50
2:D:553:PRO:HB3	2:D:649:ASN:HB3	1.93	0.50
3:B:903:POV:H39	1:C:571:HIS:HE1	1.78	0.47
2:B:627:THR:HG21	1:C:831:ILE:HB	1.98	0.45
2:B:616:ASN:OD1	2:B:616:ASN:N	2.52	0.43
3:B:903:POV:H36	3:B:903:POV:H33	1.71	0.43
1:A:619:ILE:HG22	2:D:629:LYS:HE3	2.01	0.43
2:D:570:SER:HB3	2:D:609:LEU:HD12	2.00	0.43
2:D:616:ASN:OD1	2:D:616:ASN:N	2.52	0.42
3:C:901:POV:H15B	3:C:901:POV:H11A	1.91	0.42
3:B:903:POV:H39	1:C:571:HIS:CE1	2.54	0.42
2:B:547:PRO:HB3	2:B:820:GLY:H	1.85	0.42
2:D:550:PHE:CD2	2:D:551:LEU:HG	2.55	0.42
3:B:903:POV:H218	1:C:555:MET:HE3	2.02	0.41
3:A:901:POV:H210	3:A:902:POV:H216	2.02	0.41
3:A:901:POV:H15B	3:A:901:POV:H11A	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:LEU:HA	2:B:620:VAL:HG11	2.02	0.40

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	120/847 (14%)	120 (100%)	0	0	100	100
1	C	120/847 (14%)	118 (98%)	2 (2%)	0	100	100
2	B	128/862 (15%)	124 (97%)	4 (3%)	0	100	100
2	D	128/862 (15%)	122 (95%)	6 (5%)	0	100	100
All	All	496/3418 (14%)	484 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	94/728 (13%)	94 (100%)	0	100	100
1	C	94/728 (13%)	94 (100%)	0	100	100
2	B	103/745 (14%)	102 (99%)	1 (1%)	68	88
2	D	103/745 (14%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	394/2946 (13%)	393 (100%)	1 (0%)	84	95

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

Mol	Chain	Res	Type
2	B	620	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	GLN
1	A	616	ASN
2	B	621	GLN
2	B	622	ASN
2	B	656	GLN
1	C	556	GLN
1	C	616	ASN
2	D	621	GLN
2	D	649	ASN
2	D	656	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CLR	D	901	-	31,31,31	0.37	0	48,48,48	0.47	0
3	POV	A	901	-	51,51,51	0.50	0	57,59,59	0.45	0
4	CLR	B	901	-	31,31,31	0.37	0	48,48,48	0.45	0
3	POV	B	903	-	51,51,51	0.50	0	57,59,59	0.45	0
3	POV	C	901	-	51,51,51	0.50	0	57,59,59	0.45	0
3	POV	A	902	-	51,51,51	0.50	0	57,59,59	0.45	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
4	CLR	D	901	-	-	9/10/68/68	0/4/4/4
3	POV	A	901	-	-	17/55/55/55	-
4	CLR	B	901	-	-	9/10/68/68	0/4/4/4
3	POV	B	903	-	-	22/55/55/55	-
3	POV	C	901	-	-	20/55/55/55	-
3	POV	A	902	-	-	23/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O14
3	A	901	POV	O12-C11-C12-N
3	A	902	POV	C1-O11-P-O12
3	A	902	POV	C1-O11-P-O13
3	A	902	POV	O22-C21-O21-C2
3	B	903	POV	C1-O11-P-O12
3	B	903	POV	C1-O11-P-O13
3	B	903	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
3	B	903	POV	C11-O12-P-O11
3	B	903	POV	C11-O12-P-O13
3	B	903	POV	C11-O12-P-O14
3	B	903	POV	O22-C21-O21-C2
3	C	901	POV	C1-O11-P-O14
3	C	901	POV	O12-C11-C12-N
3	A	902	POV	C22-C21-O21-C2
3	B	903	POV	C22-C21-O21-C2
4	D	901	CLR	C16-C17-C20-C21
4	D	901	CLR	C13-C17-C20-C22
4	D	901	CLR	C13-C17-C20-C21
4	D	901	CLR	C17-C20-C22-C23
4	B	901	CLR	C21-C20-C22-C23
4	B	901	CLR	C17-C20-C22-C23
4	D	901	CLR	C21-C20-C22-C23
3	B	903	POV	C21-C22-C23-C24
4	D	901	CLR	C16-C17-C20-C22
3	C	901	POV	C311-C312-C313-C314
3	B	903	POV	C34-C35-C36-C37
4	B	901	CLR	C13-C17-C20-C22
3	A	901	POV	C311-C312-C313-C314
3	A	902	POV	C34-C35-C36-C37
3	C	901	POV	C32-C33-C34-C35
3	A	902	POV	C25-C26-C27-C28
3	A	902	POV	C21-C22-C23-C24
3	B	903	POV	C25-C26-C27-C28
3	B	903	POV	C2-C1-O11-P
3	A	901	POV	C39-C310-C311-C312
3	A	901	POV	C32-C33-C34-C35
3	A	901	POV	C22-C21-O21-C2
4	B	901	CLR	C16-C17-C20-C21
3	B	903	POV	C26-C27-C28-C29
3	C	901	POV	C39-C310-C311-C312
3	C	901	POV	C25-C26-C27-C28
4	B	901	CLR	C13-C17-C20-C21
3	A	902	POV	C26-C27-C28-C29
3	A	901	POV	C25-C26-C27-C28
3	A	901	POV	C310-C311-C312-C313
3	B	903	POV	C312-C313-C314-C315
3	C	901	POV	C22-C21-O21-C2
3	A	902	POV	C311-C312-C313-C314
3	B	903	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	A	901	POV	C37-C38-C39-C310
3	A	902	POV	C2-C1-O11-P
4	B	901	CLR	C16-C17-C20-C22
3	A	902	POV	C33-C34-C35-C36
3	A	902	POV	C312-C313-C314-C315
3	C	901	POV	C37-C38-C39-C310
3	A	901	POV	O11-C1-C2-O21
3	C	901	POV	C310-C311-C312-C313
4	B	901	CLR	C23-C24-C25-C27
3	C	901	POV	O11-C1-C2-C3
3	A	901	POV	O22-C21-O21-C2
3	B	903	POV	C311-C312-C313-C314
3	C	901	POV	O22-C21-O21-C2
3	A	902	POV	O11-C1-C2-O21
3	B	903	POV	O11-C1-C2-O21
4	B	901	CLR	C23-C24-C25-C26
3	C	901	POV	C32-C31-O31-C3
3	A	902	POV	O11-C1-C2-C3
3	B	903	POV	O11-C1-C2-C3
3	C	901	POV	O11-C1-C2-O21
3	C	901	POV	O21-C2-C3-O31
3	C	901	POV	O32-C31-O31-C3
3	A	901	POV	C1-O11-P-O12
3	A	902	POV	C1-O11-P-O14
3	A	902	POV	C11-O12-P-O11
3	A	902	POV	C11-O12-P-O13
3	A	902	POV	C11-O12-P-O14
3	C	901	POV	C1-O11-P-O12
3	A	901	POV	O11-C1-C2-C3
4	D	901	CLR	C23-C24-C25-C27
4	D	901	CLR	C22-C23-C24-C25
4	B	901	CLR	C22-C23-C24-C25
3	A	902	POV	O21-C2-C3-O31
3	B	903	POV	C27-C28-C29-C210
3	A	901	POV	O32-C31-O31-C3
3	C	901	POV	C36-C37-C38-C39
3	A	901	POV	C32-C31-O31-C3
3	A	902	POV	C27-C28-C29-C210
3	C	901	POV	C1-C2-C3-O31
3	A	902	POV	C12-C11-O12-P
3	B	903	POV	C29-C210-C211-C212
4	D	901	CLR	C23-C24-C25-C26

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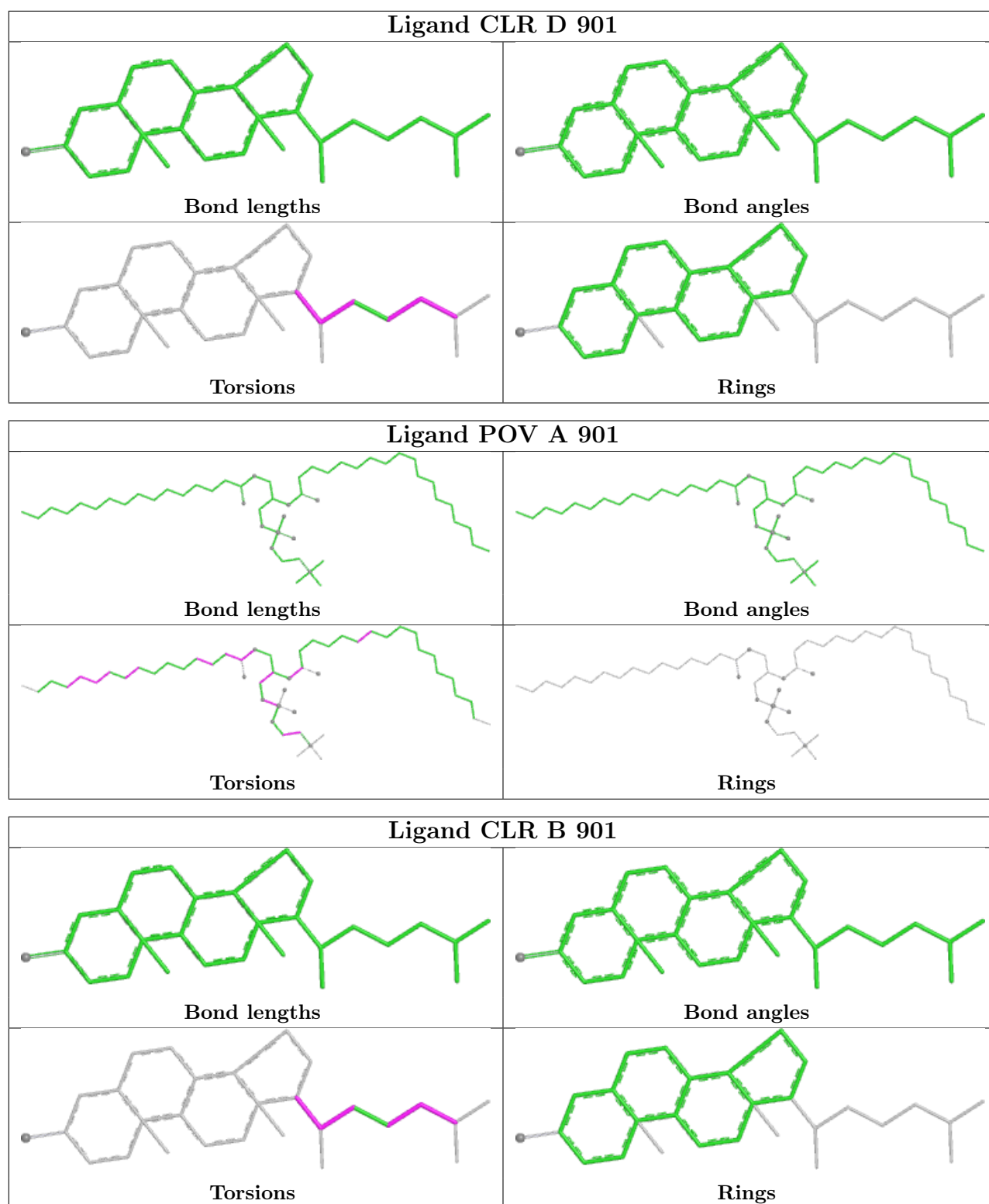
Mol	Chain	Res	Type	Atoms
3	C	901	POV	O31-C31-C32-C33
3	A	901	POV	O31-C31-C32-C33
3	B	903	POV	O31-C31-C32-C33
3	C	901	POV	O32-C31-C32-C33
3	A	902	POV	C35-C36-C37-C38
3	A	901	POV	O32-C31-C32-C33
3	A	902	POV	C29-C210-C211-C212
3	B	903	POV	O32-C31-C32-C33

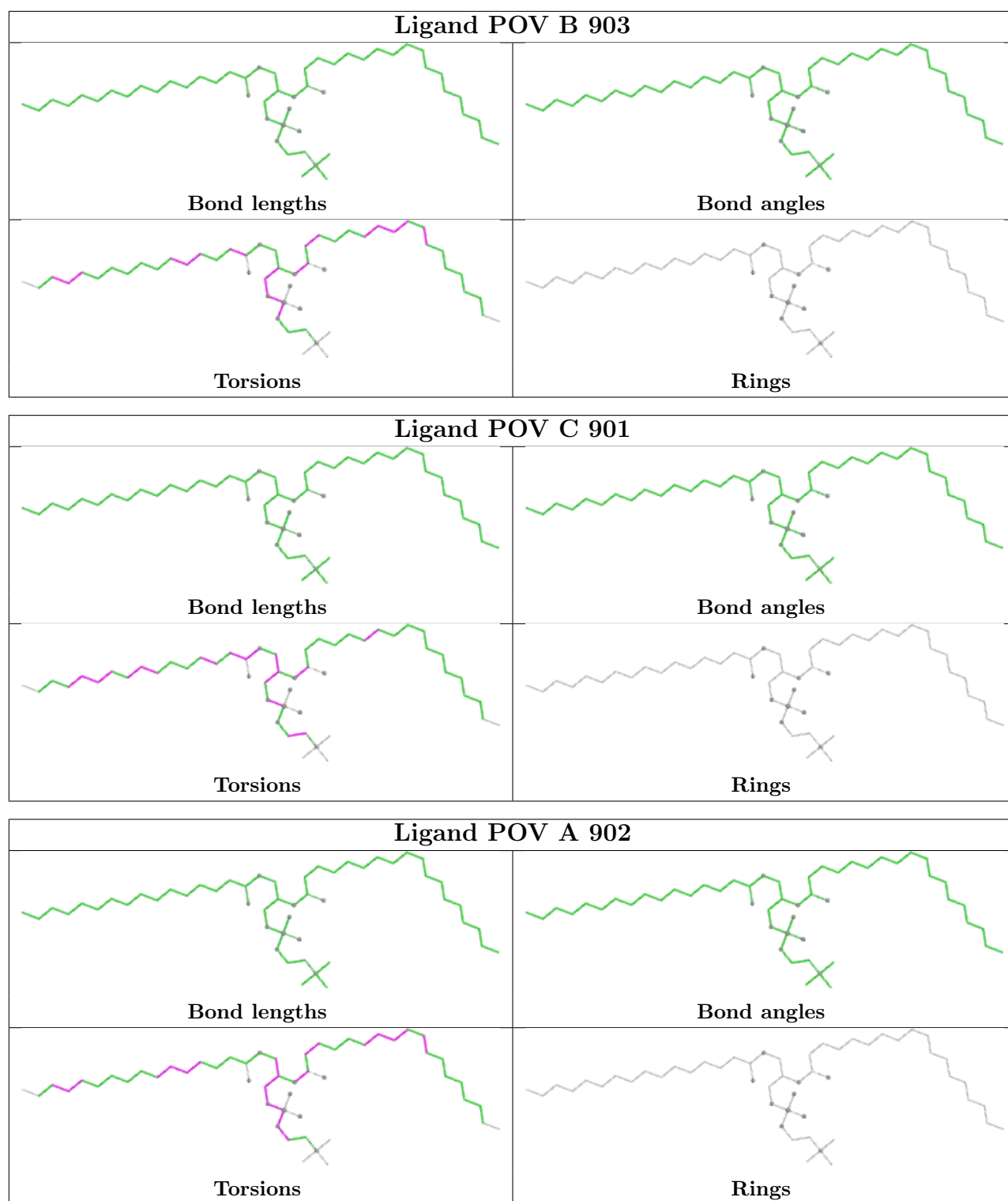
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	POV	3	0
3	B	903	POV	4	0
3	C	901	POV	1	0
3	A	902	POV	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 ⓘ

There are no chain breaks in this entry.

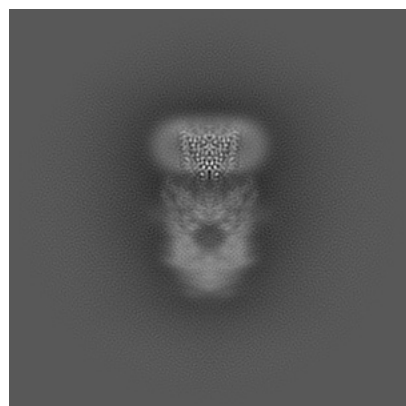
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70304. These allow visual inspection of the internal detail of the map and identification of artifacts.

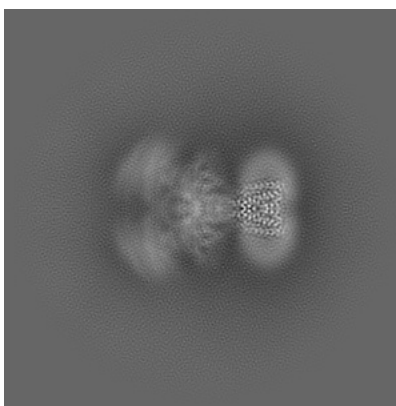
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

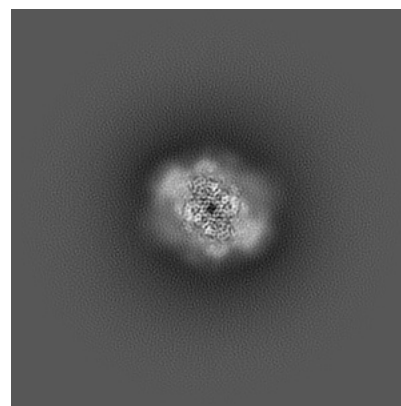
6.1.1 Primary map



X

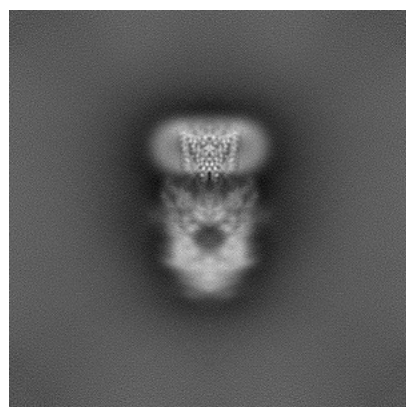


Y

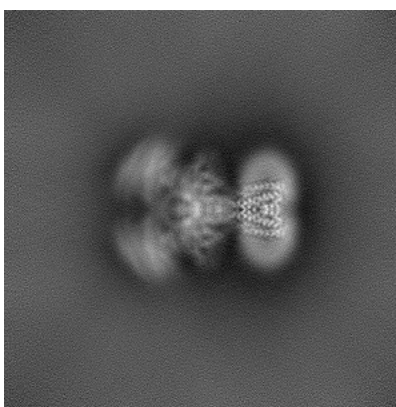


Z

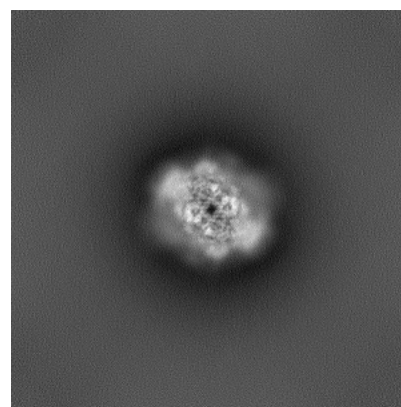
6.1.2 Raw map



X



Y

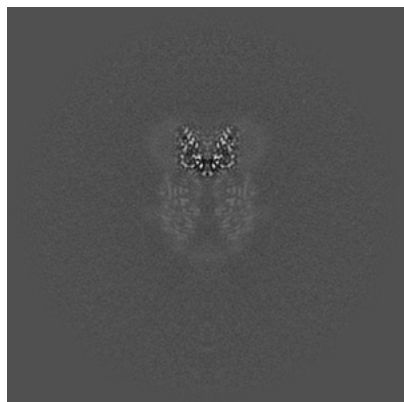


Z

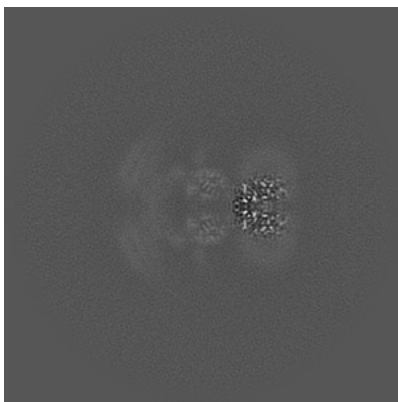
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

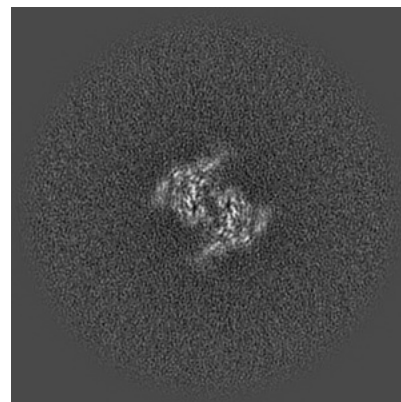
6.2.1 Primary map



X Index: 220

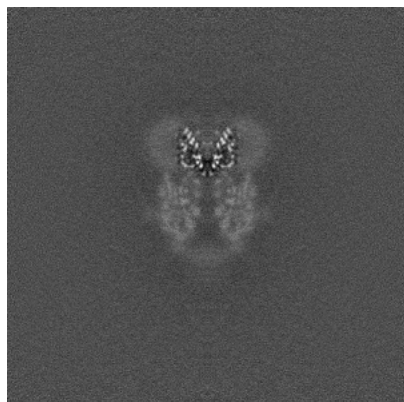


Y Index: 220

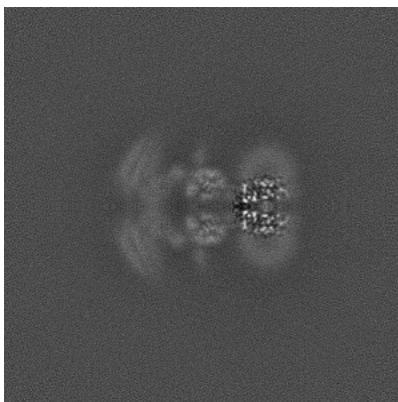


Z Index: 220

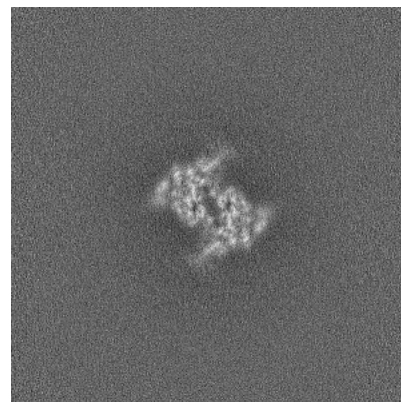
6.2.2 Raw map



X Index: 220



Y Index: 220

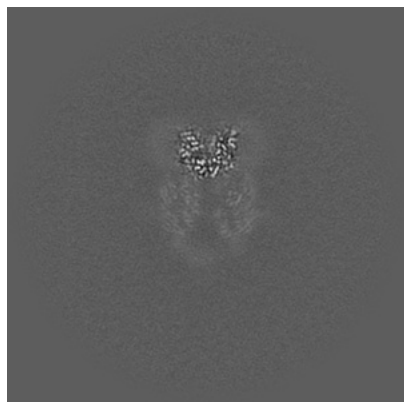


Z Index: 220

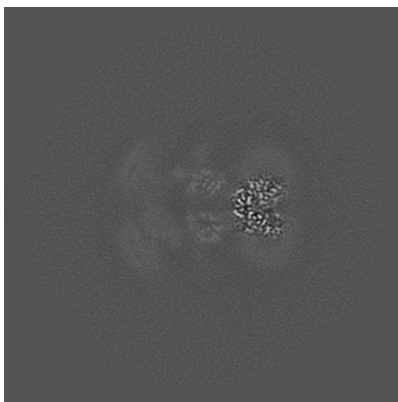
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

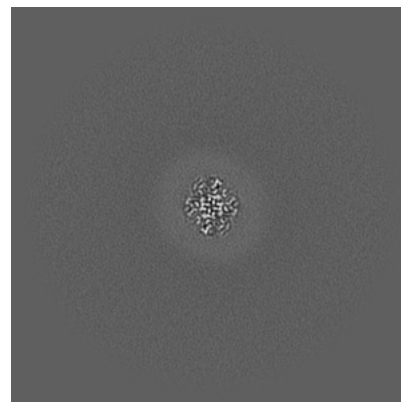
6.3.1 Primary map



X Index: 217

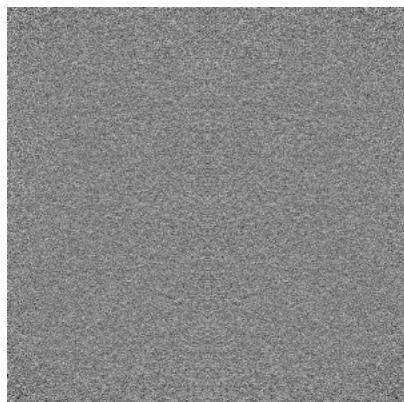


Y Index: 217

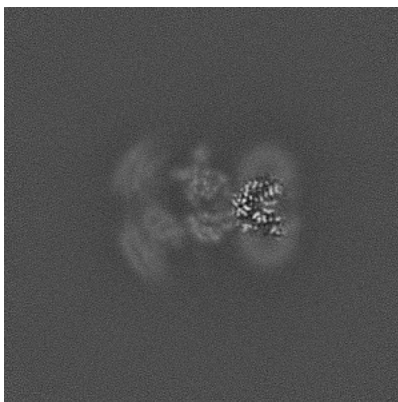


Z Index: 270

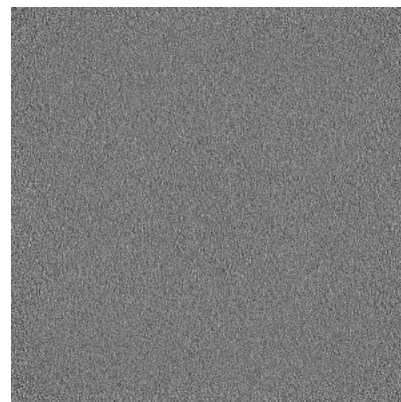
6.3.2 Raw map



X Index: 0



Y Index: 214

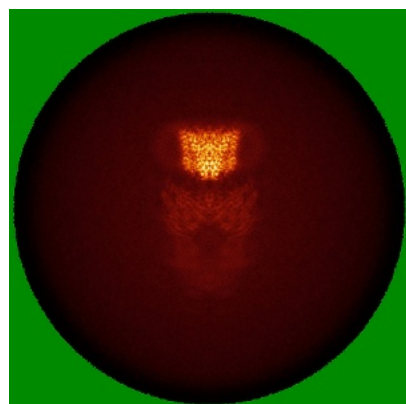


Z Index: 0

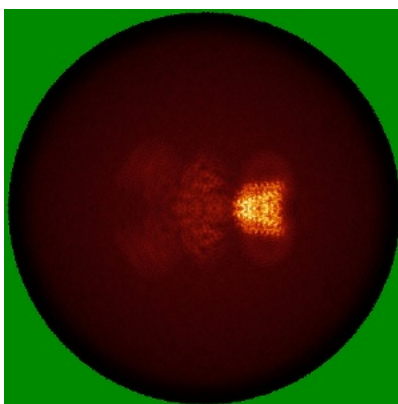
The images above show the largest variance slices of the map in three orthogonal directions.

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

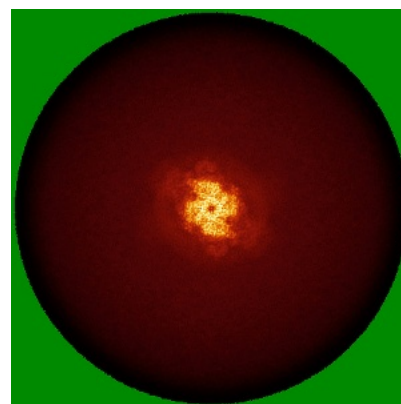
6.4.1 Primary map



X

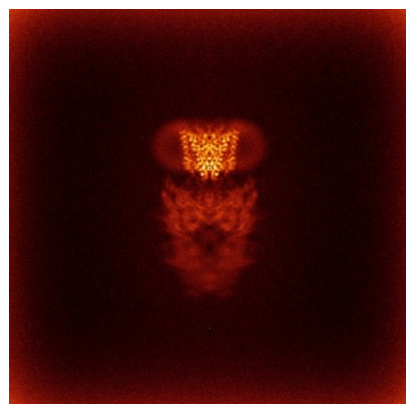


Y

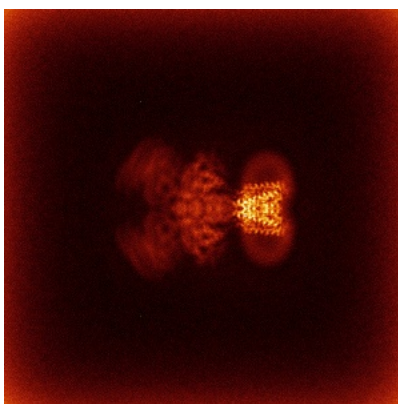


Z

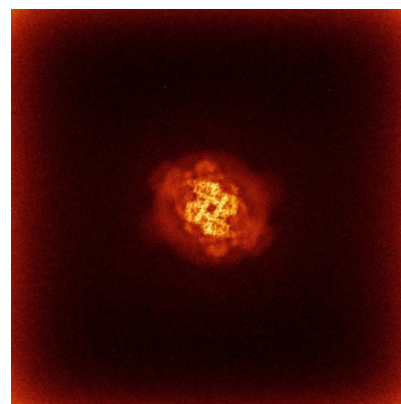
6.4.2 Raw map



X



Y

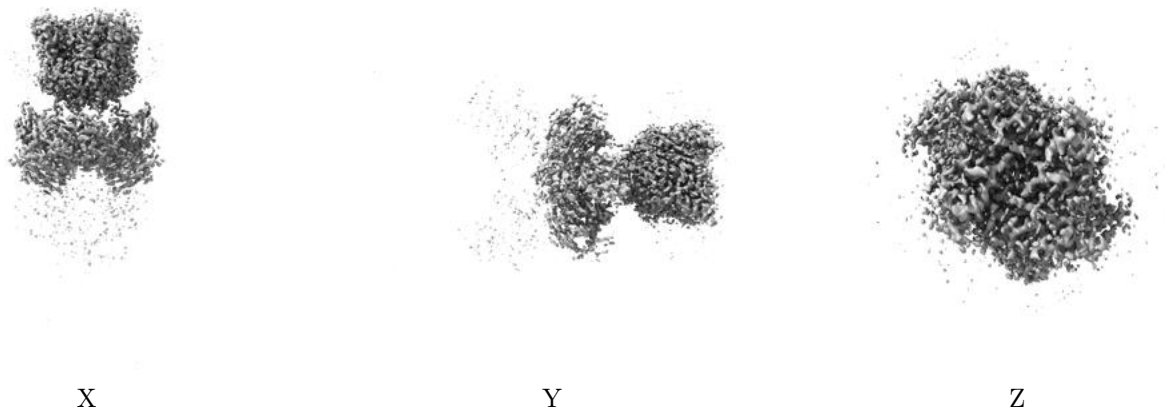


Z

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.

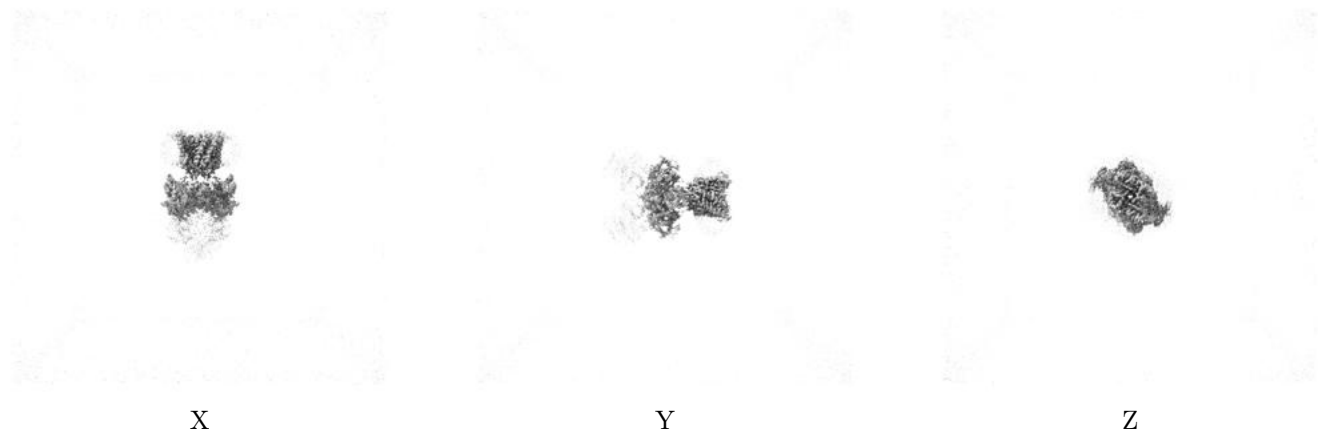
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

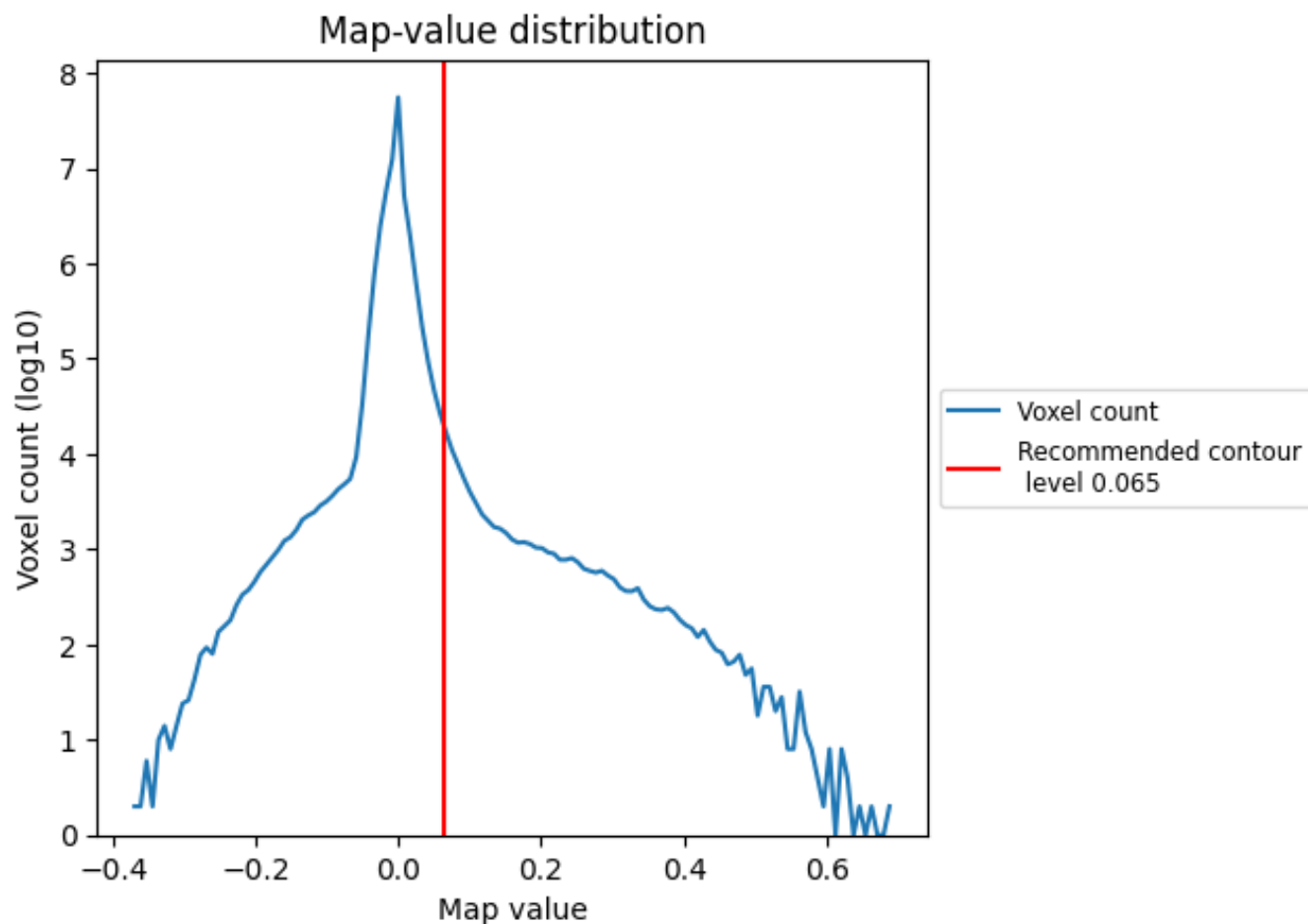
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

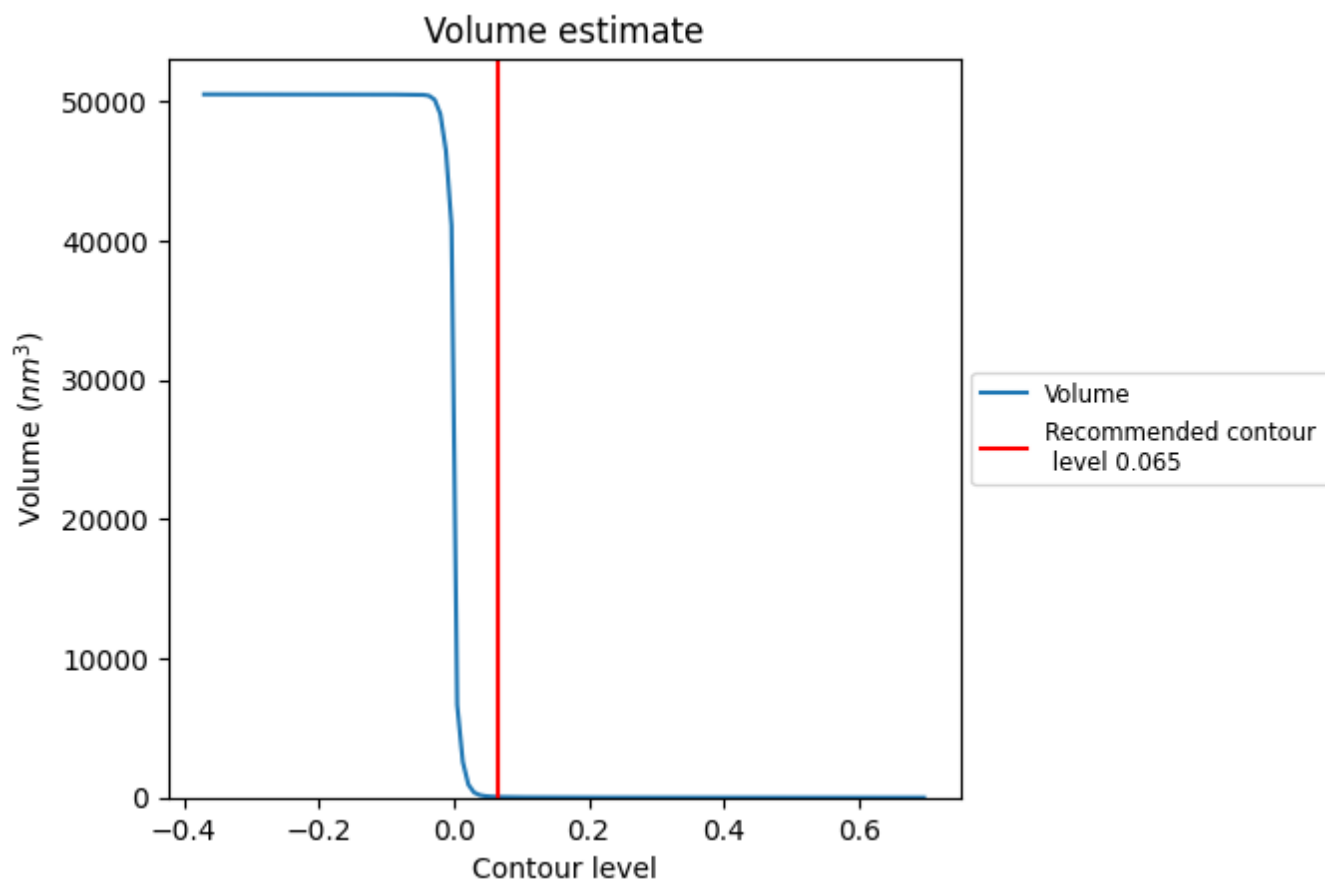
This section contains the results of statistical analysis of the map.

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.

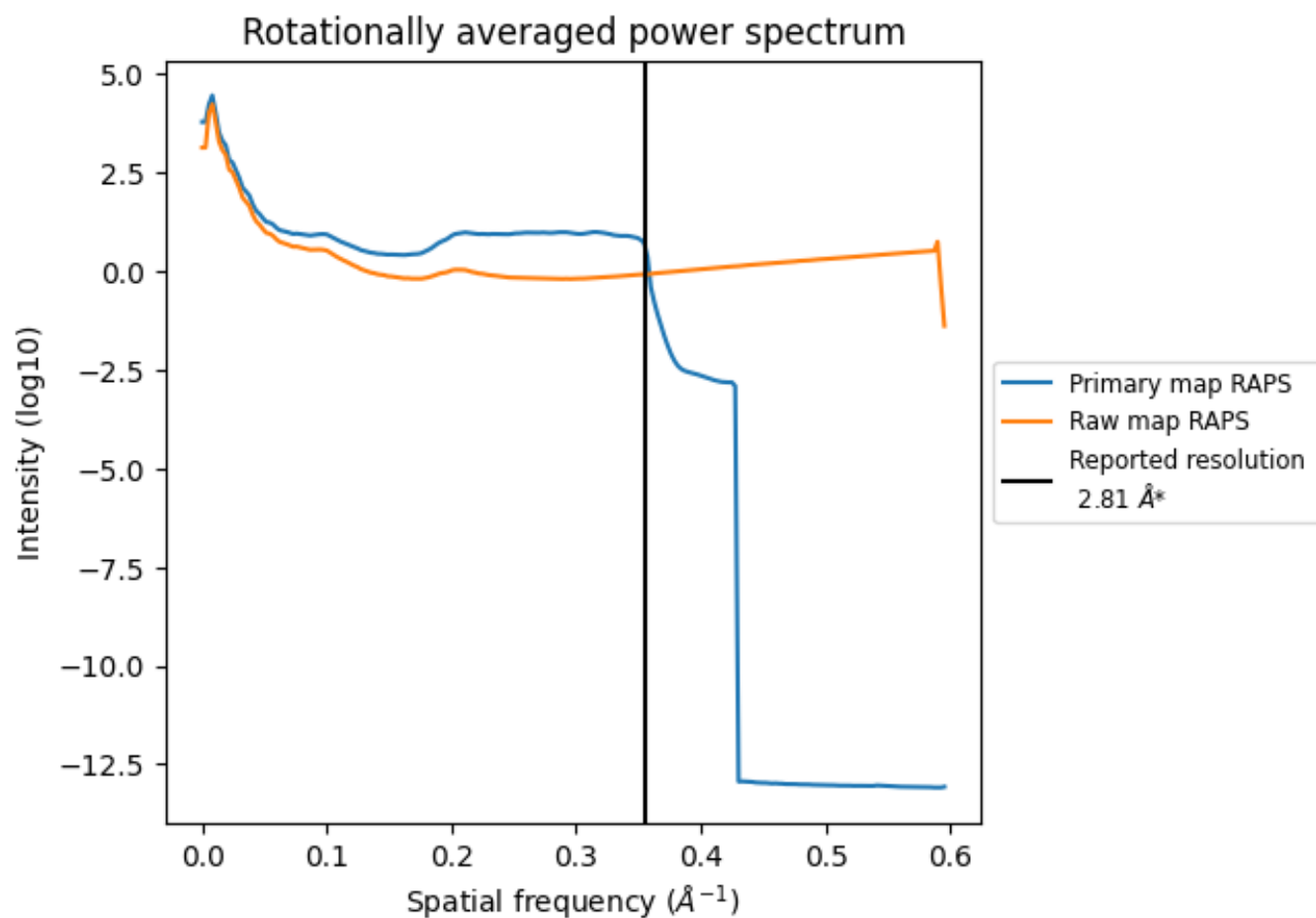
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm^3 ; this corresponds to an approximate mass of 44 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 ⓘ

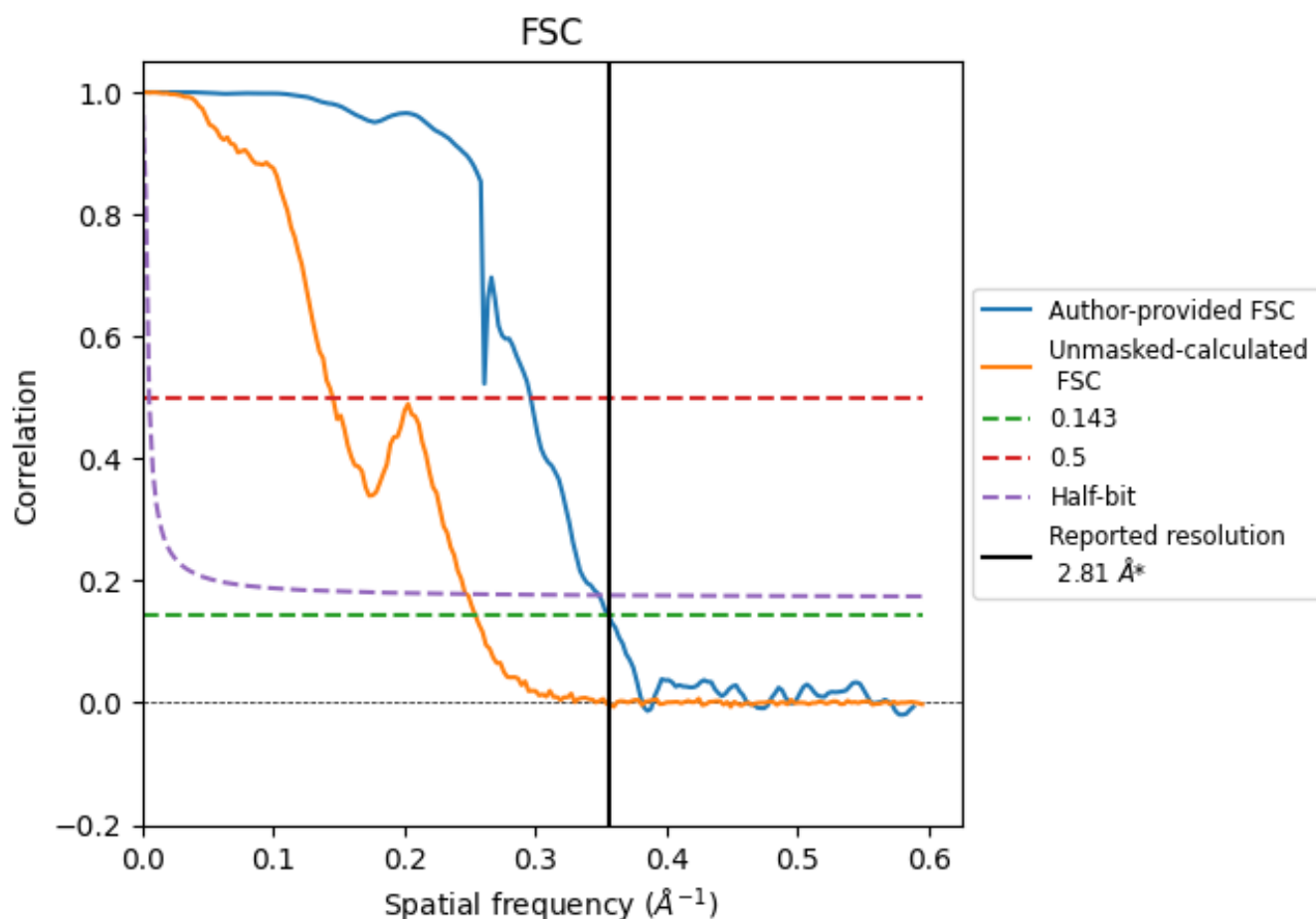


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

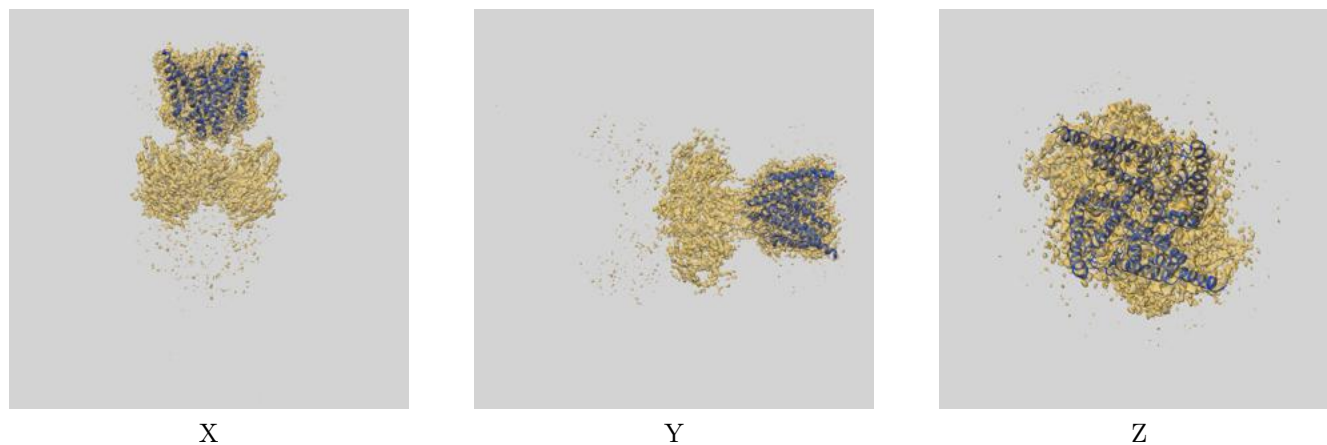
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.37	2.87
Unmasked-calculated*	3.93	6.88	4.04

*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 3.93 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

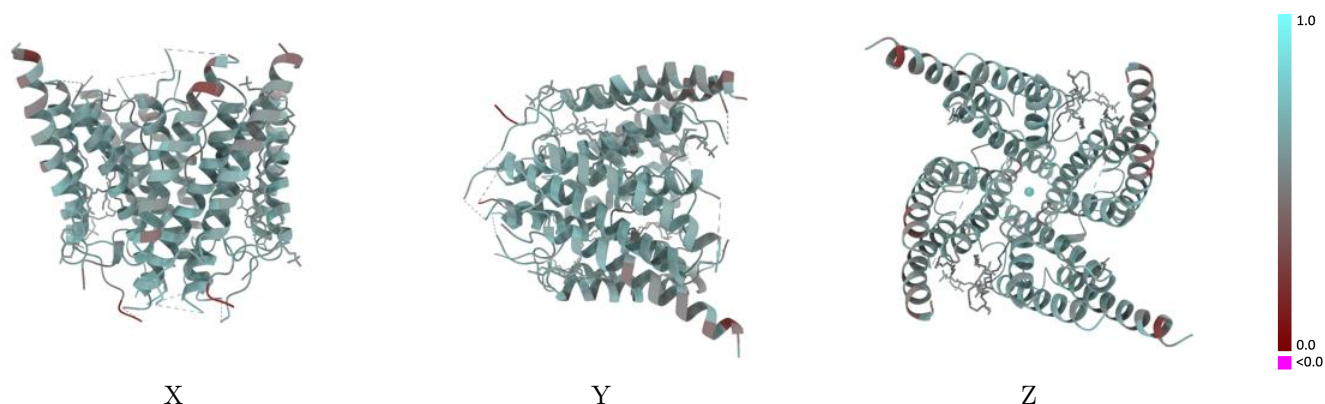
This section contains information regarding the fit between EMDB map EMD-70304 and PDB model 9OBZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



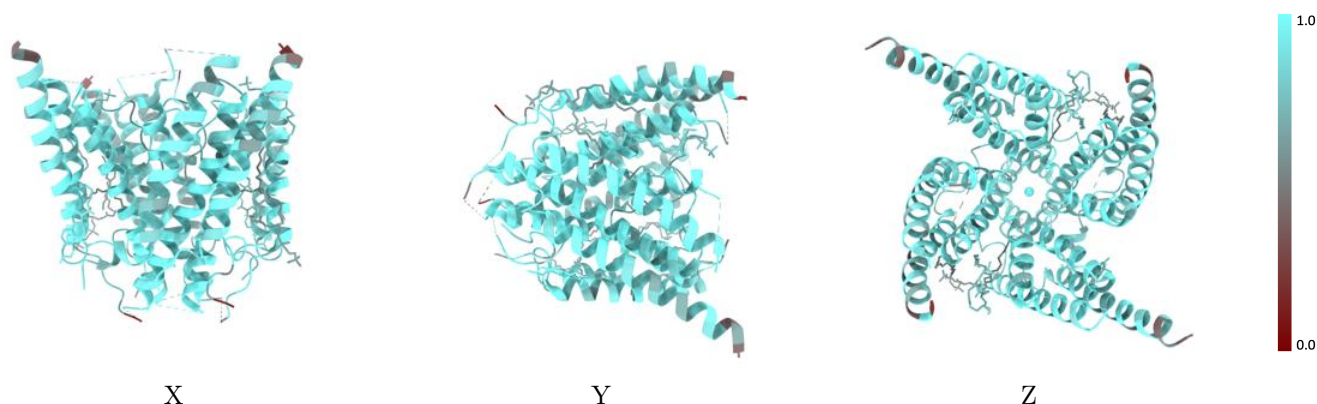
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



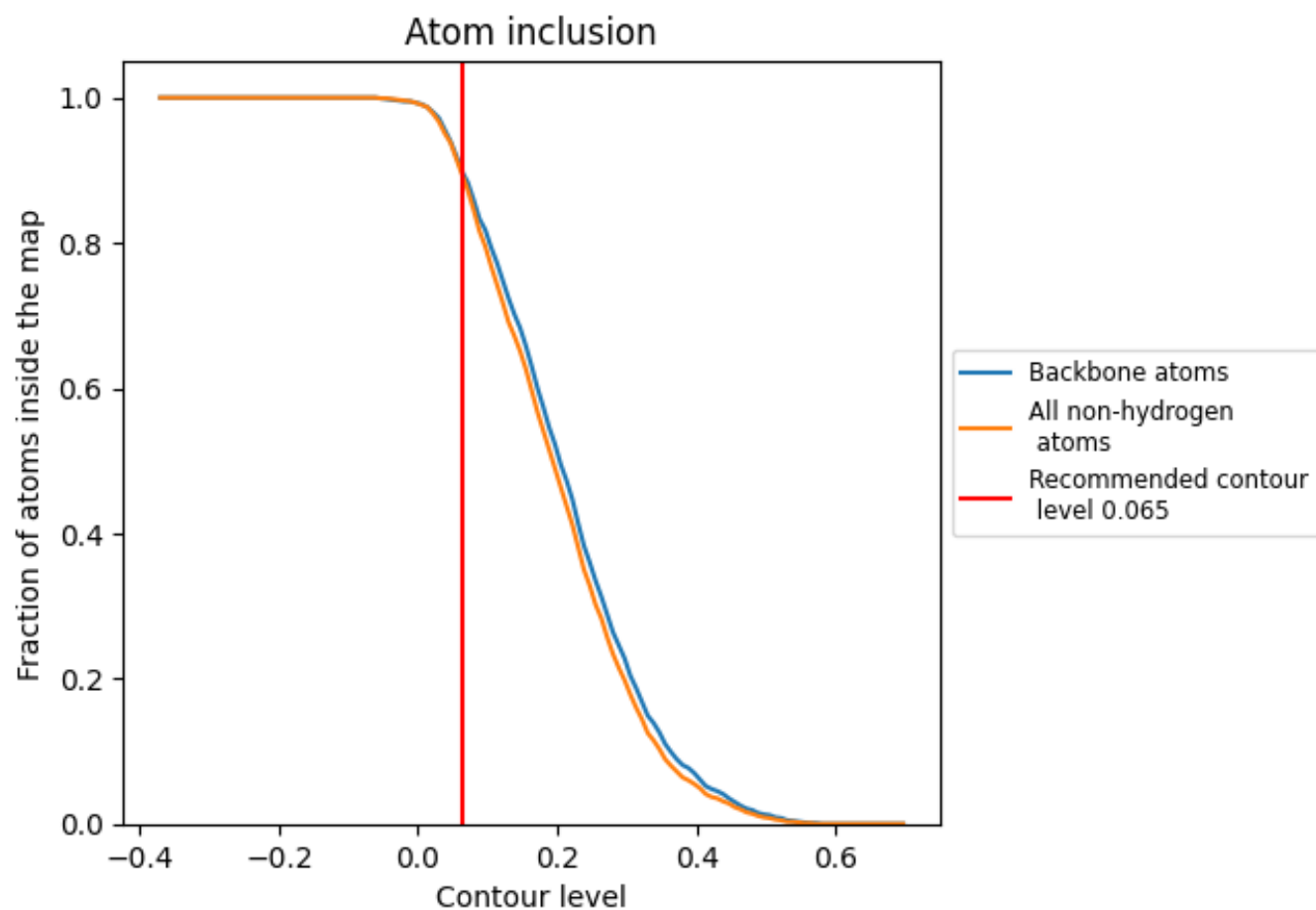
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.5820
A	0.8940	0.5910
B	0.8790	0.5720
C	0.9000	0.5910
D	0.8880	0.5740

