Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:35 AM UTC

PDB ID	:	6MMB / pdb_00006mmb
EMDB ID	:	EMD-9149
Title	:	Diheteromeric NMDA receptor GluN1/GluN2A in the 'Super-Splayed' conformation, in complex with glycine and glutamate, in the presence of 1 micromolar zinc chloride, and at pH 6.1
Authors	:	Jalali-Yazdi, F.; Chowdhury, S.; Yoshioka, C.; Gouaux, E.
Deposited on	:	2018-09-30
Resolution	:	12.70 Å(reported)
Based on initial models	:	5TQ0, 5I57, 5UOW, 4PE5

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:

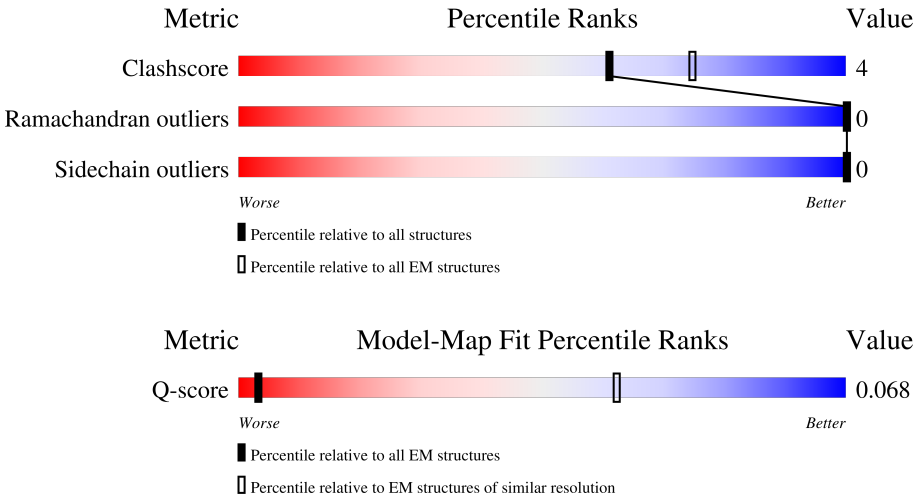
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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 (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 12.70 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	58 (12.20 - 13.20)

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 <=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	838	21% 79% 12% 8%
1	C	838	10% 80% 13% 7%
2	B	837	25% 80% 10% 11%
2	D	837	16% 78% 11% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24494 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	767	Total	C	N	O	S	0	0
			6064	3870	1046	1113	35		
1	C	778	Total	C	N	O	S	0	0
			6152	3922	1061	1134	35		

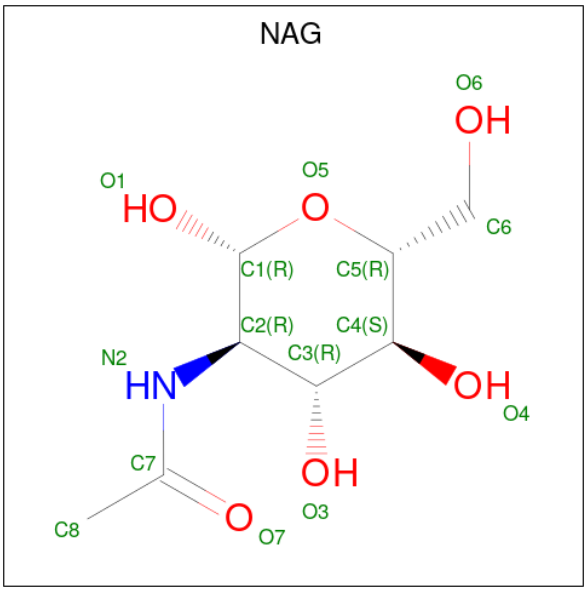
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	748	Total	C	N	O	S	0	0
			5907	3817	965	1091	34		
2	D	746	Total	C	N	O	S	0	0
			5895	3811	963	1087	34		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	758	THR	SER	conflict	UNP Q00959
D	758	THR	SER	conflict	UNP Q00959

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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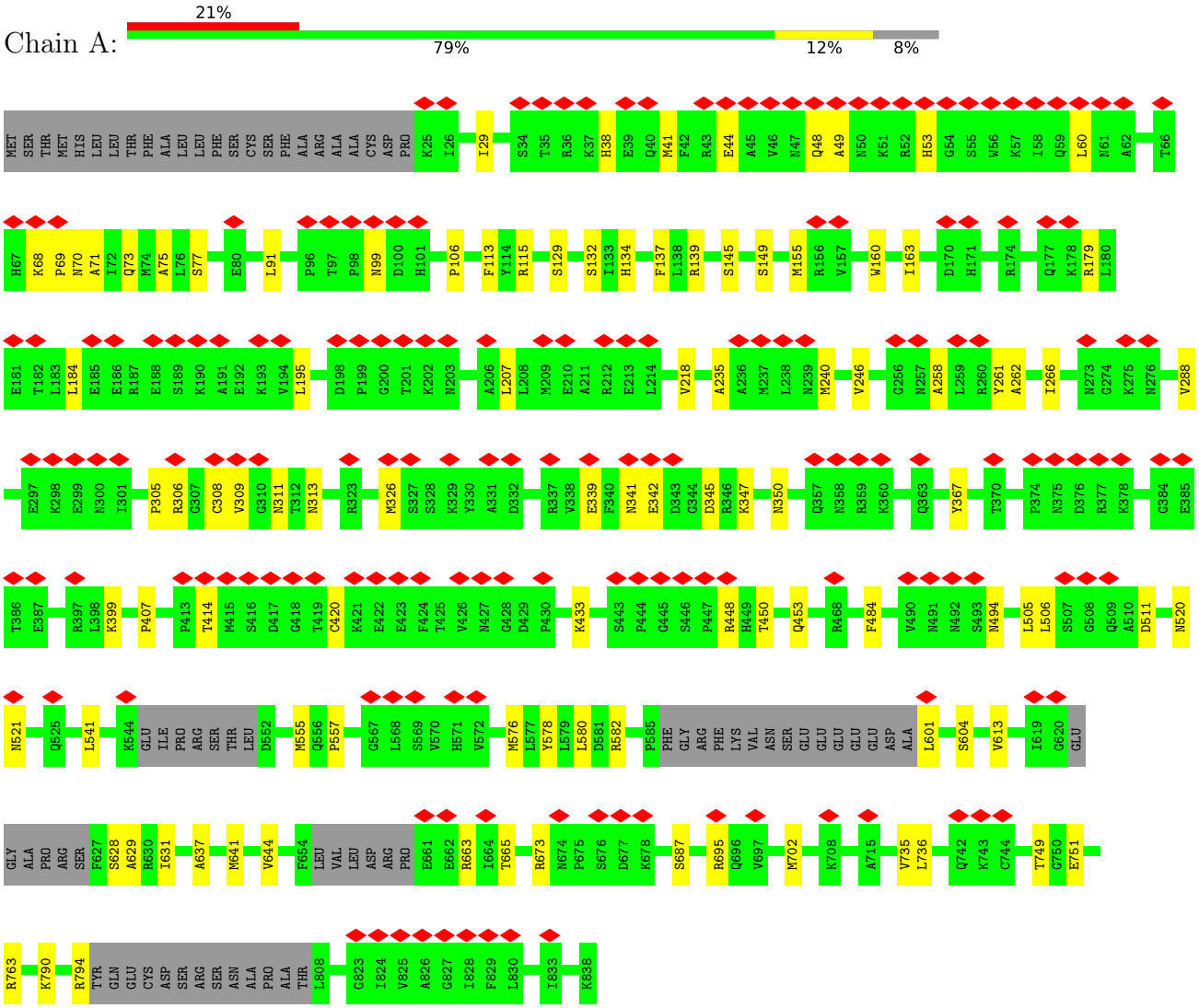
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3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

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.

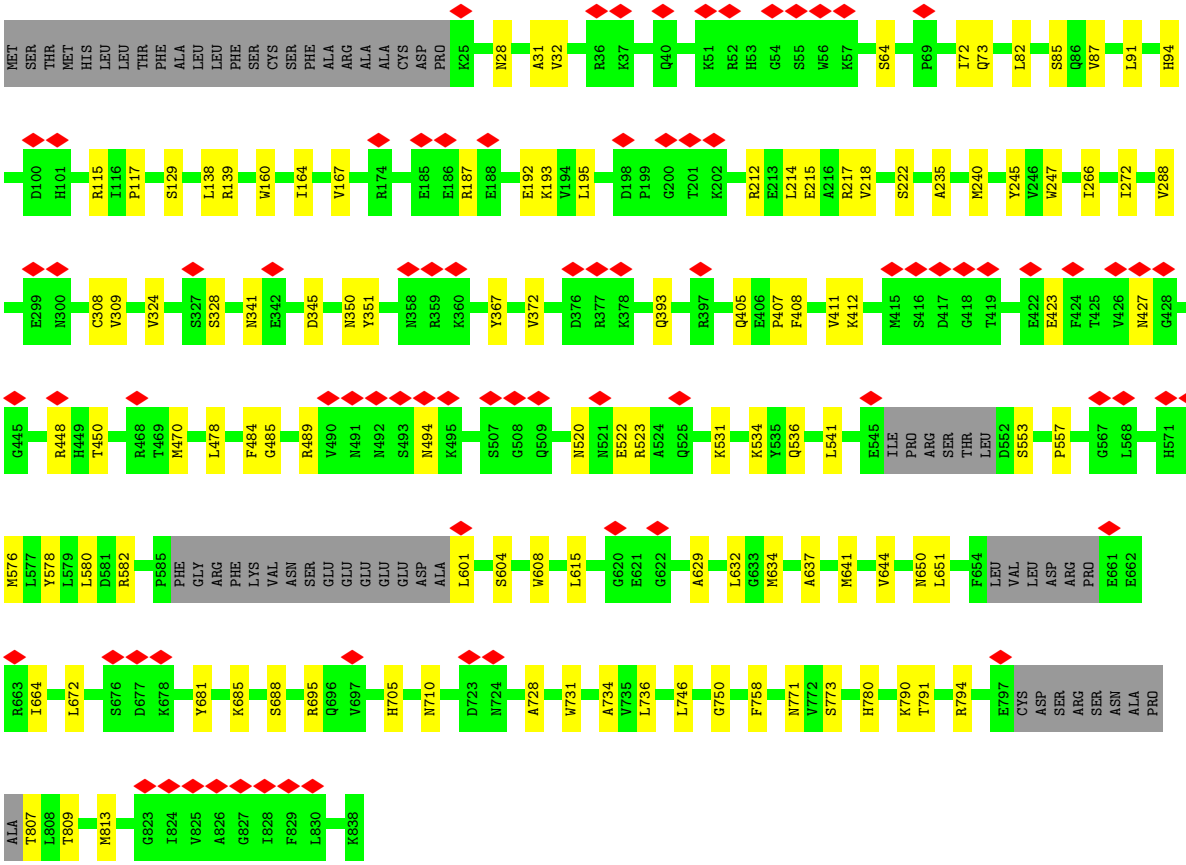
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

Chain A:



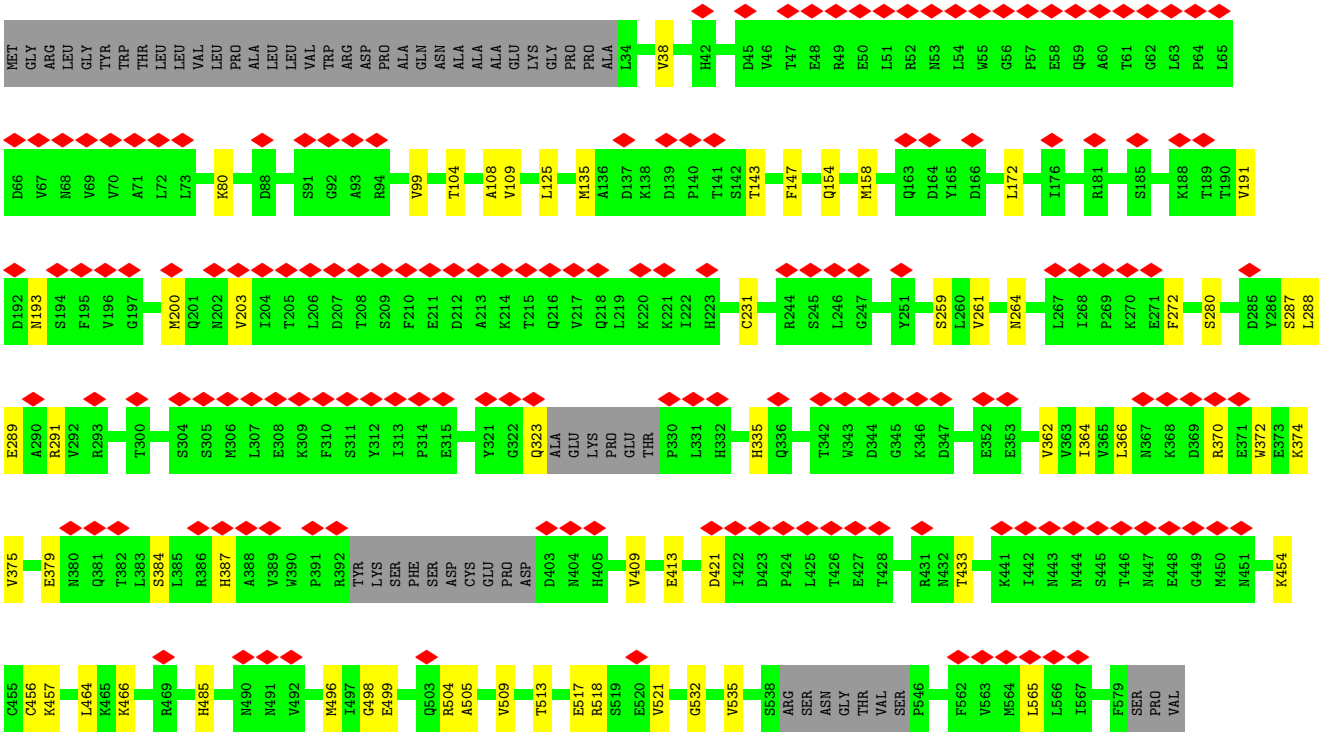
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

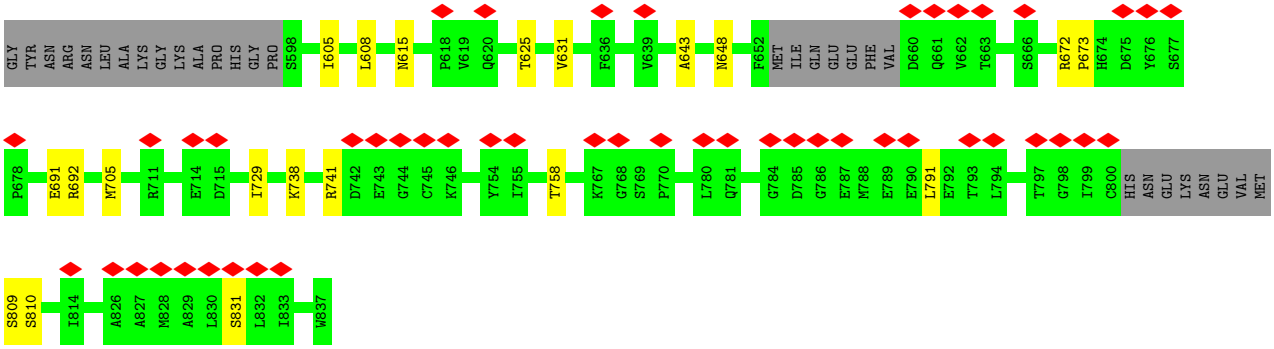
Chain C:



• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

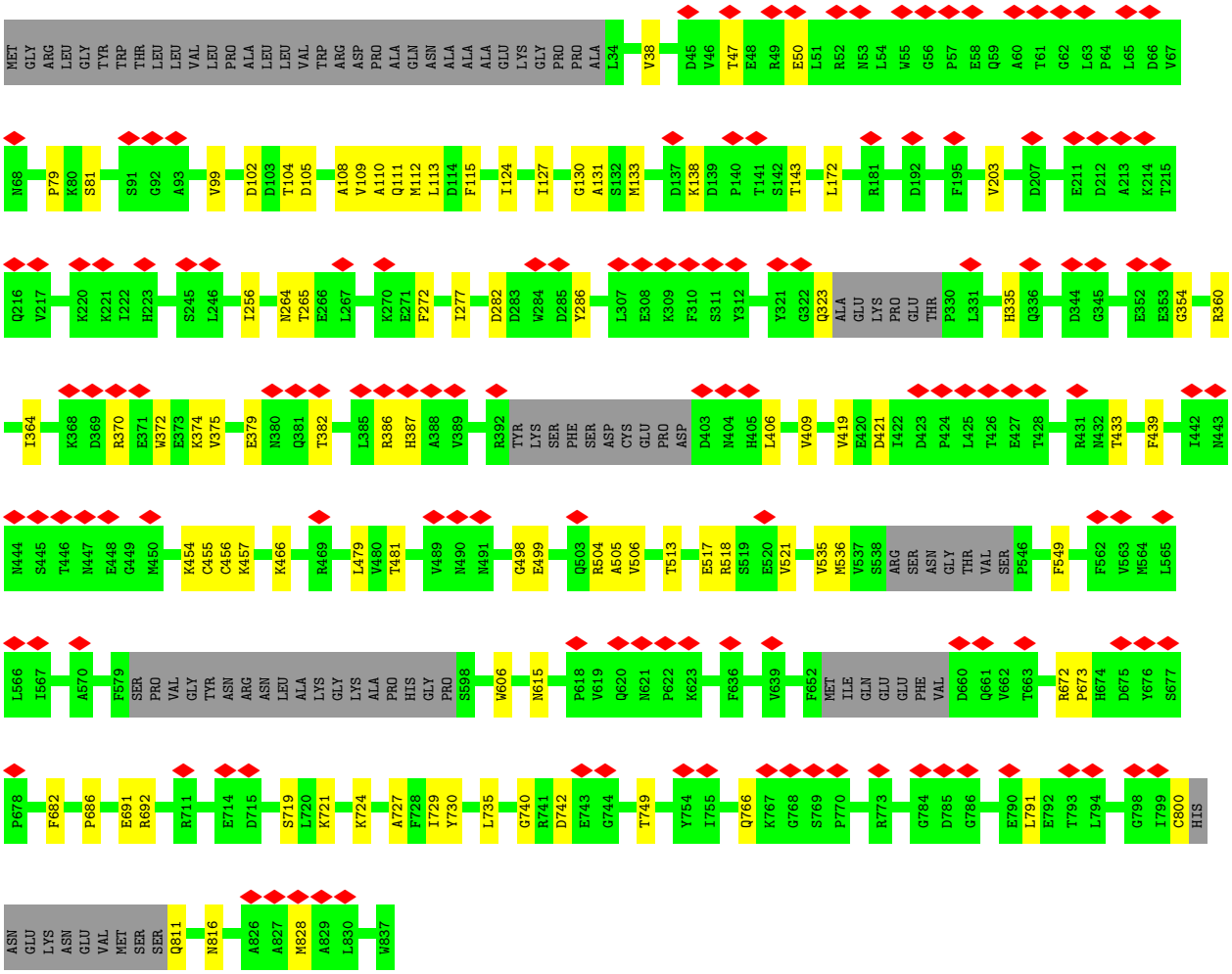
Chain B:





• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	328.32, 328.32, 328.32	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	Depositor

5 Model quality

5.1 Standard geometry

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	0.16	0/6197	0.38	0/8388
1	C	0.16	0/6288	0.39	0/8513
2	B	0.16	0/6044	0.39	0/8203
2	D	0.16	0/6032	0.38	0/8187
All	All	0.16	0/24561	0.38	0/33291

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	6064	0	6037	60	0
1	C	6152	0	6114	67	0
2	B	5907	0	5855	51	0
2	D	5895	0	5843	57	0
3	A	154	0	143	0	0
3	B	84	0	78	1	0
3	C	154	0	143	0	0
3	D	84	0	78	0	0
All	All	24494	0	24291	213	0

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

All (213) 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:413:GLU:OE2	2:B:485:HIS:NE2	2.17	0.76
2:D:433:THR:HA	2:D:456:CYS:O	1.86	0.74
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.78	0.66
2:B:280:SER:O	2:B:362:VAL:HB	1.97	0.65
1:A:44:GLU:OE2	1:A:48:GLN:NE2	2.30	0.65
2:D:272:PHE:HB2	2:D:370:ARG:HH12	1.62	0.65
1:A:663:ARG:HG2	1:A:665:THR:H	1.63	0.63
1:A:350:ASN:HA	1:A:367:TYR:O	1.98	0.63
2:D:112:MET:O	2:D:115:PHE:HB3	1.98	0.63
1:C:32:VAL:HG12	1:C:94:HIS:HD2	1.63	0.62
1:A:134:HIS:HB3	1:A:137:PHE:HB3	1.83	0.60
1:A:580:LEU:HD22	1:A:629:ALA:HB2	1.84	0.59
2:D:265:THR:OG1	2:D:282:ASP:OD2	2.16	0.59
1:A:38:HIS:HA	1:A:41:MET:HG3	1.85	0.59
1:C:167:VAL:HG22	1:C:222:SER:HB3	1.85	0.59
1:A:521:ASN:H	1:A:695:ARG:HH12	1.49	0.59
2:B:433:THR:HG22	2:B:457:LYS:HB3	1.84	0.58
1:A:145:SER:HB2	1:A:179:ARG:HG2	1.86	0.58
1:A:70:ASN:OD1	1:A:73:GLN:NE2	2.37	0.57
2:B:272:PHE:HB2	2:B:370:ARG:HH12	1.70	0.57
2:D:419:VAL:HG11	2:D:479:LEU:HD11	1.86	0.56
2:D:517:GLU:OE1	2:D:692:ARG:NH2	2.39	0.56
1:A:601:LEU:HB3	1:A:604:SER:HB2	1.88	0.56
1:A:258:ALA:HA	1:A:261:TYR:HB2	1.87	0.55
2:D:721:LYS:NZ	2:D:742:ASP:OD1	2.40	0.55
1:C:247:TRP:HB3	1:C:266:ILE:HG13	1.88	0.55
2:B:421:ASP:OD1	2:B:454:LYS:NZ	2.40	0.54
1:C:809:THR:HA	1:C:813:MET:HB2	1.88	0.54
2:D:421:ASP:OD1	2:D:454:LYS:NZ	2.40	0.54
1:A:673:ARG:HD3	1:A:702:MET:HE3	1.90	0.54
1:A:790:LYS:HG2	1:A:794:ARG:HE	1.73	0.54
1:A:115:ARG:HH22	2:B:109:VAL:HG23	1.73	0.53
1:C:129:SER:OG	1:C:139:ARG:NH2	2.41	0.53
1:C:427:ASN:HD22	1:C:791:THR:HG22	1.73	0.53
1:C:601:LEU:HB3	1:C:604:SER:HB2	1.89	0.53
2:B:191:VAL:HG11	2:B:200:MET:HB2	1.89	0.53
2:B:565:LEU:HD23	2:B:608:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:740:GLY:HA2	2:D:800:CYS:HB2	1.90	0.53
1:A:306:ARG:O	1:A:311:ASN:ND2	2.42	0.53
1:C:534:LYS:HB3	1:C:758:PHE:HB2	1.90	0.53
1:A:506:LEU:HD23	1:A:763:ARG:HH22	1.74	0.52
2:B:513:THR:OG1	2:B:518:ARG:NH1	2.41	0.52
2:B:625:THR:HG23	1:C:608:TRP:HE1	1.75	0.52
1:A:68:LYS:HD2	1:A:73:GLN:HB3	1.90	0.52
1:A:555:MET:HG2	1:A:557:PRO:HD2	1.90	0.52
1:C:522:GLU:OE1	1:C:695:ARG:NH1	2.43	0.52
1:A:75:ALA:HB2	1:A:106:PRO:HB2	1.91	0.52
1:C:31:ALA:O	1:C:64:SER:HA	2.10	0.52
2:B:409:VAL:HG13	2:B:496:MET:HG2	1.92	0.52
2:D:513:THR:OG1	2:D:518:ARG:NH1	2.42	0.52
1:C:91:LEU:HD11	1:C:288:VAL:HG21	1.92	0.52
1:C:351:TYR:HB2	1:C:367:TYR:HB3	1.91	0.52
1:A:308:CYS:SG	1:A:309:VAL:N	2.83	0.52
2:B:375:VAL:HG13	2:B:387:HIS:HD2	1.74	0.52
1:C:541:LEU:HD21	1:C:746:LEU:HD22	1.92	0.52
2:D:433:THR:HG22	2:D:457:LYS:HB3	1.91	0.52
1:A:484:PHE:HB2	1:A:687:SER:HA	1.92	0.51
2:D:143:THR:HG22	2:D:335:HIS:HB2	1.91	0.51
1:A:641:MET:HA	1:A:644:VAL:HG22	1.92	0.51
1:A:326:MET:HE1	1:A:342:GLU:HA	1.93	0.51
2:B:535:VAL:HG22	2:B:729:ILE:HG12	1.92	0.51
2:B:631:VAL:HG12	1:C:615:LEU:HD11	1.93	0.51
1:C:576:MET:HE1	2:D:828:MET:HE3	1.91	0.51
2:B:517:GLU:OE1	2:B:692:ARG:NH2	2.44	0.51
1:C:405:GLN:HG3	1:C:407:PRO:HD2	1.91	0.51
1:C:489:ARG:NH2	1:C:494:ASN:OD1	2.43	0.51
1:C:541:LEU:O	1:C:728:ALA:HA	2.10	0.51
2:D:99:VAL:HG13	2:D:127:ILE:HG13	1.92	0.51
2:D:109:VAL:O	2:D:112:MET:HB2	2.11	0.51
1:C:637:ALA:HB1	2:D:615:ASN:HD22	1.76	0.51
2:D:433:THR:HB	2:D:455:CYS:HB3	1.93	0.51
1:A:494:ASN:ND2	2:B:193:ASN:O	2.44	0.50
2:B:104:THR:O	2:B:264:ASN:ND2	2.44	0.50
2:D:172:LEU:HD23	2:D:203:VAL:HG22	1.93	0.50
2:D:374:LYS:O	2:D:386:ARG:NH1	2.45	0.50
2:B:498:GLY:O	2:B:504:ARG:NH2	2.43	0.50
1:C:664:ILE:HD12	1:C:672:LEU:HD11	1.93	0.50
1:C:650:ASN:HB2	2:D:811:GLN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HE3	1:A:77:SER:HB2	1.93	0.50
2:B:691:GLU:HG2	2:B:705:MET:HE1	1.94	0.50
1:C:531:LYS:NZ	1:C:773:SER:OG	2.45	0.50
1:A:69:PRO:O	1:A:99:ASN:ND2	2.45	0.49
2:B:379:GLU:HB2	2:B:384:SER:HB2	1.93	0.49
1:A:115:ARG:HH21	2:B:108:ALA:H	1.59	0.49
2:B:231:CYS:H	2:B:261:VAL:HG22	1.77	0.49
2:B:364:ILE:HD12	2:B:372:TRP:HB3	1.93	0.49
2:D:104:THR:O	2:D:264:ASN:ND2	2.45	0.49
1:A:132:SER:HB3	2:B:135:MET:HB2	1.94	0.49
1:A:448:ARG:NH1	1:A:450:THR:OG1	2.44	0.49
2:B:466:LYS:HZ2	2:B:791:LEU:HD11	1.77	0.49
2:D:672:ARG:HD2	2:D:673:PRO:HD2	1.93	0.49
1:A:407:PRO:HG3	1:A:735:VAL:HG13	1.94	0.49
1:A:341:ASN:HD21	1:A:345:ASP:HB2	1.78	0.49
1:C:308:CYS:SG	1:C:309:VAL:N	2.85	0.49
2:B:648:ASN:HB2	1:C:807:THR:HG21	1.94	0.49
2:D:409:VAL:HG21	2:D:499:GLU:HG3	1.94	0.48
2:B:143:THR:HG22	2:B:335:HIS:HB2	1.95	0.48
1:A:129:SER:OG	1:A:139:ARG:NH2	2.47	0.48
1:C:520:ASN:HB2	1:C:695:ARG:HH12	1.79	0.48
1:A:305:PRO:HG3	1:A:313:ASN:HB2	1.96	0.48
1:C:650:ASN:ND2	2:D:811:GLN:O	2.46	0.48
2:B:464:LEU:HD13	2:B:509:VAL:HG21	1.96	0.48
1:C:193:LYS:HE2	1:C:195:LEU:HD21	1.96	0.47
1:C:731:TRP:HD1	1:C:736:LEU:HG	1.79	0.47
2:D:375:VAL:HG13	2:D:387:HIS:HD2	1.79	0.47
2:D:466:LYS:HZ2	2:D:791:LEU:HD21	1.79	0.47
1:C:192:GLU:OE2	1:C:214:LEU:HB3	2.14	0.47
1:A:520:ASN:HB2	1:A:695:ARG:HH12	1.80	0.47
2:D:110:ALA:HB2	2:D:131:ALA:HA	1.96	0.47
1:C:790:LYS:HG2	1:C:794:ARG:HE	1.79	0.47
2:D:138:LYS:NZ	2:D:354:GLY:O	2.48	0.47
2:D:549:PHE:HE2	2:D:816:ASN:HD22	1.63	0.46
1:A:155:MET:HG2	1:A:160:TRP:HB2	1.97	0.46
2:D:38:VAL:HA	2:D:99:VAL:HB	1.97	0.46
1:A:218:VAL:HA	1:A:246:VAL:HB	1.98	0.46
1:A:613:VAL:HG13	1:A:637:ALA:HB2	1.98	0.46
2:B:672:ARG:HD2	2:B:673:PRO:HD2	1.97	0.46
1:A:91:LEU:HD11	1:A:288:VAL:HG21	1.98	0.46
2:D:406:LEU:HD22	2:D:506:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:O	1:C:328:SER:OG	2.33	0.45
1:C:536:GLN:HE21	1:C:734:ALA:H	1.65	0.45
1:C:681:TYR:H	1:C:705:HIS:HE1	1.64	0.45
1:C:217:ARG:HE	1:C:393:GLN:HE22	1.63	0.45
2:B:364:ILE:HG22	2:B:374:LYS:HA	1.98	0.45
2:D:113:LEU:HD22	2:D:124:ILE:HD13	1.98	0.45
2:D:535:VAL:HG22	2:D:729:ILE:HG12	1.97	0.45
1:C:576:MET:HE3	1:C:632:LEU:HD11	1.98	0.45
2:B:38:VAL:HA	2:B:99:VAL:HB	1.97	0.45
2:D:439:PHE:HB3	2:D:481:THR:HG21	1.98	0.45
2:D:498:GLY:O	2:D:504:ARG:NH2	2.49	0.45
1:A:749:THR:HG23	1:A:751:GLU:H	1.82	0.45
1:C:685:LYS:HB2	1:C:710:ASN:HB3	1.98	0.45
1:A:399:LYS:H	1:A:511:ASP:HB2	1.81	0.45
1:C:634:MET:HE2	2:D:606:TRP:HD1	1.82	0.45
2:B:433:THR:HA	2:B:456:CYS:O	2.16	0.45
2:B:565:LEU:HD22	2:B:605:ILE:HA	1.99	0.45
3:B:906:NAG:O4	1:C:780:HIS:O	2.35	0.45
1:C:405:GLN:HB3	1:C:408:PHE:HB2	1.98	0.45
2:D:105:ASP:HA	2:D:133:MET:HE1	1.98	0.45
1:A:49:ALA:O	1:A:53:HIS:ND1	2.48	0.44
2:B:154:GLN:HE22	2:B:259:SER:H	1.65	0.44
1:A:637:ALA:HB1	2:B:615:ASN:HD21	1.81	0.44
1:C:235:ALA:HB1	1:C:240:MET:HB2	1.99	0.44
1:C:308:CYS:O	2:D:81:SER:OG	2.34	0.44
1:C:448:ARG:NH1	1:C:450:THR:OG1	2.45	0.44
1:A:29:ILE:HD11	1:A:60:LEU:HD22	1.99	0.44
2:D:286:TYR:HE1	2:D:360:ARG:HH11	1.66	0.44
2:B:499:GLU:O	2:B:505:ALA:N	2.48	0.44
1:C:115:ARG:HH12	2:D:108:ALA:HB2	1.83	0.44
1:C:367:TYR:HD1	1:C:372:VAL:HG22	1.81	0.44
2:D:536:MET:HA	2:D:749:THR:HG22	2.00	0.44
1:C:411:VAL:HG21	1:C:478:LEU:HD21	1.99	0.44
2:B:532:GLY:HA2	2:B:758:THR:HA	1.99	0.44
2:B:672:ARG:HB3	1:C:750:GLY:HA2	1.99	0.44
2:B:518:ARG:HA	2:B:521:VAL:HG22	1.99	0.44
1:C:82:LEU:HD22	1:C:87:VAL:HG21	2.00	0.44
1:A:70:ASN:ND2	2:B:323:GLN:OE1	2.50	0.44
1:C:72:ILE:HD12	2:D:323:GLN:HE22	1.82	0.43
2:D:364:ILE:HG22	2:D:374:LYS:HA	2.00	0.43
2:D:379:GLU:OE1	2:D:382:THR:OG1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HD11	1:A:184:LEU:HD11	2.01	0.43
2:B:287:SER:OG	2:B:289:GLU:OE1	2.33	0.43
1:C:485:GLY:O	1:C:523:ARG:NH2	2.52	0.43
1:C:578:TYR:OH	1:C:582:ARG:NH1	2.44	0.43
2:D:102:ASP:HB3	2:D:130:GLY:H	1.83	0.43
1:C:470:MET:HE2	1:C:771:ASN:HB3	2.00	0.43
2:D:256:ILE:HG12	2:D:277:ILE:HB	2.00	0.42
1:A:541:LEU:HD13	1:A:736:LEU:HD22	2.00	0.42
1:C:212:ARG:NH1	1:C:245:TYR:OH	2.52	0.42
1:C:272:ILE:HD12	1:C:350:ASN:HB3	2.01	0.42
1:A:113:PHE:O	1:A:115:ARG:NH1	2.44	0.42
1:C:160:TRP:O	1:C:187:ARG:NH2	2.52	0.42
2:D:505:ALA:O	2:D:766:GLN:NE2	2.49	0.42
1:A:262:ALA:HB1	1:A:266:ILE:HG21	2.01	0.42
2:B:288:LEU:HD12	2:B:291:ARG:HD2	2.01	0.42
1:C:117:PRO:HB3	1:C:138:LEU:HD13	2.00	0.42
1:A:339:GLU:HB3	1:A:347:LYS:HD2	2.02	0.42
2:B:643:ALA:HB1	1:C:651:LEU:HD21	2.01	0.42
1:A:149:SER:OG	1:A:179:ARG:NH2	2.53	0.41
1:A:420:CYS:HB3	1:A:433:LYS:HD2	2.01	0.41
1:C:341:ASN:HD21	1:C:345:ASP:HB2	1.85	0.41
2:D:47:THR:OG1	2:D:50:GLU:OE1	2.36	0.41
2:B:172:LEU:HD23	2:B:203:VAL:HG22	2.02	0.41
1:C:412:LYS:NZ	1:C:423:GLU:OE2	2.47	0.41
1:C:580:LEU:HD22	1:C:629:ALA:HB2	2.02	0.41
2:D:730:TYR:HB3	2:D:735:LEU:HD11	2.02	0.41
1:C:641:MET:HA	1:C:644:VAL:HG22	2.01	0.41
1:C:553:SER:HA	1:C:557:PRO:HB2	2.02	0.41
1:A:576:MET:HE3	2:B:831:SER:HB2	2.02	0.41
1:C:73:GLN:HE22	2:D:323:GLN:HG3	1.86	0.41
2:B:125:LEU:HB3	2:B:147:PHE:HE2	1.86	0.41
2:B:738:LYS:HA	2:B:741:ARG:HG2	2.02	0.41
1:C:164:ILE:HB	1:C:218:VAL:O	2.21	0.41
2:D:364:ILE:HD12	2:D:372:TRP:HB3	2.02	0.41
2:D:686:PRO:HA	2:D:691:GLU:OE2	2.21	0.41
1:A:414:THR:HG23	1:A:453:GLN:HA	2.03	0.41
1:A:628:SER:HA	1:A:631:ILE:HD12	2.03	0.41
2:D:518:ARG:HA	2:D:521:VAL:HG22	2.02	0.41
2:D:682:PHE:HB3	2:D:727:ALA:HB3	2.03	0.41
2:D:719:SER:O	2:D:724:LYS:N	2.54	0.41
2:B:154:GLN:HG2	2:B:158:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:CYS:HA	2:B:80:LYS:HD3	2.03	0.40
1:A:578:TYR:OH	1:A:582:ARG:NH2	2.48	0.40
2:B:809:SER:OG	2:B:810:SER:N	2.54	0.40
2:D:79:PRO:HB3	2:D:112:MET:HE2	2.03	0.40
2:D:108:ALA:O	2:D:111:GLN:HB3	2.20	0.40
1:A:195:LEU:HD22	1:A:207:LEU:HD12	2.03	0.40
1:A:235:ALA:HB1	1:A:240:MET:HB2	2.03	0.40
1:C:28:ASN:HD22	1:C:85:SER:HB3	1.84	0.40
1:C:192:GLU:OE2	1:C:215:GLU:N	2.49	0.40
1:C:484:PHE:HD2	1:C:688:SER:H	1.70	0.40
2:B:366:LEU:HD13	2:B:372:TRP:HE1	1.86	0.40
1:A:505:LEU:HD11	1:A:763:ARG:HD3	2.03	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	755/838 (90%)	725 (96%)	30 (4%)	0	100	100
1	C	768/838 (92%)	722 (94%)	46 (6%)	0	100	100
2	B	734/837 (88%)	688 (94%)	46 (6%)	0	100	100
2	D	732/837 (88%)	686 (94%)	46 (6%)	0	100	100
All	All	2989/3350 (89%)	2821 (94%)	168 (6%)	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	661/722 (92%)	661 (100%)	0	100	100
1	C	670/722 (93%)	670 (100%)	0	100	100
2	B	653/726 (90%)	653 (100%)	0	100	100
2	D	651/726 (90%)	651 (100%)	0	100	100
All	All	2635/2896 (91%)	2635 (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. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	73	GLN
1	A	94	HIS
1	A	162	HIS
1	A	311	ASN
1	A	405	GLN
1	A	477	HIS
1	A	536	GLN
1	A	727	HIS
1	A	780	HIS
2	B	42	HIS
2	B	106	GLN
2	B	223	HIS
2	B	332	HIS
2	B	387	HIS
2	B	702	HIS
2	B	709	ASN
1	C	94	HIS
1	C	99	ASN
1	C	196	GLN
1	C	270	GLN
1	C	405	GLN
1	C	427	ASN
1	C	536	GLN
1	C	616	ASN
1	C	709	HIS

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Mol	Chain	Res	Type
1	C	780	HIS
1	C	812	ASN
2	D	53	ASN
2	D	218	GLN
2	D	323	GLN
2	D	332	HIS
2	D	335	HIS
2	D	336	GLN
2	D	358	HIS
2	D	387	HIS
2	D	620	GLN
2	D	674	HIS
2	D	702	HIS
2	D	774	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)

34 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	NAG	C	907	1	14,14,15	0.42	0	17,19,21	0.80	1 (5%)
3	NAG	D	901	2	14,14,15	0.56	0	17,19,21	0.61	0
3	NAG	A	904	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
3	NAG	D	904	2	14,14,15	0.66	1 (7%)	17,19,21	2.08	4 (23%)
3	NAG	C	910	1	14,14,15	0.41	0	17,19,21	0.96	1 (5%)
3	NAG	D	903	2	14,14,15	0.43	0	17,19,21	1.03	1 (5%)
3	NAG	A	911	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
3	NAG	C	901	1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
3	NAG	C	904	1	14,14,15	0.37	0	17,19,21	0.80	1 (5%)
3	NAG	C	903	1	14,14,15	0.36	0	17,19,21	0.84	1 (5%)
3	NAG	B	905	2	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
3	NAG	B	906	2	14,14,15	0.46	0	17,19,21	1.20	3 (17%)
3	NAG	B	904	2	14,14,15	0.60	0	17,19,21	1.19	2 (11%)
3	NAG	C	911	1	14,14,15	0.54	0	17,19,21	1.28	3 (17%)
3	NAG	A	908	1	14,14,15	0.37	0	17,19,21	0.84	1 (5%)
3	NAG	D	905	2	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
3	NAG	C	902	1	14,14,15	0.36	0	17,19,21	0.82	1 (5%)
3	NAG	A	910	1	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
3	NAG	D	902	2	14,14,15	0.46	0	17,19,21	1.79	1 (5%)
3	NAG	C	908	1	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
3	NAG	A	905	1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
3	NAG	A	901	1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
3	NAG	A	906	1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
3	NAG	A	909	1	14,14,15	0.67	1 (7%)	17,19,21	1.23	4 (23%)
3	NAG	B	902	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
3	NAG	C	905	1	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
3	NAG	C	906	1	14,14,15	0.50	0	17,19,21	1.14	1 (5%)
3	NAG	B	901	2	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
3	NAG	A	907	1	14,14,15	0.35	0	17,19,21	0.91	1 (5%)
3	NAG	C	909	1	14,14,15	0.50	0	17,19,21	0.65	0
3	NAG	A	902	1	14,14,15	0.39	0	17,19,21	0.77	1 (5%)
3	NAG	B	903	2	14,14,15	0.40	0	17,19,21	0.96	1 (5%)
3	NAG	A	903	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
3	NAG	D	906	2	14,14,15	0.37	0	17,19,21	0.83	1 (5%)

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	NAG	C	907	1	-	3/6/23/26	0/1/1/1
3	NAG	D	901	2	-	3/6/23/26	0/1/1/1
3	NAG	A	904	1	-	0/6/23/26	0/1/1/1
3	NAG	D	904	2	-	4/6/23/26	0/1/1/1
3	NAG	C	910	1	-	3/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	A	911	1	-	0/6/23/26	0/1/1/1
3	NAG	C	901	1	-	0/6/23/26	0/1/1/1
3	NAG	C	904	1	-	2/6/23/26	0/1/1/1
3	NAG	C	903	1	-	2/6/23/26	0/1/1/1
3	NAG	B	905	2	-	3/6/23/26	0/1/1/1
3	NAG	B	906	2	-	4/6/23/26	0/1/1/1
3	NAG	B	904	2	-	3/6/23/26	0/1/1/1
3	NAG	C	911	1	-	3/6/23/26	0/1/1/1
3	NAG	A	908	1	-	2/6/23/26	0/1/1/1
3	NAG	D	905	2	-	3/6/23/26	0/1/1/1
3	NAG	C	902	1	-	0/6/23/26	0/1/1/1
3	NAG	A	910	1	-	3/6/23/26	0/1/1/1
3	NAG	D	902	2	-	4/6/23/26	0/1/1/1
3	NAG	C	908	1	-	2/6/23/26	0/1/1/1
3	NAG	A	905	1	-	3/6/23/26	0/1/1/1
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	NAG	A	906	1	-	2/6/23/26	0/1/1/1
3	NAG	A	909	1	-	4/6/23/26	0/1/1/1
3	NAG	B	902	2	-	4/6/23/26	0/1/1/1
3	NAG	C	905	1	-	0/6/23/26	0/1/1/1
3	NAG	C	906	1	-	2/6/23/26	0/1/1/1
3	NAG	B	901	2	-	2/6/23/26	0/1/1/1
3	NAG	A	907	1	-	0/6/23/26	0/1/1/1
3	NAG	C	909	1	-	0/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	B	903	2	-	3/6/23/26	0/1/1/1
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	906	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	NAG	C1-C2	2.17	1.55	1.52
3	D	904	NAG	C1-C2	2.03	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	902	NAG	C1-O5-C5	6.72	121.19	112.19
3	D	904	NAG	C1-O5-C5	6.66	121.11	112.19
3	C	906	NAG	C1-O5-C5	3.92	117.44	112.19
3	D	903	NAG	C1-O5-C5	3.82	117.30	112.19
3	C	911	NAG	C1-O5-C5	3.39	116.73	112.19
3	B	904	NAG	C1-O5-C5	3.38	116.71	112.19
3	B	903	NAG	C1-O5-C5	3.28	116.59	112.19
3	C	910	NAG	C1-O5-C5	3.24	116.52	112.19
3	B	902	NAG	C1-O5-C5	3.19	116.46	112.19
3	A	906	NAG	C1-O5-C5	3.13	116.39	112.19
3	A	907	NAG	C1-O5-C5	3.09	116.32	112.19
3	D	904	NAG	O5-C1-C2	3.07	116.04	111.29
3	C	903	NAG	C1-O5-C5	3.02	116.23	112.19
3	B	906	NAG	C1-O5-C5	3.01	116.22	112.19
3	C	908	NAG	C1-O5-C5	2.97	116.17	112.19
3	B	905	NAG	C1-O5-C5	2.96	116.15	112.19
3	D	904	NAG	C4-C3-C2	2.95	115.34	111.02
3	A	910	NAG	C1-O5-C5	2.93	116.11	112.19
3	A	908	NAG	C1-O5-C5	2.92	116.10	112.19
3	D	905	NAG	C1-O5-C5	2.87	116.03	112.19
3	C	902	NAG	C1-O5-C5	2.83	115.98	112.19
3	C	904	NAG	C1-O5-C5	2.80	115.93	112.19
3	A	904	NAG	C1-O5-C5	2.78	115.92	112.19
3	A	903	NAG	C1-O5-C5	2.76	115.88	112.19
3	A	911	NAG	C1-O5-C5	2.76	115.88	112.19
3	B	901	NAG	C1-O5-C5	2.76	115.88	112.19
3	C	907	NAG	C1-O5-C5	2.74	115.86	112.19
3	D	904	NAG	C2-N2-C7	2.72	126.55	122.90
3	C	905	NAG	C1-O5-C5	2.71	115.82	112.19
3	A	901	NAG	C1-O5-C5	2.70	115.80	112.19
3	C	901	NAG	C1-O5-C5	2.68	115.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	911	NAG	C2-N2-C7	2.66	126.46	122.90
3	D	906	NAG	C1-O5-C5	2.65	115.74	112.19
3	A	905	NAG	C1-O5-C5	2.64	115.73	112.19
3	A	902	NAG	C1-O5-C5	2.62	115.70	112.19
3	B	906	NAG	C2-N2-C7	2.44	126.17	122.90
3	B	906	NAG	C1-C2-N2	2.41	114.23	110.43
3	B	904	NAG	C2-N2-C7	2.41	126.12	122.90
3	A	909	NAG	O5-C1-C2	-2.40	107.58	111.29
3	A	909	NAG	C1-C2-N2	2.39	114.21	110.43
3	A	909	NAG	C4-C3-C2	2.33	114.44	111.02
3	A	909	NAG	C2-N2-C7	2.30	125.99	122.90
3	C	911	NAG	C1-C2-N2	2.04	113.64	110.43

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	NAG	C8-C7-N2-C2
3	A	903	NAG	O7-C7-N2-C2
3	A	905	NAG	C1-C2-N2-C7
3	A	905	NAG	C8-C7-N2-C2
3	A	905	NAG	O7-C7-N2-C2
3	A	906	NAG	C8-C7-N2-C2
3	A	906	NAG	O7-C7-N2-C2
3	A	909	NAG	C1-C2-N2-C7
3	A	909	NAG	C8-C7-N2-C2
3	A	909	NAG	O7-C7-N2-C2
3	A	910	NAG	C1-C2-N2-C7
3	A	910	NAG	C8-C7-N2-C2
3	A	910	NAG	O7-C7-N2-C2
3	B	901	NAG	C8-C7-N2-C2
3	B	901	NAG	O7-C7-N2-C2
3	B	903	NAG	C1-C2-N2-C7
3	B	903	NAG	C8-C7-N2-C2
3	B	903	NAG	O7-C7-N2-C2
3	B	904	NAG	C1-C2-N2-C7
3	B	904	NAG	C8-C7-N2-C2
3	B	904	NAG	O7-C7-N2-C2
3	B	905	NAG	C1-C2-N2-C7
3	B	905	NAG	C8-C7-N2-C2
3	B	905	NAG	O7-C7-N2-C2
3	B	906	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	906	NAG	C8-C7-N2-C2
3	B	906	NAG	O7-C7-N2-C2
3	C	903	NAG	O7-C7-N2-C2
3	C	906	NAG	C8-C7-N2-C2
3	C	906	NAG	O7-C7-N2-C2
3	C	907	NAG	C8-C7-N2-C2
3	C	907	NAG	O7-C7-N2-C2
3	C	910	NAG	C1-C2-N2-C7
3	C	910	NAG	C8-C7-N2-C2
3	C	910	NAG	O7-C7-N2-C2
3	C	911	NAG	C1-C2-N2-C7
3	C	911	NAG	C8-C7-N2-C2
3	C	911	NAG	O7-C7-N2-C2
3	D	902	NAG	C8-C7-N2-C2
3	D	902	NAG	O7-C7-N2-C2
3	D	903	NAG	C8-C7-N2-C2
3	D	903	NAG	O7-C7-N2-C2
3	D	904	NAG	C3-C2-N2-C7
3	D	904	NAG	C8-C7-N2-C2
3	D	904	NAG	O7-C7-N2-C2
3	D	905	NAG	C1-C2-N2-C7
3	D	905	NAG	C8-C7-N2-C2
3	D	905	NAG	O7-C7-N2-C2
3	D	906	NAG	C3-C2-N2-C7
3	D	906	NAG	C8-C7-N2-C2
3	D	906	NAG	O7-C7-N2-C2
3	C	903	NAG	C8-C7-N2-C2
3	A	908	NAG	C8-C7-N2-C2
3	A	908	NAG	O7-C7-N2-C2
3	C	908	NAG	C8-C7-N2-C2
3	C	908	NAG	O7-C7-N2-C2
3	A	902	NAG	C8-C7-N2-C2
3	A	902	NAG	O7-C7-N2-C2
3	D	901	NAG	C8-C7-N2-C2
3	D	901	NAG	O7-C7-N2-C2
3	B	902	NAG	C8-C7-N2-C2
3	D	901	NAG	O5-C5-C6-O6
3	D	902	NAG	O5-C5-C6-O6
3	A	909	NAG	O5-C5-C6-O6
3	D	904	NAG	O5-C5-C6-O6
3	C	907	NAG	O5-C5-C6-O6
3	B	906	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	902	NAG	O7-C7-N2-C2
3	B	902	NAG	C4-C5-C6-O6
3	B	902	NAG	O5-C5-C6-O6
3	C	904	NAG	C8-C7-N2-C2
3	D	902	NAG	C1-C2-N2-C7
3	C	904	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	906	NAG	1	0

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.

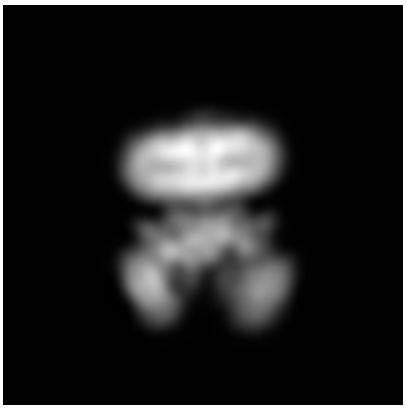
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9149. 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.

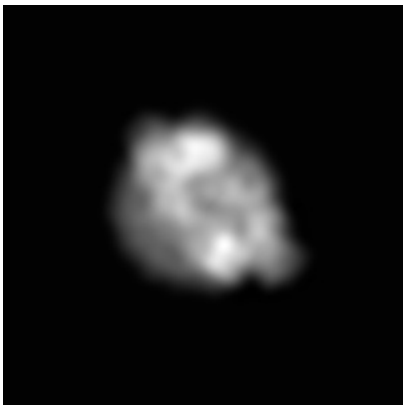
6.1 Orthogonal projections

6.1.1 Primary map



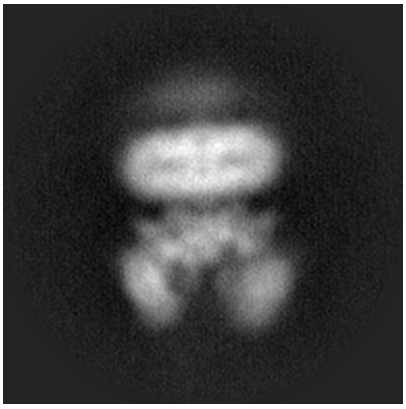
X

Y

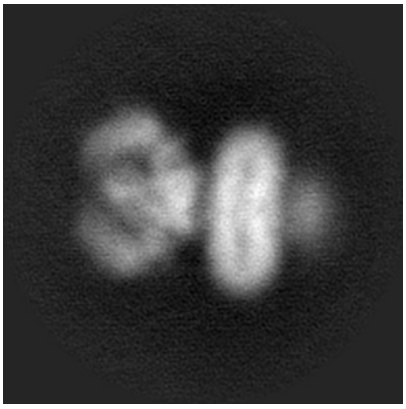


Z

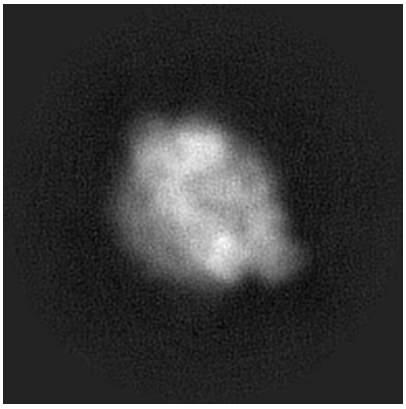
6.1.2 Raw map



X



Y



Z

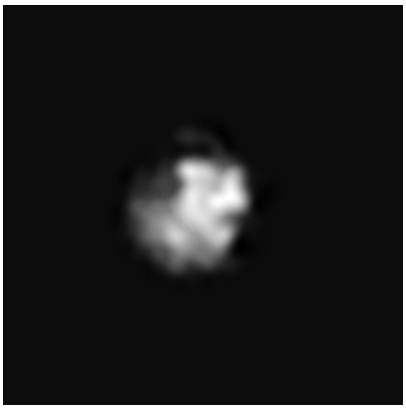
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

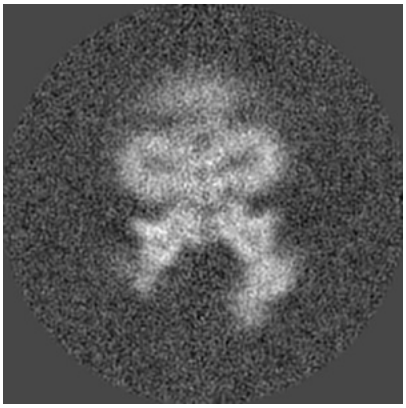
X Index: 96

Y Index: 96

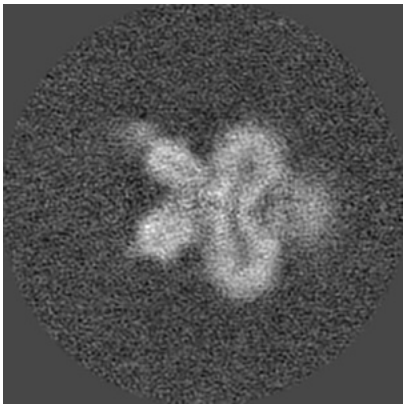


Z Index: 96

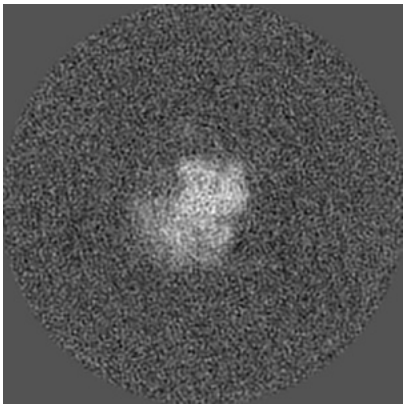
6.2.2 Raw map



X Index: 96



Y Index: 96

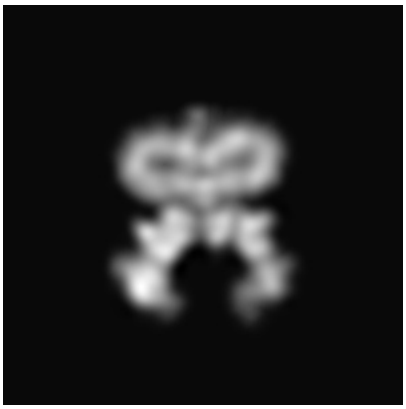


Z Index: 96

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

6.3 Largest variance slices (i)

6.3.1 Primary map

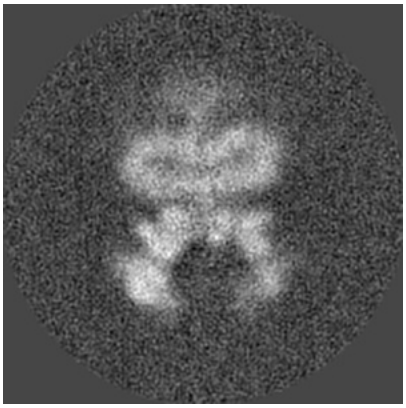


X Index: 102

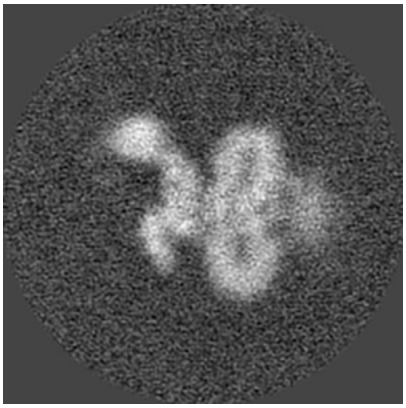
Y Index: 74

Z Index: 122

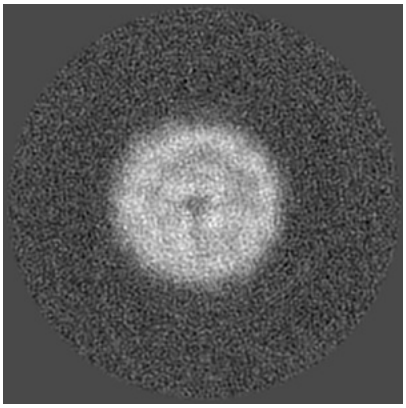
6.3.2 Raw map



X Index: 103



Y Index: 89

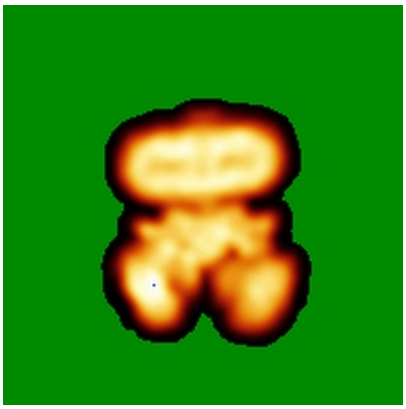


Z Index: 122

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

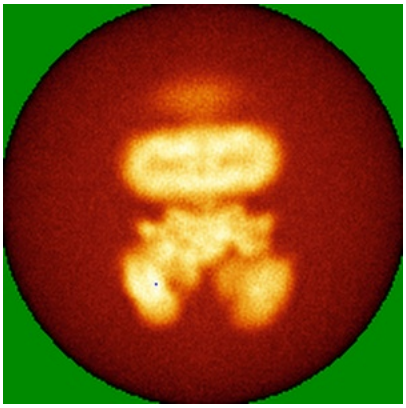


X

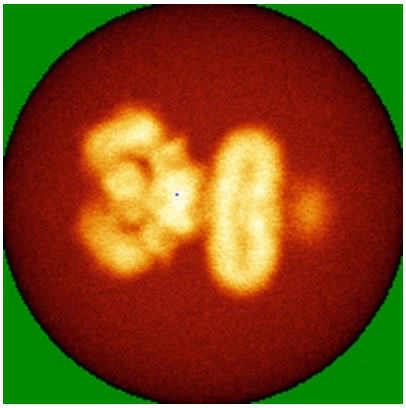
Y

Z

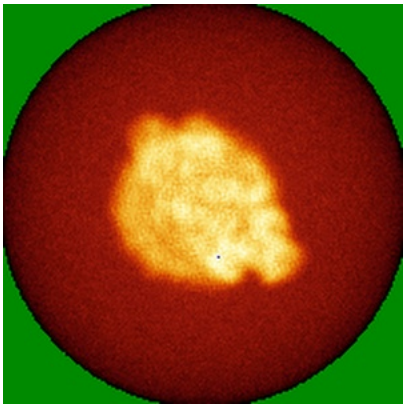
6.4.2 Raw map



X



Y

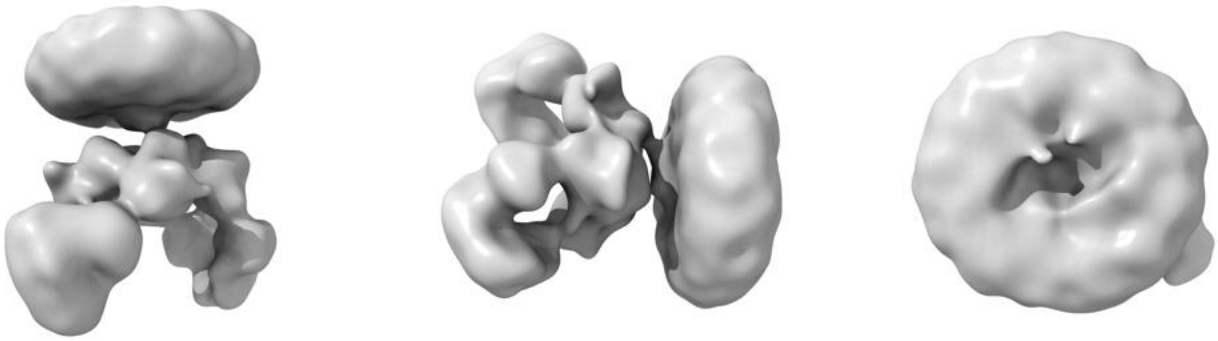


Z

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)

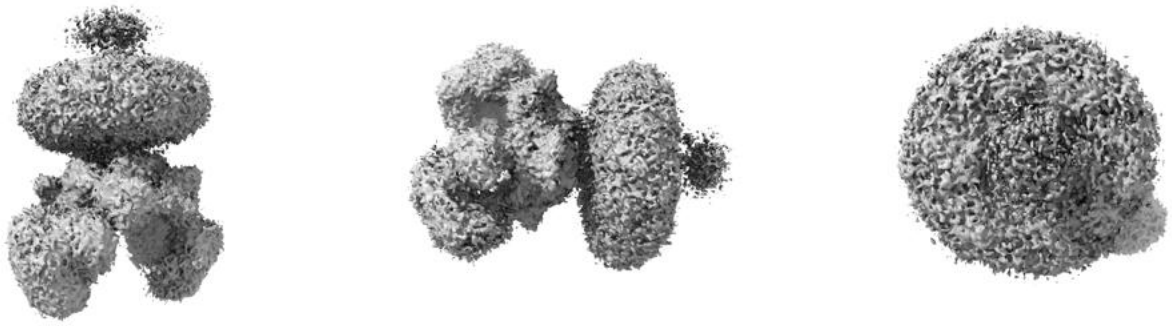
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

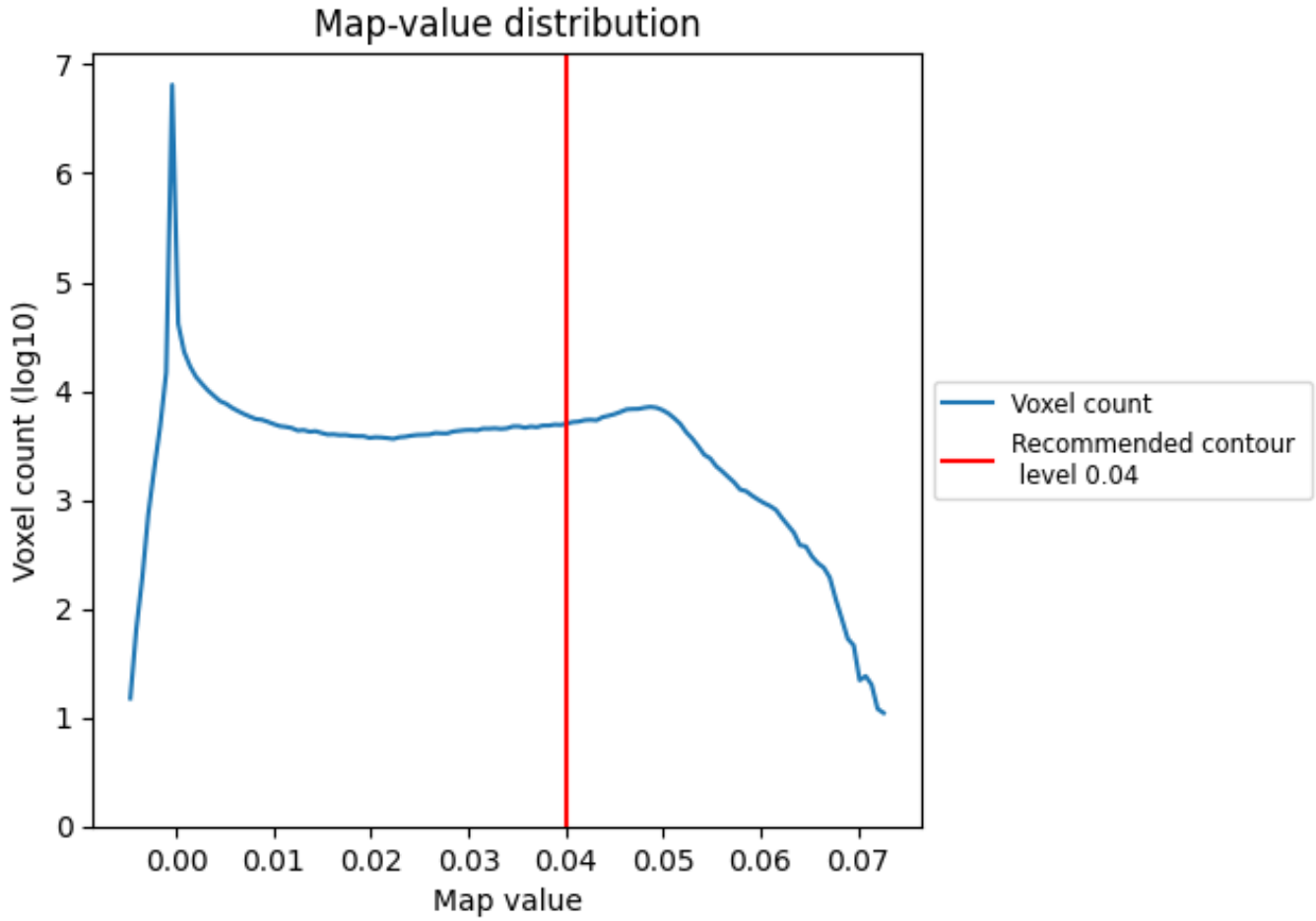
6.6 Mask visualisation (i)

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

7 Map analysis

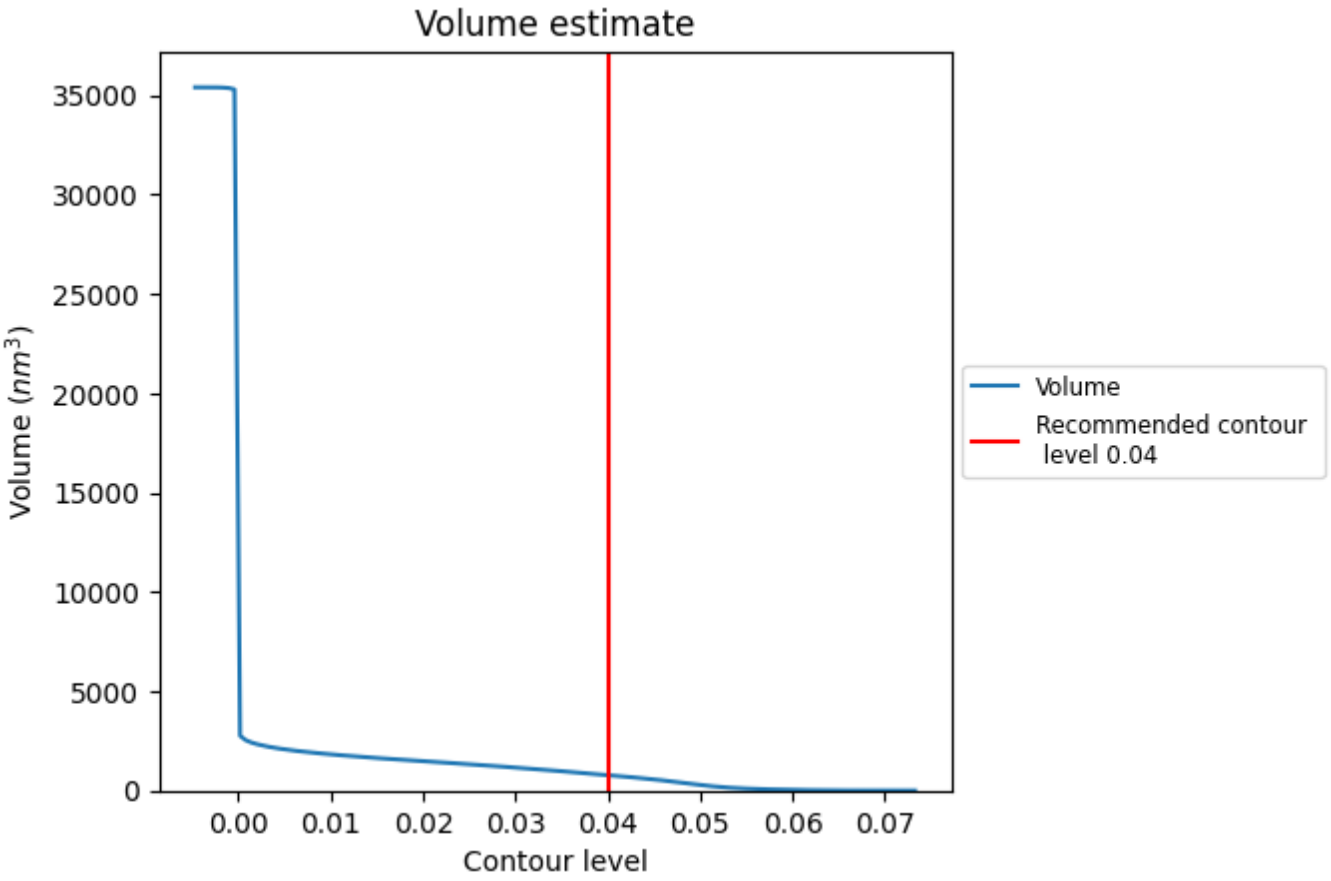
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

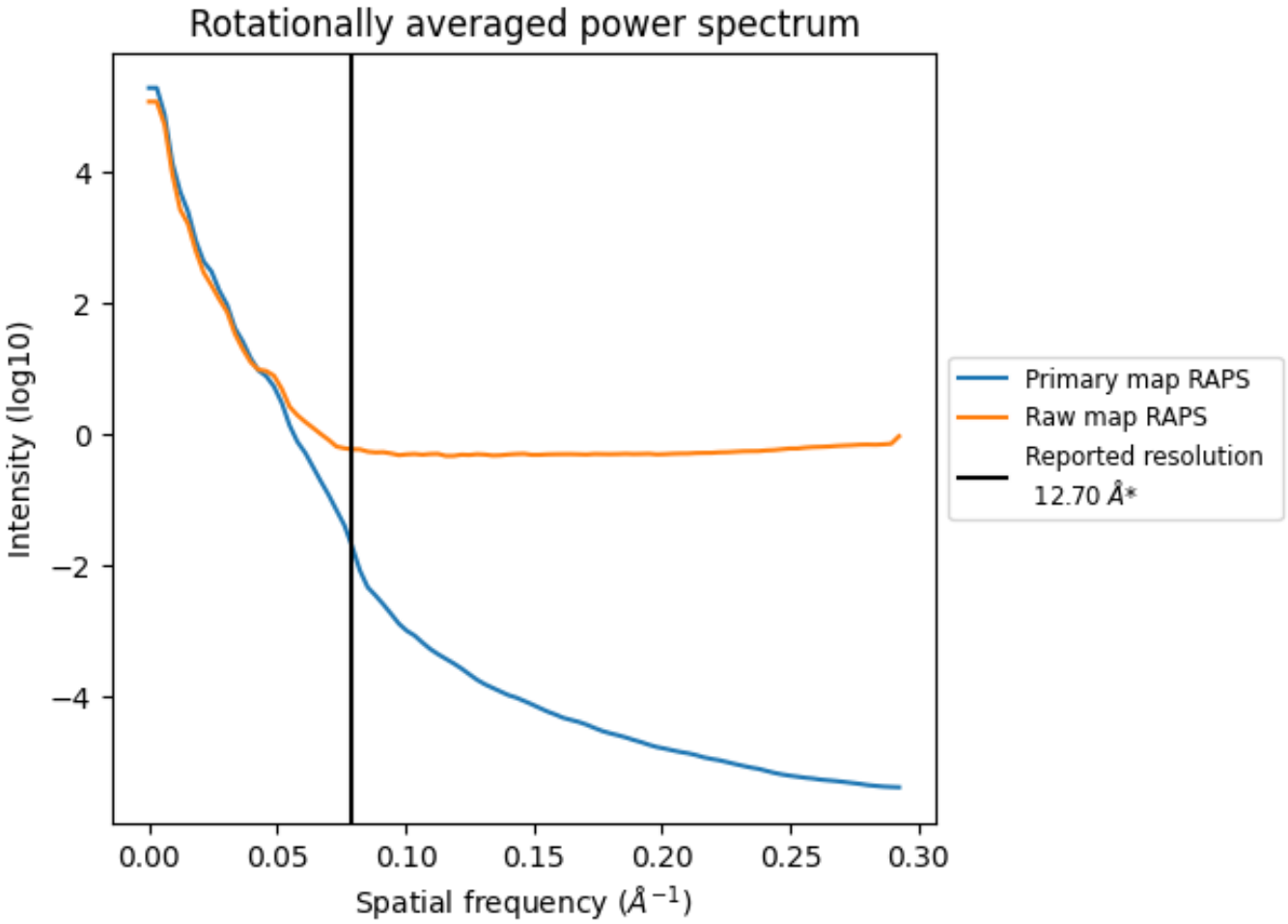
7.2 Volume estimate



The volume at the recommended contour level is 780 nm^3; this corresponds to an approximate mass of 704 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 (i)

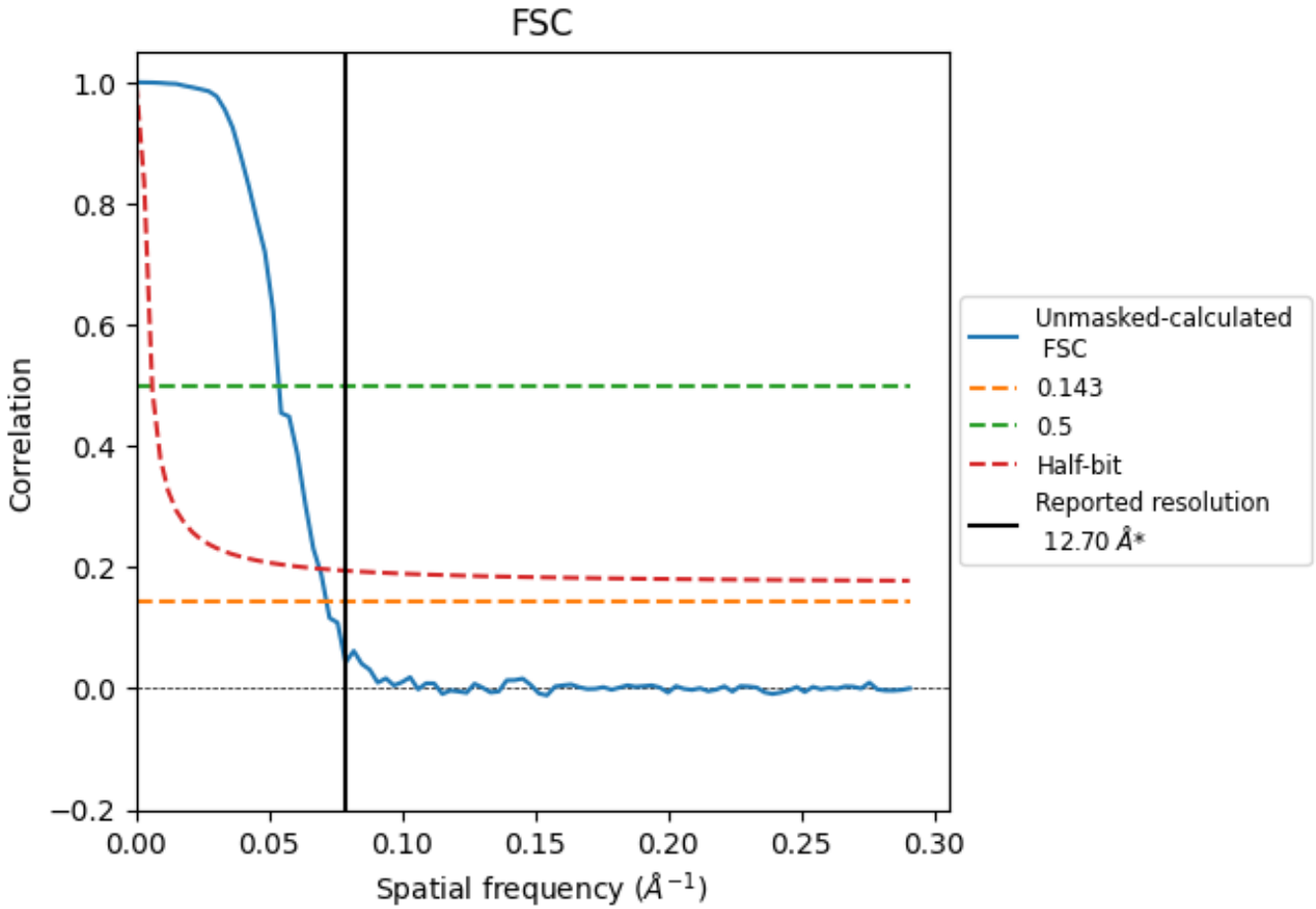


*Reported resolution corresponds to spatial frequency of 0.079 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.079 Å^{-1}

8.2 Resolution estimates (i)

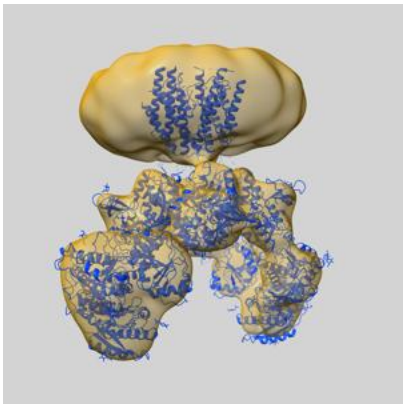
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.99	18.62	14.49

*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 13.99 differs from the reported value 12.7 by more than 10 %

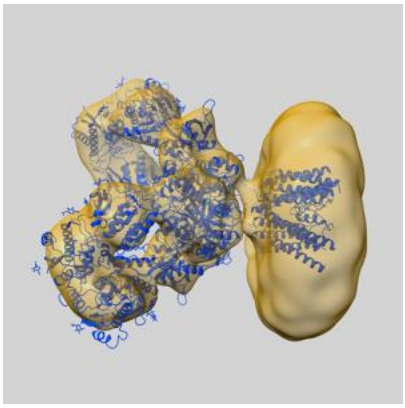
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9149 and PDB model 6MMB. Per-residue inclusion information can be found in section 3 on page 6.

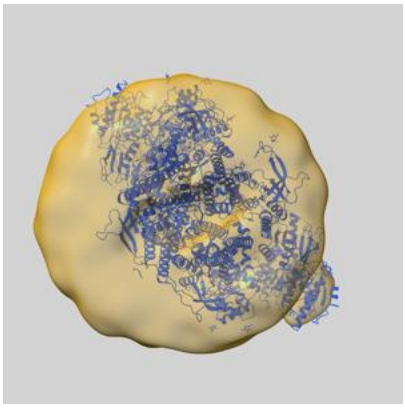
9.1 Map-model overlay



X



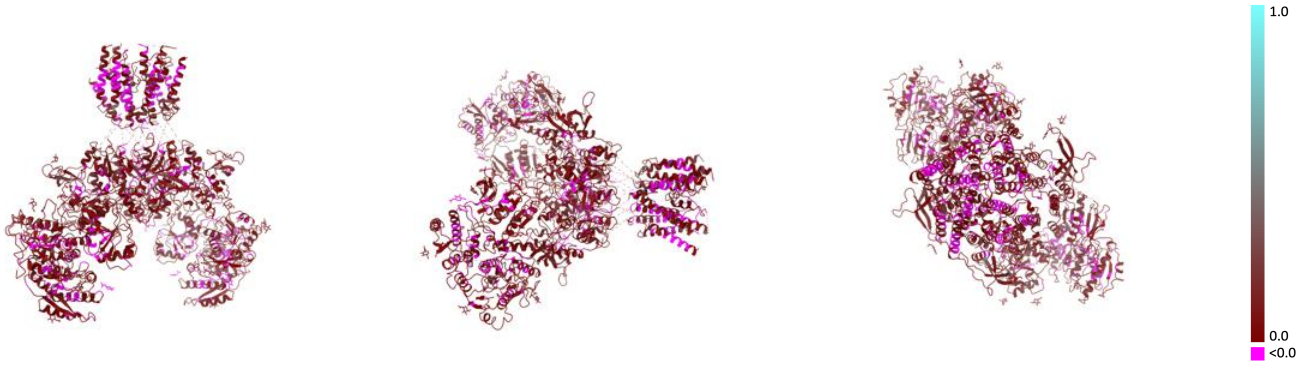
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

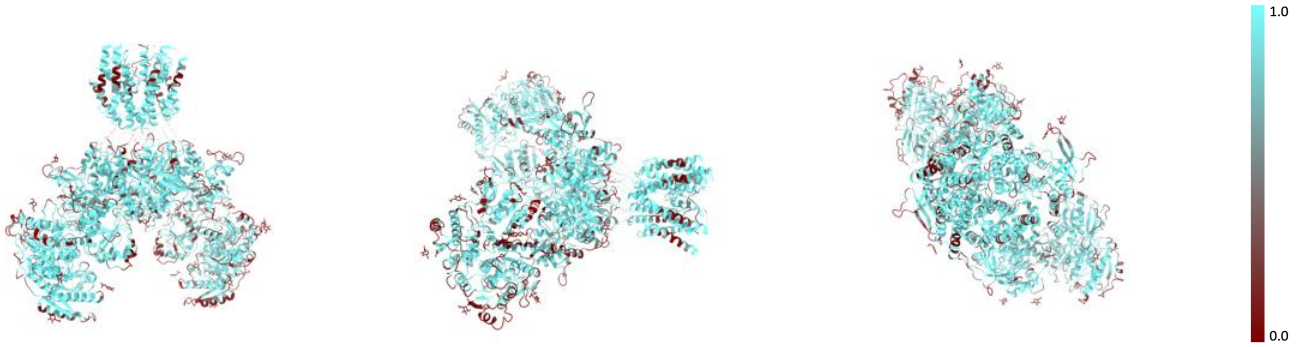
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

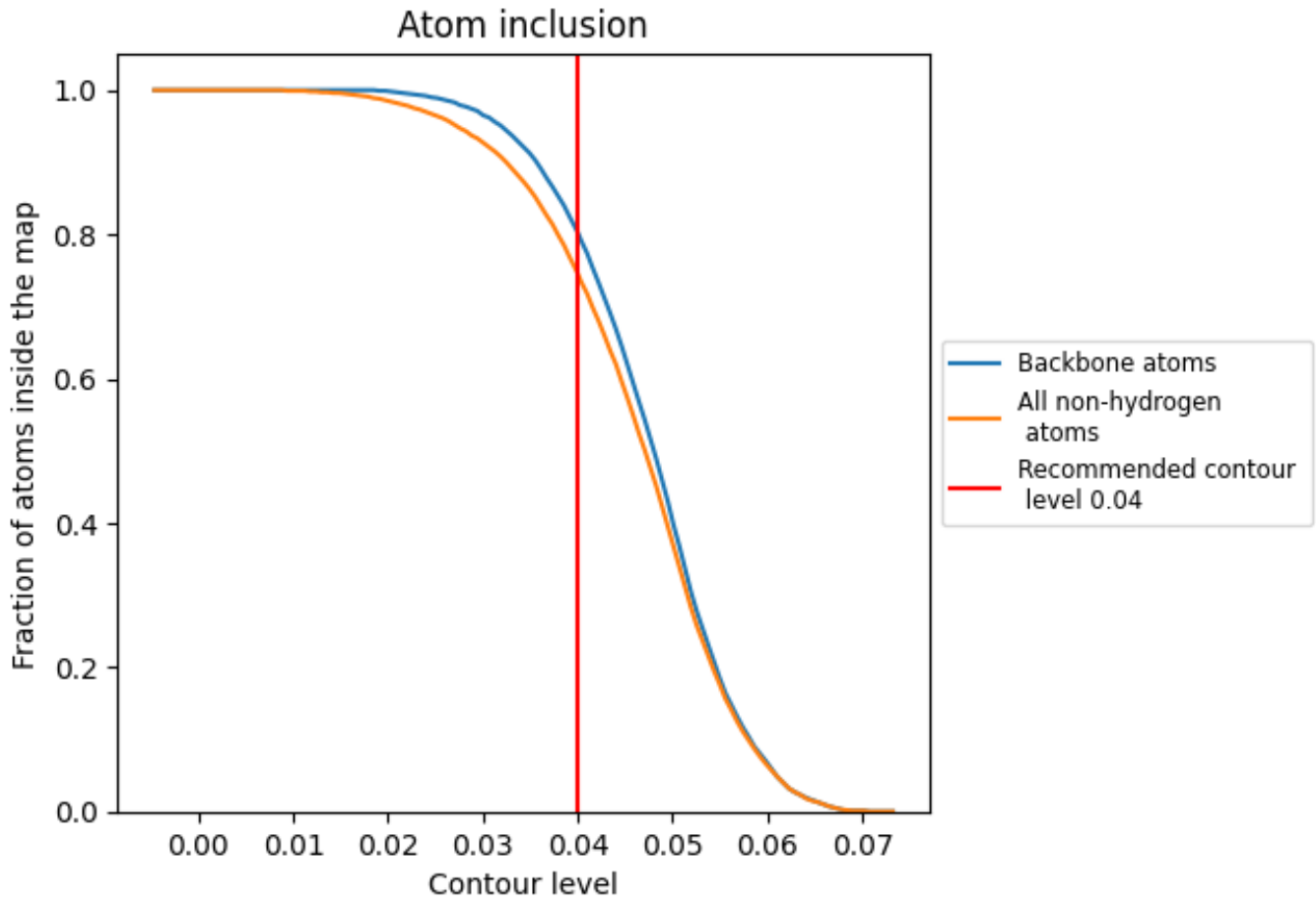
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.0680
A	0.7080	0.0650
B	0.6760	0.0650
C	0.8260	0.0730
D	0.7700	0.0690