Full wwPDB EM Validation Report (i)

Oct 19, 2026 – 05:45 PM JST

PDB ID	:	9X5N / pdb_00009x5n
EMDB ID	:	EMD-66591
Title	:	Cryo-EM structure of SLC4A10 bound K+ and HCO3-
Authors	:	Yang, H.; Sun, P.
Deposited on	:	2025-10-13
Resolution	:	2.52 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 (i) 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 (i)) were used in the production of this report:

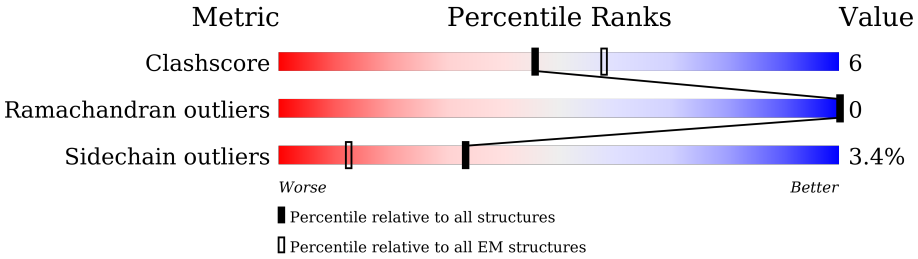
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

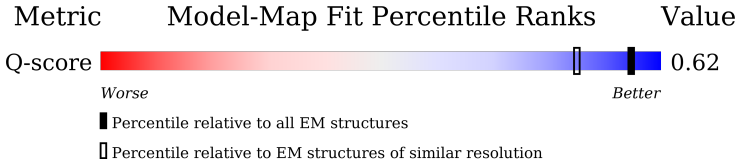
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 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	7226 (2.02 - 3.02)

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	1118	41% 10% 49%
1	B	1118	43% 8% 48%

2 Entry composition (i)

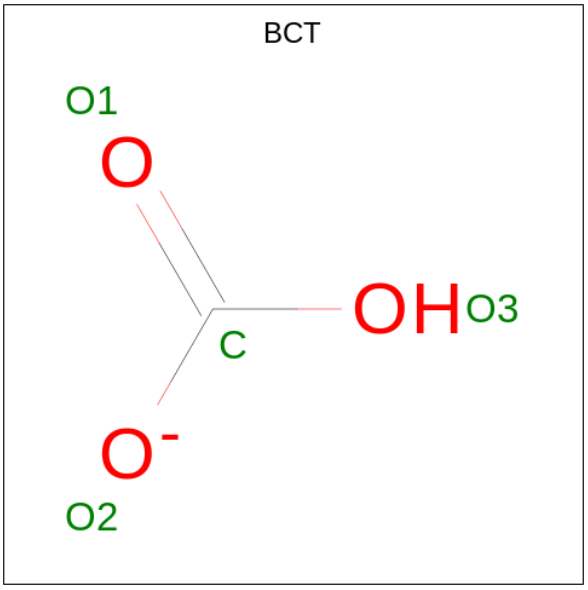
There are 5 unique types of molecules in this entry. The entry contains 9213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sodium-driven chloride bicarbonate exchanger.

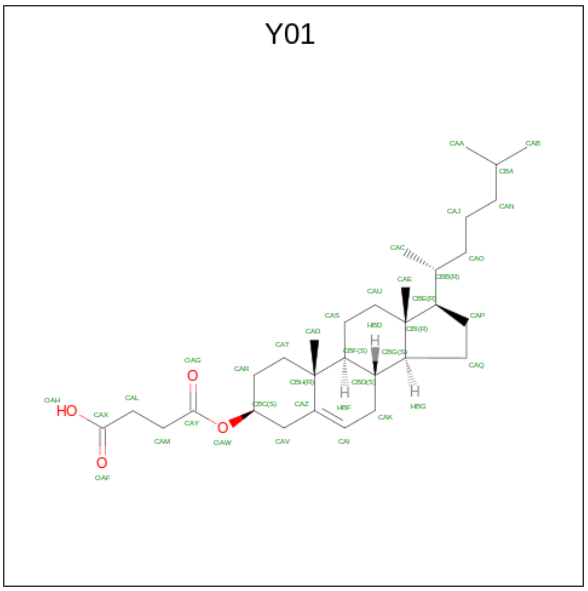
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	574	4547	3002	729	781	35	0	0
1	B	578	4582	3023	734	789	36	1	0

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	4	1	3	0
2	B	1	4	1	3	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	35	31	4	0
3	B	1	35	31	4	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
4	A	1	1	1	0
4	B	1	1	1	0

- Molecule 5 is water.

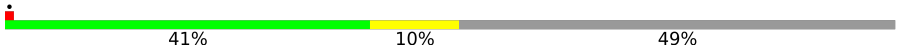
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	A	2	2	2	0
5	B	2	2	2	0

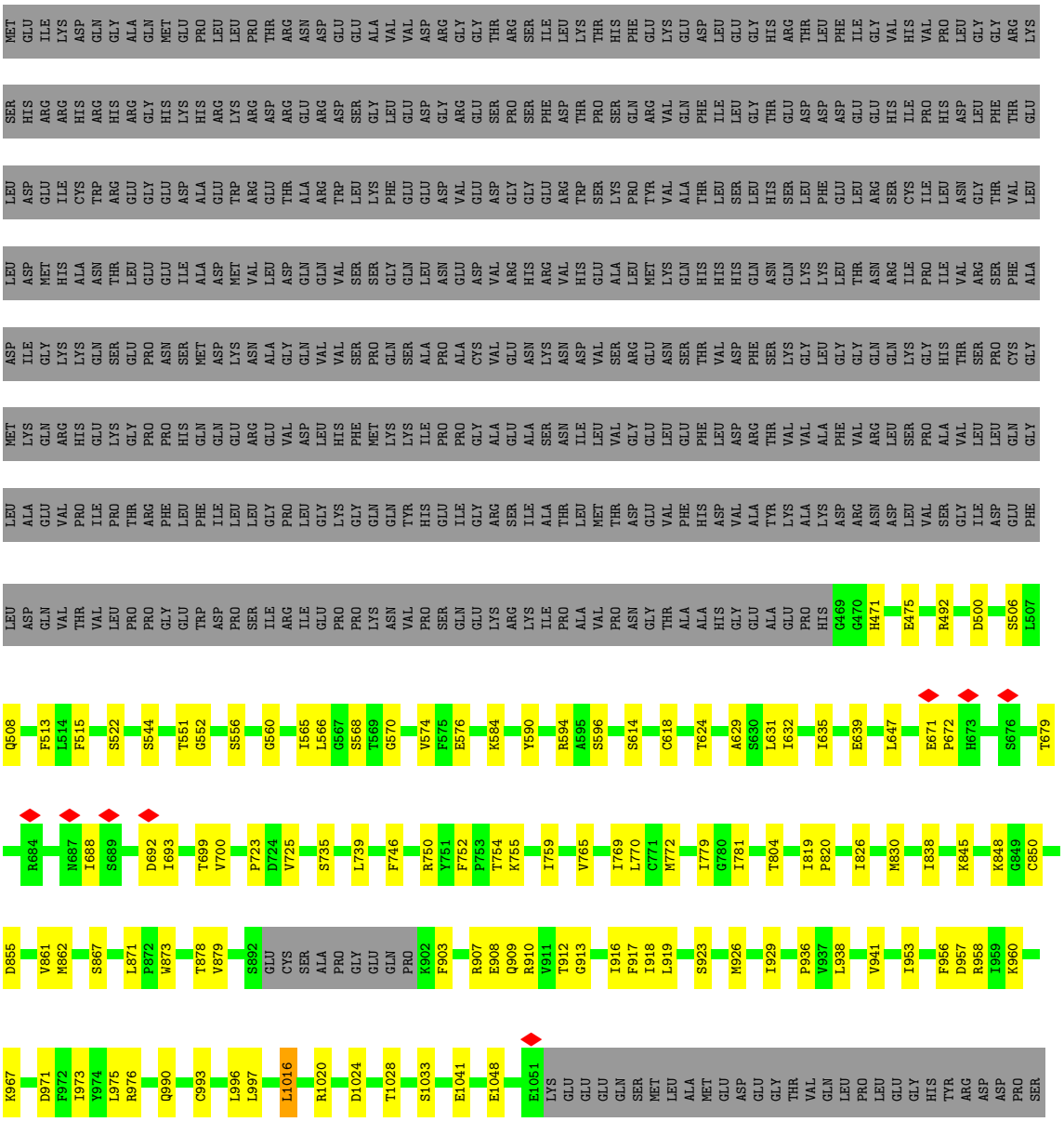
3 Residue-property plots (i)

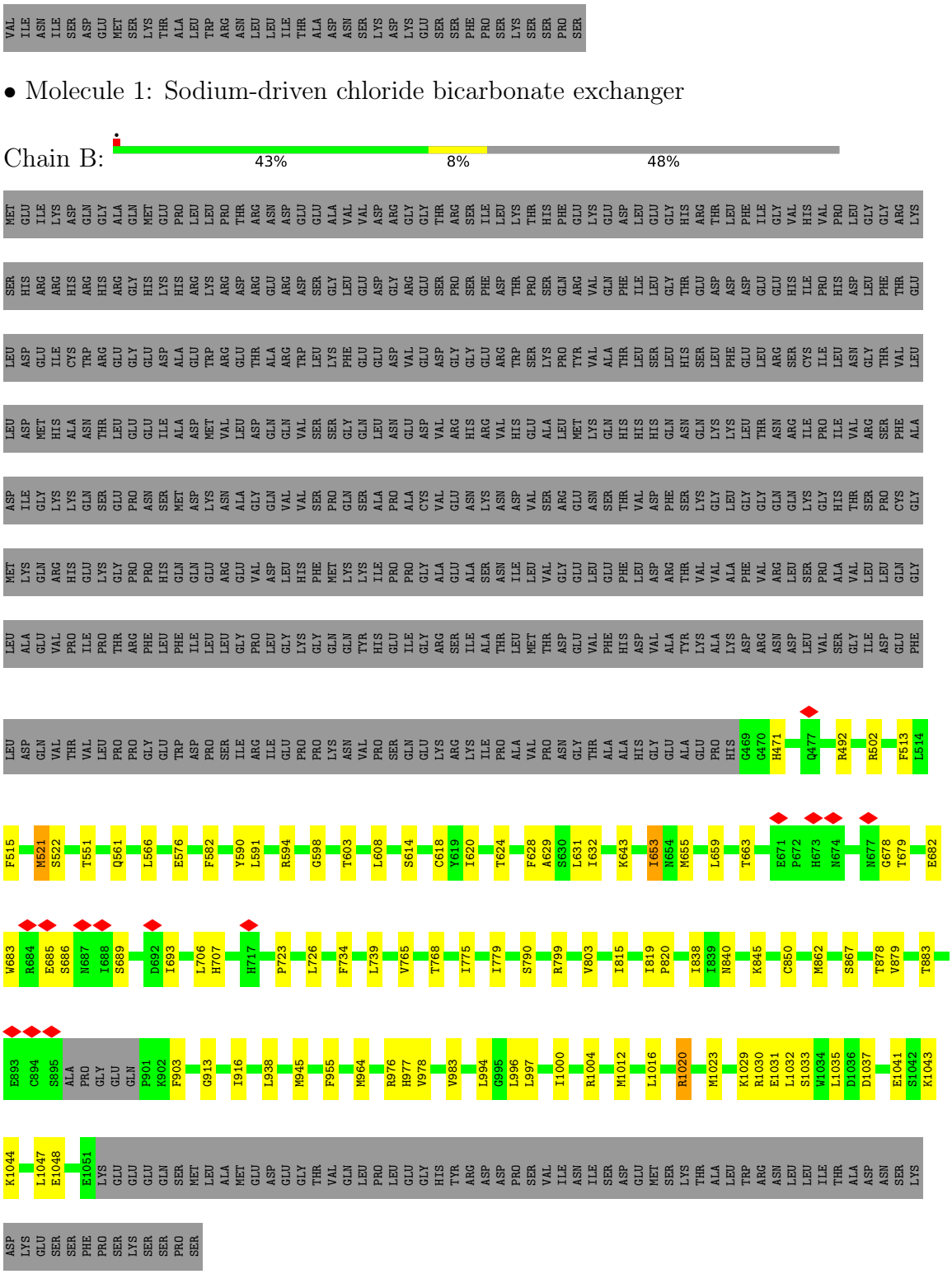
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium-driven chloride bicarbonate exchanger

Chain A:







VAL ILE ASN ILE SER ASP GLU MET SER LYS THR ALA LEU TRP ARG ASN LEU LEU ILE THR ALA ASP ASN SER LYS ASP LYS GLU SER SER PHE PRO SER LYS SER SER PRO SER

- Molecule 1: Sodium-driven chloride bicarbonate exchanger

Chain B: 43% 8% 48%

MET GLU ILE LYS ASP GLN GLY ALA GLN MET GLU PRO LEU LEU PRO THR ARG ASN ASP GLU GLU ALA VAL VAL ASP ARG GLY GLY THR ARG SER ILE LEU LYS THR HIS PHE GLU LYS GLU ASP LEU GLU GLY HIS ARG THR LEU PHE ILE GLY VAL HIS VAL PRO LEU GLY GLY ARG LYS

SER HIS ARG ARG HIS ARG HIS ARG GLY HIS LYS HIS ARG LYS ARG ASP ARG GLU ARG ASP SER GLY LEU GLU ASP GLY ARG GLU SER PRO SER PHE ASP THR PRO SER GLN ARG VAL GLN PHE ILE LEU GLY THR GLU ASP ASP ASP GLU GLU HIS ILE PRO HIS ASP LEU PHE THR GLU

LEU ASP GLU ILE CYS TRP ARG GLU GLY GLU ASP ALA GLU TRP ARG GLU THR ALA ARG TRP LEU LYS PHE GLU GLU ASP VAL GLU ASP GLY GLY GLU ARG TRP SER LYS PRO TYR VAL ALA THR LEU SER LEU HIS SER LEU PHE GLU LEU ARG SER CYS ILE LEU ASN GLY THR VAL LEU

LEU ASP MET HIS ALA ASN THR LEU GLU GLU ILE ALA ASP MET VAL LEU ASP GLN GLN VAL SER SER GLY GLN LEU ASN GLU ASP VAL ARG HIS ARG VAL HIS GLU ALA LEU MET LYS GLN HIS HIS HIS GLN ASN GLN LYS LYS LEU THR ASN ARG ILE PRO ILE VAL ARG SER PHE ALA

ASP ILE GLY LYS LYS GLN SER GLU PRO ASN SER MET ASP LYS ASN ALA GLY GLN VAL VAL SER PRO GLN SER ALA PRO ALA CYS VAL GLU ASN LYS ASN ASP VAL SER ARG GLU ASN SER THR VAL ASP PHE SER LYS GLY LEU GLY GLY GLN GLN LYS GLY HIS THR SER PRO CYS GLY

MET LYS GLN ARG HIS GLU LYS GLY PRO PRO HIS GLN GLN GLU ARG GLU VAL ASP LEU HIS PHE MET LYS LYS ILE PRO PRO GLY ALA GLU ALA SER ASN ILE LEU VAL GLY GLU LEU GLU PHE LEU ASP ARG THR VAL VAL ALA PHE VAL ARG LEU SER PRO ALA VAL LEU LEU GLN GLY

LEU ALA GLU VAL PRO ILE PRO THR ARG PHE LEU PHE ILE LEU LEU GLY PRO LEU GLY LYS GLY GLN GLN TYR HIS GLU ILE GLY ARG SER ILE ALA THR LEU MET THR ASP GLU VAL PHE HIS ASP VAL ALA TYR LYS ALA LYS ASP ARG ASN ASP LEU VAL SER GLY ILE ASP GLU PHE

LEU ASP GLN VAL THR VAL LEU PRO PRO GLY GLU TRP ASP PRO SER ILE ARG ILE GLU PRO PRO LYS ASN VAL PRO SER GLN GLU LYS ARG LYS ILE PRO ALA VAL PRO ASN GLY THR ALA ALA HIS GLY GLU ALA GLU PRO HIS G469 G470 H471 Q477 R492 R502 F513 L514

F515 M521 S522 T551 Q561 L566 E576 F582 Y590 L591 R594 G598 T603 L608 S614 C618 Y619 I620 T624 F628 A629 S630 L631 I632 K643 I653 N654 M655 L659 T663 E671 P672 H673 N674 N677 G678 T679 E682

W683 R684 E685 S686 N687 I688 S689 D692 I693 L706 H707 H717 P723 L726 F734 L739 V765 T768 I775 I779 S790 R799 V803 I815 I819 P820 I838 I839 N840 K845 C850 M862 S867 T878 V879 T883

E893 C894 S895 ALA PRO GLY GLU GLN P901 K902 F903 G913 I916 L938 M945 F955 M964 R976 H977 V978 V983 L994 G995 L996 L997 I1000 R1004 M1012 L1016 R1020 M1023 K1029 R1030 E1031 L1032 S1033 W1034 L1035 D1036 D1037 E1041 S1042 K1043

K1044 L1047 E1048 E1051 LYS GLU GLU GLU GLN SER MET LEU ALA MET GLU ASP GLU GLY THR VAL GLN LEU PRO LEU GLU GLY HIS TYR ARG ASP ASP PRO SER VAL ILE ASN ILE SER ASP GLU MET SER LYS THR ALA LEU TRP ARG ASN LEU LEU ILE THR ALA ASP ASN SER LYS

ASP LYS GLU SER SER PHE PRO SER LYS SER SER PRO SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221965	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 ($e^-/Å^2$)	51.22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.223	Depositor
Minimum map value	-0.751	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.114	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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: K, Y01, BCT

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	0.12	0/4665	0.26	0/6327
1	B	0.13	0/4701	0.27	0/6376
All	All	0.13	0/9366	0.26	0/12703

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	4547	0	4679	61	0
1	B	4582	0	4711	58	0
2	A	4	0	1	0	0
2	B	4	0	0	1	0
3	A	35	0	49	0	0
3	B	35	0	49	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
All	All	9213	0	9489	116	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 6.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:GLU:OE2	1:B:594:ARG:NH2	2.25	0.69
1:A:513:PHE:HZ	1:A:919:LEU:HD21	1.57	0.69
1:B:631:LEU:HD22	1:B:997:LEU:HB3	1.74	0.68
1:B:1029:LYS:O	1:B:1029:LYS:NZ	2.22	0.67
1:B:679:THR:HG1	1:B:707:HIS:HD1	1.41	0.66
1:A:629:ALA:HB2	1:A:838:ILE:HD13	1.78	0.65
1:B:978:VAL:HG13	1:B:1031:GLU:HG2	1.78	0.64
1:B:561:GLN:NE2	1:B:840:ASN:OD1	2.31	0.63
1:A:635:ILE:O	1:A:639:GLU:HG2	1.99	0.60
1:A:492:ARG:NH1	1:A:850:CYS:O	2.34	0.60
1:B:632:ILE:HG22	1:B:879:VAL:HG23	1.84	0.60
1:A:551:THR:HG22	1:A:566:LEU:HD12	1.85	0.59
1:A:958:ARG:NH2	1:A:990:GLN:OE1	2.33	0.59
1:A:976:ARG:NH1	1:A:1048:GLU:OE1	2.36	0.57
1:A:471:HIS:HB2	1:A:618:CYS:HA	1.85	0.57
1:B:629:ALA:HB2	1:B:838:ILE:HD13	1.87	0.57
1:A:508:GLN:OE1	1:A:907:ARG:NH1	2.37	0.57
1:A:551:THR:HA	1:A:862:MET:HG3	1.88	0.56
1:B:591:LEU:HB3	1:B:803:VAL:HG11	1.89	0.55
1:B:913:GLY:HA2	1:B:916:ILE:HD12	1.88	0.55
1:A:867:SER:OG	1:A:873:TRP:NE1	2.41	0.54
1:A:522:SER:HB2	1:A:938:LEU:HD13	1.88	0.54
1:A:725:VAL:HG21	1:B:659:LEU:HD11	1.89	0.54
1:A:735:SER:HB2	1:A:772:MET:HE2	1.90	0.54
1:A:723:PRO:HB3	1:B:723:PRO:HB3	1.90	0.53
1:A:631:LEU:HD22	1:A:997:LEU:HB3	1.90	0.53
1:B:996:LEU:O	1:B:1000:ILE:HD12	2.08	0.53
1:B:983:VAL:HG22	1:B:1035:LEU:HD21	1.90	0.53
1:B:693:ILE:HD13	1:B:706:LEU:HD13	1.90	0.53
1:B:977:HIS:NE2	1:B:1048:GLU:OE2	2.40	0.52
1:A:993:CYS:HB3	1:A:1016:LEU:HD11	1.91	0.52
1:B:551:THR:HA	1:B:862:MET:HG3	1.91	0.52
1:A:560:GLY:N	1:A:855:ASP:OD1	2.43	0.52
1:B:1004:ARG:N	1:B:1004:ARG:HD3	2.25	0.52
1:A:953:ILE:HG22	1:A:956:PHE:H	1.75	0.52
1:A:746:PHE:HZ	1:A:752:PHE:HD2	1.58	0.52
1:A:826:ILE:HG23	1:A:830:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:ILE:HG22	1:A:781:ILE:HG12	1.93	0.51
1:B:734:PHE:HE2	3:B:1202:Y01:HAP1	1.75	0.51
1:A:624:THR:HG23	1:A:1016:LEU:HB3	1.93	0.50
1:A:861:VAL:HG12	1:A:862:MET:HE2	1.93	0.50
1:A:632:ILE:HG22	1:A:879:VAL:HG23	1.94	0.49
1:A:750:ARG:HB2	1:B:964:MET:HE2	1.93	0.49
1:A:570:GLY:O	1:A:574:VAL:HG23	2.12	0.49
1:B:632:ILE:HG21	1:B:878:THR:HB	1.93	0.49
1:A:671:GLU:HG3	1:A:672:PRO:HD2	1.94	0.49
1:B:1043:LYS:O	1:B:1047:LEU:HG	2.12	0.49
1:B:679:THR:OG1	1:B:707:HIS:ND1	2.37	0.48
1:B:739:LEU:HB3	1:B:768:THR:HG23	1.95	0.48
1:B:689:SER:O	1:B:693:ILE:HG13	2.13	0.48
1:B:471:HIS:ND1	1:B:620:ILE:O	2.35	0.48
1:A:967:LYS:HE3	1:A:967:LYS:HA	1.96	0.47
1:B:734:PHE:CE2	3:B:1202:Y01:HAP1	2.49	0.47
1:B:1012:MET:HA	1:B:1012:MET:HE2	1.95	0.47
1:B:819:ILE:HB	1:B:820:PRO:HD3	1.97	0.47
2:B:1201:BCT:O1	5:B:1301:HOH:O	2.20	0.47
1:B:955:PHE:HE2	1:B:994:LEU:HD13	1.79	0.47
1:A:913:GLY:HA2	1:A:916:ILE:HD12	1.97	0.47
1:B:845:LYS:HE3	1:B:903:PHE:HD2	1.80	0.47
1:A:755:LYS:HE3	1:A:759:ILE:HD11	1.95	0.47
1:B:775:ILE:O	1:B:779:ILE:HG12	2.15	0.47
1:A:971:ASP:OD2	1:A:976:ARG:NH2	2.42	0.47
1:B:978:VAL:HG11	1:B:1035:LEU:HD11	1.97	0.46
1:A:1020:ARG:NH1	1:A:1024:ASP:OD1	2.48	0.46
1:B:598:GLY:HA3	1:B:867:SER:OG	2.16	0.46
1:B:643:LYS:HD3	1:B:643:LYS:HA	1.62	0.46
1:A:552:GLY:HA3	1:A:917:PHE:CG	2.51	0.46
1:A:692:ASP:OD1	1:A:692:ASP:N	2.45	0.46
1:B:576:GLU:OE1	1:B:590:TYR:OH	2.30	0.45
1:A:769:ILE:HD11	1:A:941:VAL:HG21	1.98	0.45
1:B:471:HIS:HB2	1:B:618:CYS:HA	1.99	0.45
1:A:688:ILE:HD12	1:A:693:ILE:HD11	1.96	0.45
1:B:1030:ARG:NH1	1:B:1030:ARG:HB3	2.30	0.45
1:A:576:GLU:OE2	1:A:590:TYR:OH	2.35	0.45
1:B:653:ILE:HG12	1:B:726:LEU:HD23	2.00	0.44
1:B:591:LEU:HD11	1:B:799:ARG:HD2	1.98	0.44
3:B:1202:Y01:HAP1	3:B:1202:Y01:HAO1	1.71	0.44
1:A:515:PHE:CE1	1:A:765:VAL:HG11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:LYS:NZ	1:A:908:GLU:O	2.47	0.44
1:A:584:LYS:HB3	1:A:584:LYS:HE2	1.86	0.44
1:B:1020:ARG:HH21	1:B:1032:LEU:HD13	1.82	0.43
1:B:678:GLY:O	1:B:682:GLU:HG3	2.18	0.43
1:B:1029:LYS:NZ	1:B:1033:SER:HB3	2.32	0.43
1:B:522:SER:HB2	1:B:938:LEU:HD13	1.98	0.43
1:B:551:THR:HG22	1:B:566:LEU:HD12	2.01	0.43
1:A:746:PHE:HZ	1:A:752:PHE:CD2	2.37	0.43
1:A:647:LEU:HD11	1:A:936:PRO:HG3	2.01	0.43
1:B:1037:ASP:OD2	1:B:1044:LYS:NZ	2.51	0.43
1:B:683:TRP:C	1:B:685:GLU:H	2.27	0.43
1:A:923:SER:HA	1:A:926:MET:HB2	2.00	0.42
1:A:513:PHE:CD1	1:A:513:PHE:C	2.97	0.42
1:A:594:ARG:NH2	1:A:871:LEU:O	2.44	0.42
1:B:515:PHE:CE1	1:B:765:VAL:HG11	2.54	0.42
1:A:700:VAL:HG22	1:B:663:THR:HG23	2.00	0.42
1:B:883:THR:HG21	1:B:945:MET:HG2	2.00	0.42
1:A:513:PHE:CZ	1:A:919:LEU:HD21	2.45	0.42
1:A:957:ASP:HA	1:A:960:LYS:HE3	2.01	0.42
1:B:620:ILE:HG23	1:B:624:THR:HB	2.01	0.42
1:A:500:ASP:HB3	1:A:910:ARG:HG3	2.01	0.41
1:A:819:ILE:HB	1:A:820:PRO:HD3	2.02	0.41
1:A:779:ILE:O	1:B:655:MET:HG2	2.20	0.41
1:A:973:ILE:HG22	1:A:1041:GLU:HG2	2.02	0.41
1:A:779:ILE:CG2	1:A:781:ILE:HG12	2.50	0.41
1:A:779:ILE:HD11	3:B:1202:Y01:CAS	2.50	0.41
1:A:923:SER:HA	1:A:926:MET:HE2	2.03	0.41
1:B:1020:ARG:HD2	1:B:1023:MET:HE3	2.03	0.41
1:A:551:THR:HG23	1:A:862:MET:HB3	2.01	0.41
1:A:632:ILE:HG21	1:A:878:THR:HB	2.01	0.41
1:B:521:MET:HE3	1:B:521:MET:HB3	1.76	0.41
1:B:582:PHE:CD1	1:B:582:PHE:C	2.99	0.41
1:B:628:PHE:O	1:B:632:ILE:HG12	2.21	0.41
1:A:845:LYS:NZ	1:A:903:PHE:O	2.54	0.40
1:A:975:LEU:HD23	1:A:975:LEU:HA	1.96	0.40
1:A:565:ILE:HG23	1:A:917:PHE:HZ	1.85	0.40
1:B:492:ARG:NH1	1:B:850:CYS:O	2.54	0.40
1:B:608:LEU:HD23	1:B:608:LEU:HA	1.95	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	570/1118 (51%)	560 (98%)	10 (2%)	0	100	100
1	B	575/1118 (51%)	564 (98%)	11 (2%)	0	100	100
All	All	1145/2236 (51%)	1124 (98%)	21 (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	504/982 (51%)	483 (96%)	21 (4%)	26	49
1	B	509/982 (52%)	496 (97%)	13 (3%)	40	66
All	All	1013/1964 (52%)	979 (97%)	34 (3%)	33	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	GLU
1	A	506	SER
1	A	544	SER
1	A	556	SER
1	A	568	SER
1	A	596	SER
1	A	614	SER
1	A	679	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	699	THR
1	A	739	LEU
1	A	754	THR
1	A	770	LEU
1	A	804	THR
1	A	909	GLN
1	A	912	THR
1	A	918	ILE
1	A	929	ILE
1	A	996	LEU
1	A	1016	LEU
1	A	1028	THR
1	A	1033	SER
1	B	502	ARG
1	B	513	PHE
1	B	521	MET
1	B	603	THR
1	B	614	SER
1	B	653	ILE
1	B	686	SER
1	B	790	SER
1	B	815	ILE
1	B	976	ARG
1	B	1016	LEU
1	B	1020	ARG
1	B	1041	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	707	HIS
1	B	668	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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	BCT	B	1201	4	2,3,3	1.29	0	2,3,3	4.15	2 (100%)
2	BCT	A	1201	4	2,3,3	1.26	0	2,3,3	4.22	2 (100%)
3	Y01	B	1202	-	38,38,38	0.57	0	57,57,57	0.69	0
3	Y01	A	1202	-	38,38,38	0.54	0	57,57,57	0.60	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
3	Y01	B	1202	-	-	4/19/77/77	0/4/4/4
3	Y01	A	1202	-	-	12/19/77/77	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	BCT	O2-C-O1	5.61	134.09	119.55
2	B	1201	BCT	O2-C-O1	5.49	133.79	119.55
2	A	1201	BCT	O3-C-O1	-2.07	114.19	119.55
2	B	1201	BCT	O3-C-O1	-2.06	114.20	119.55

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	Y01	CAO-CBB-CBE-CAP
3	A	1202	Y01	CAO-CBB-CBE-CBI
3	A	1202	Y01	CAC-CBB-CBE-CBI
3	A	1202	Y01	OAG-CAY-OAW-CBC
3	B	1202	Y01	CAM-CAY-OAW-CBC
3	A	1202	Y01	CAC-CBB-CBE-CAP
3	B	1202	Y01	OAG-CAY-OAW-CBC
3	A	1202	Y01	CAM-CAY-OAW-CBC
3	A	1202	Y01	CAJ-CAO-CBB-CAC
3	A	1202	Y01	CAJ-CAO-CBB-CBE
3	A	1202	Y01	CAM-CAL-CAX-OAH
3	A	1202	Y01	CAM-CAL-CAX-OAF
3	B	1202	Y01	CAL-CAM-CAY-OAW
3	A	1202	Y01	CAJ-CAN-CBA-CAB
3	B	1202	Y01	CAL-CAM-CAY-OAG
3	A	1202	Y01	CAN-CAJ-CAO-CBB

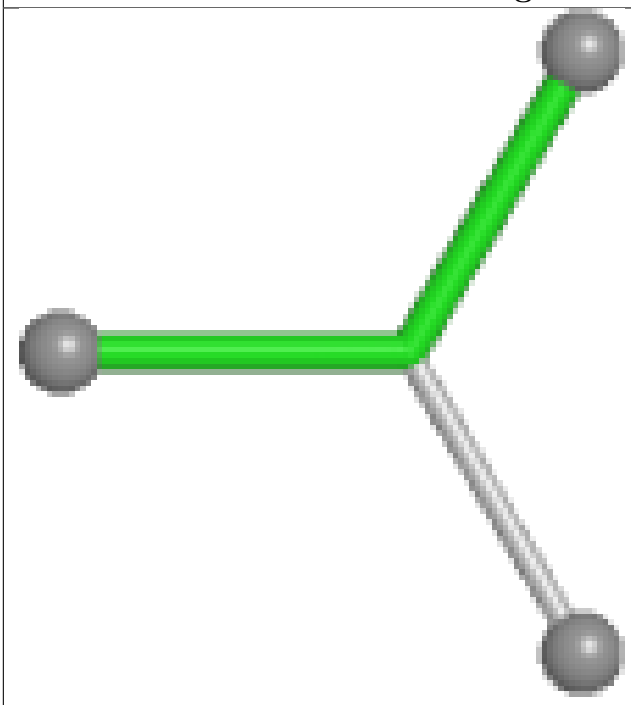
There are no ring outliers.

2 monomers are involved in 5 short contacts:

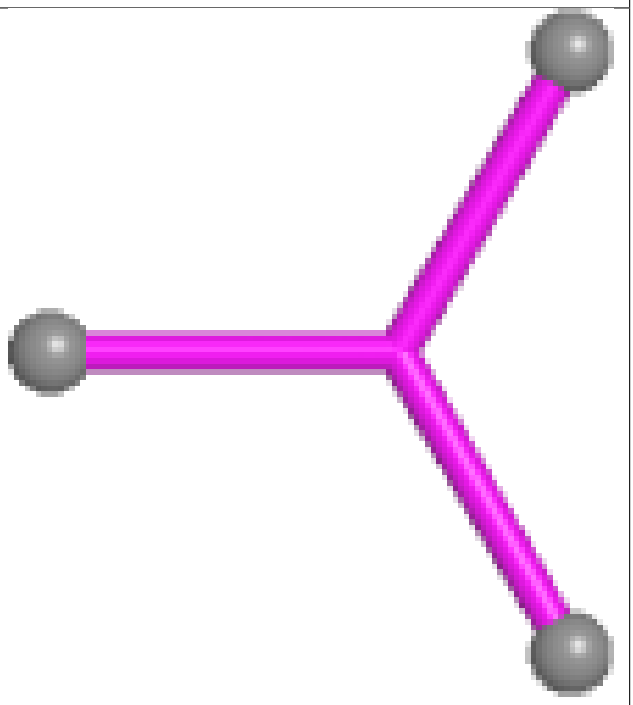
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	BCT	1	0
3	B	1202	Y01	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

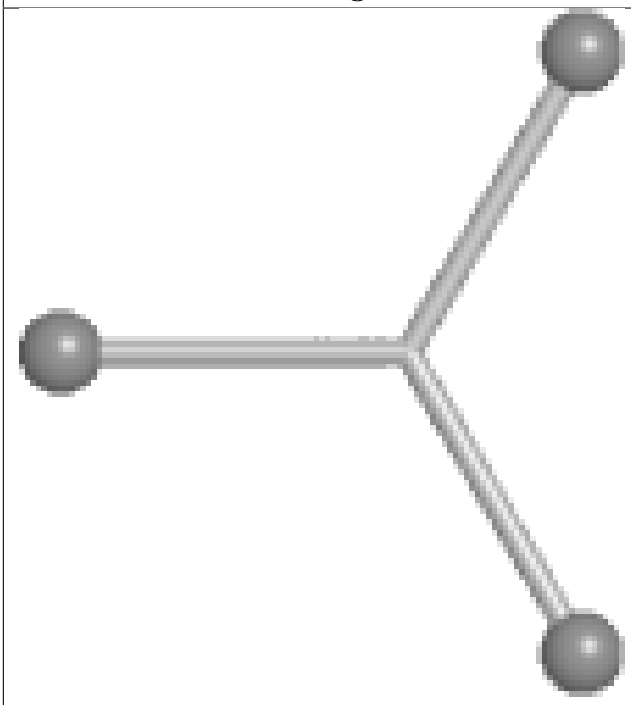
Ligand BCT B 1201



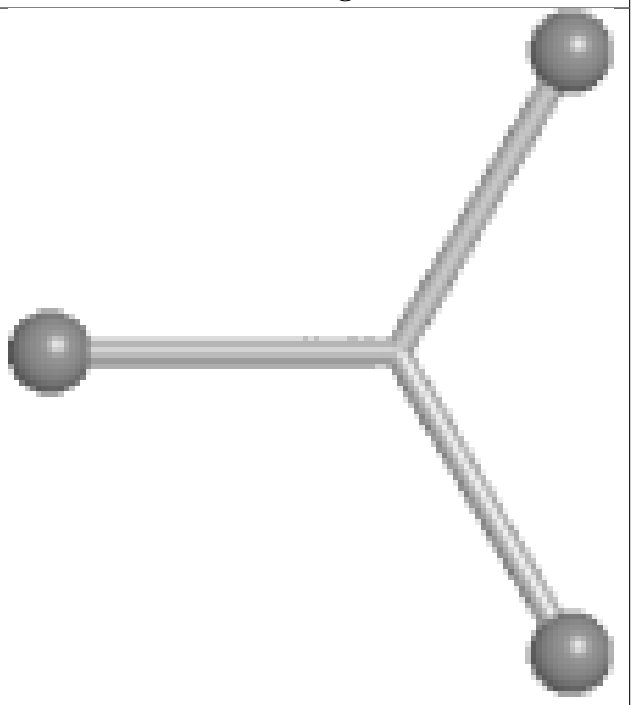
Bond lengths



Bond angles

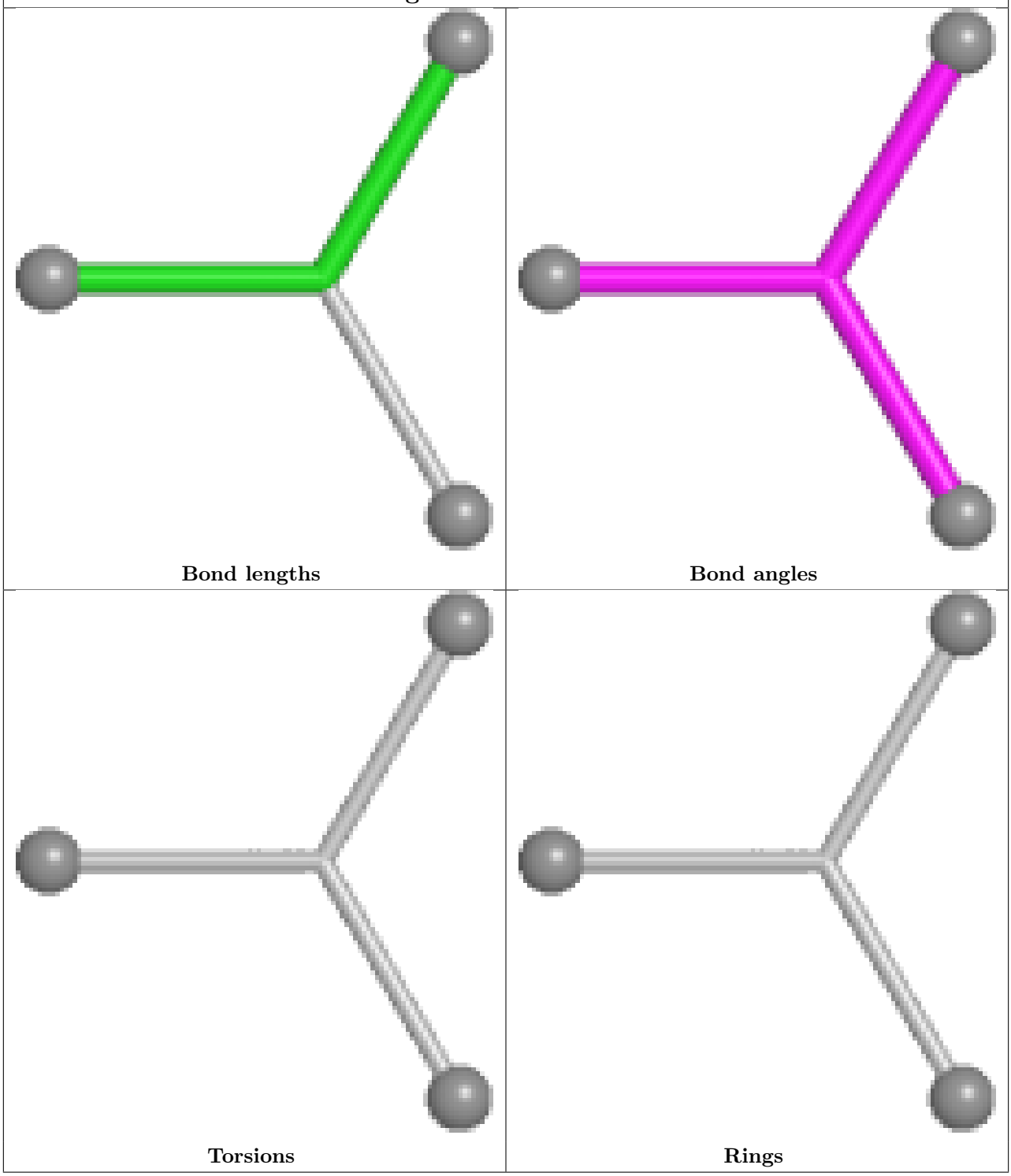


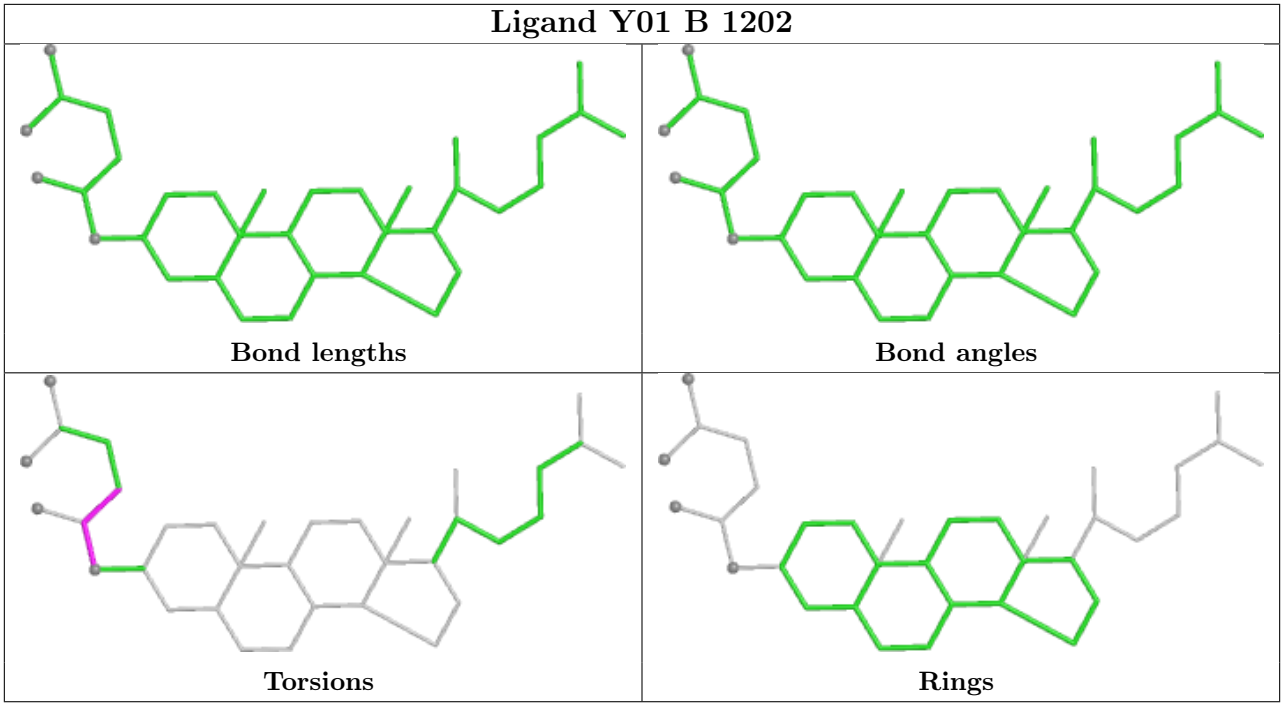
Torsions

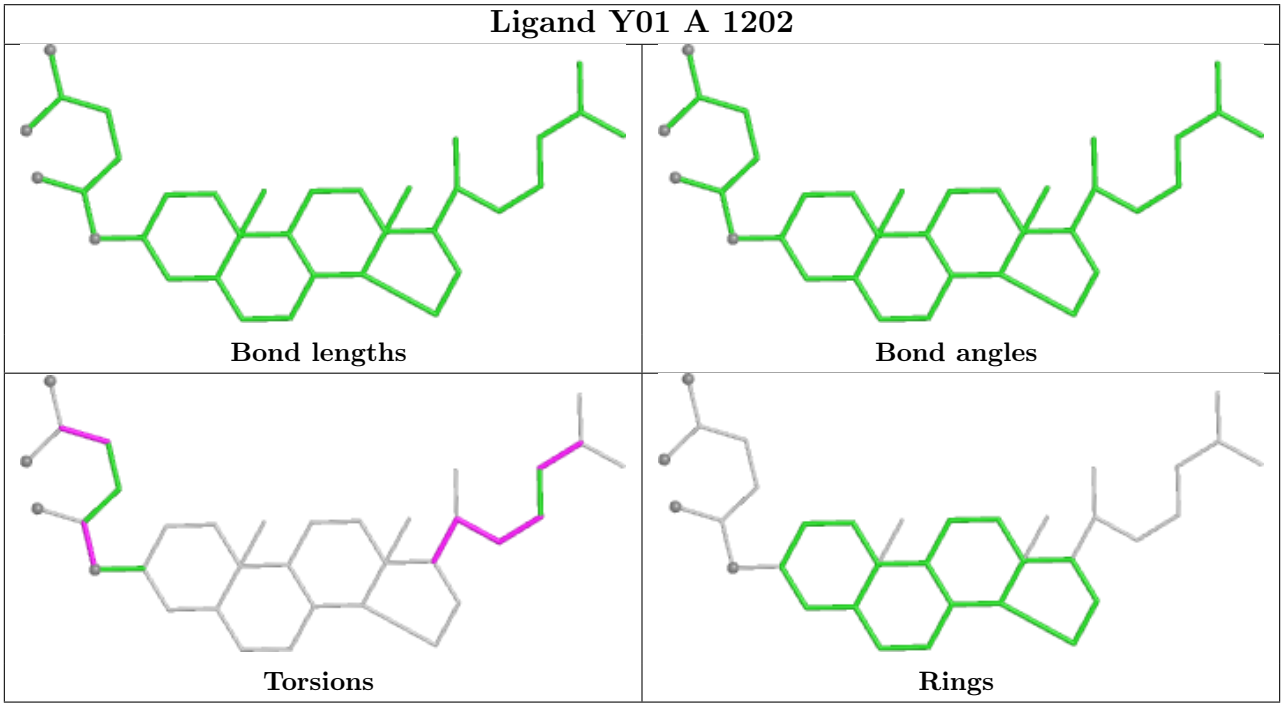


Rings

Ligand BCT A 1201







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.

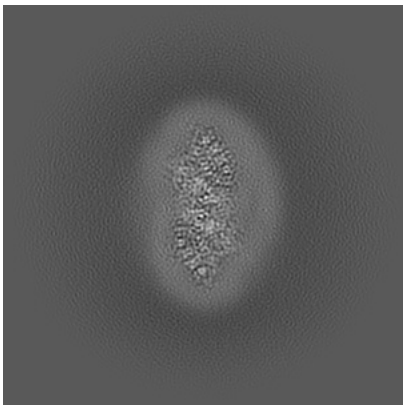
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-66591. These allow visual inspection of the internal detail of the map and identification of artifacts.

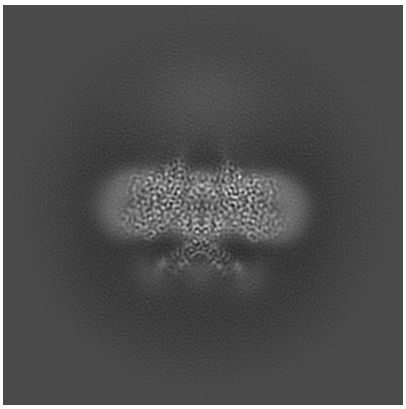
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

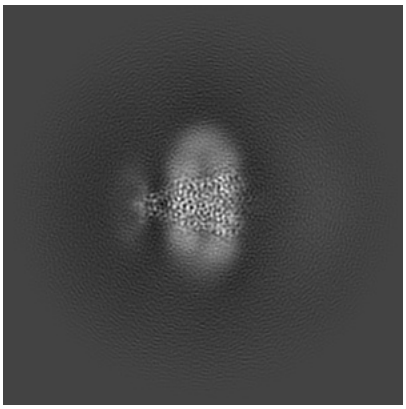
6.1.1 Primary map



X

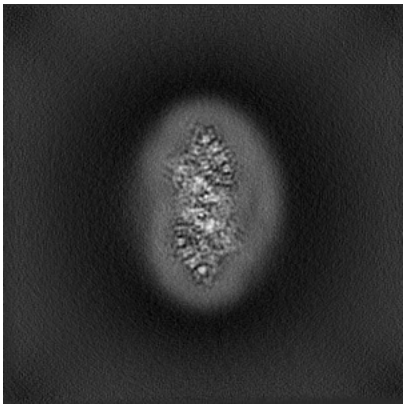


Y

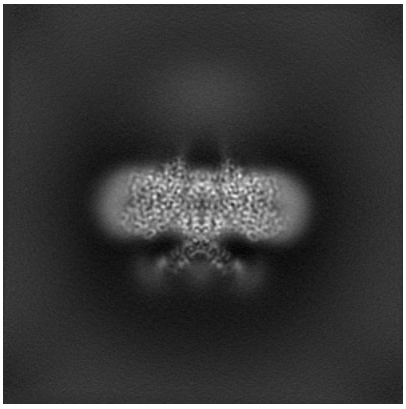


Z

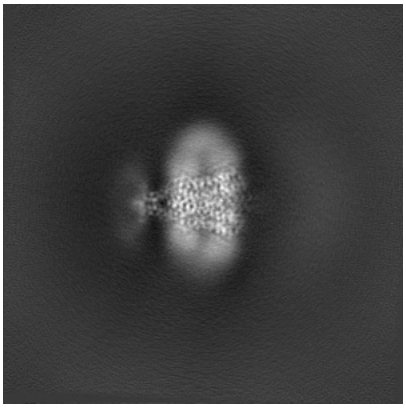
6.1.2 Raw map



X



Y

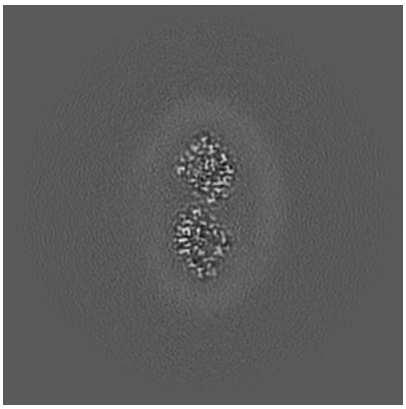


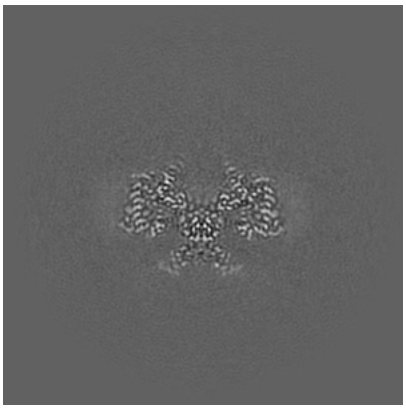
Z

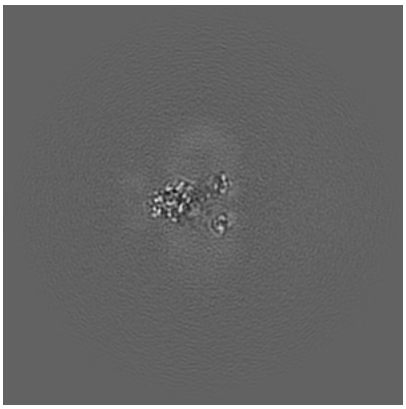
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

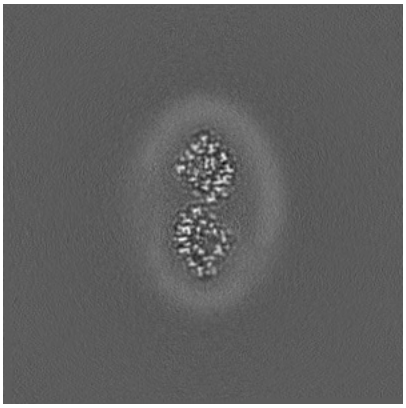
6.2.1 Primary map

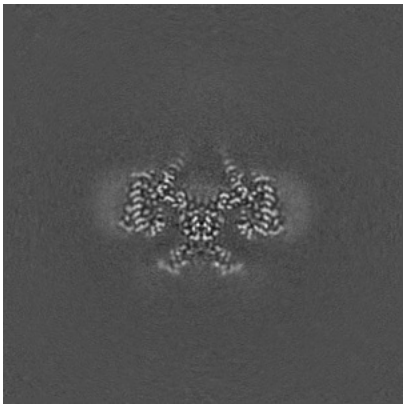

X Index: 160

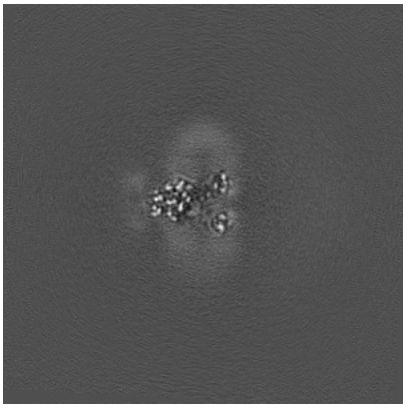

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

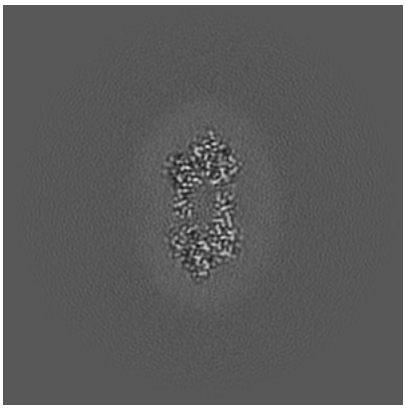

Y Index: 160

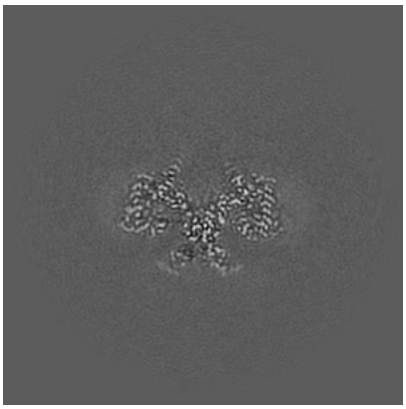

Z Index: 160

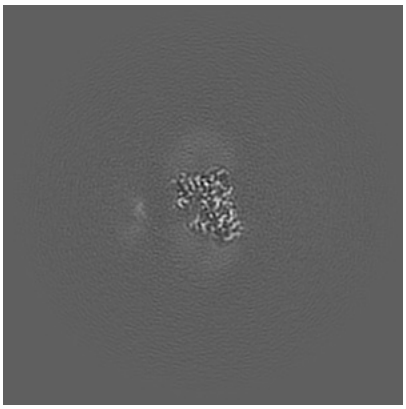
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

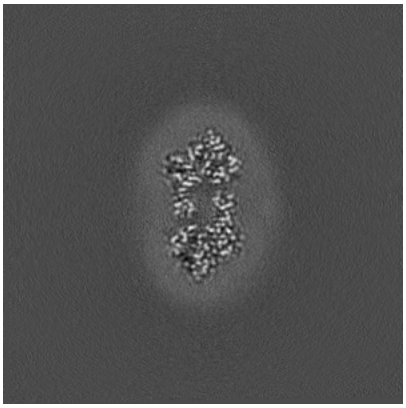
6.3.1 Primary map

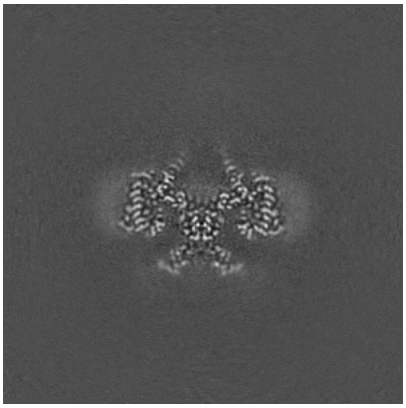

X Index: 174

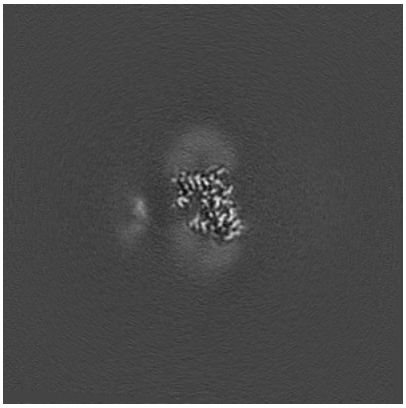

Y Index: 161


Z Index: 189

6.3.2 Raw map


X Index: 175

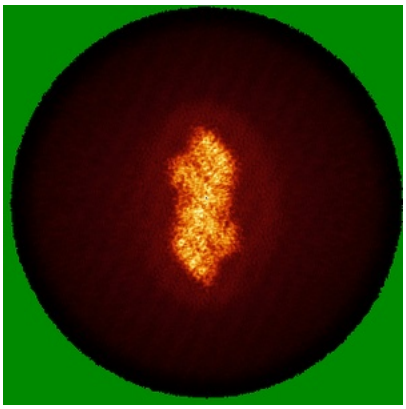

Y Index: 160

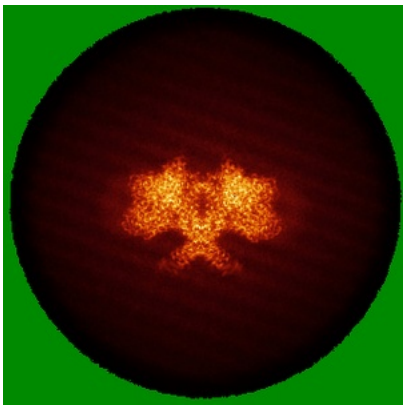

Z Index: 189

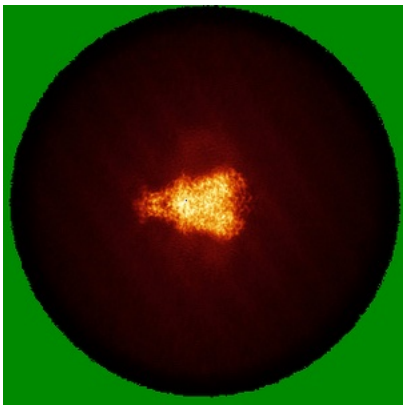
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

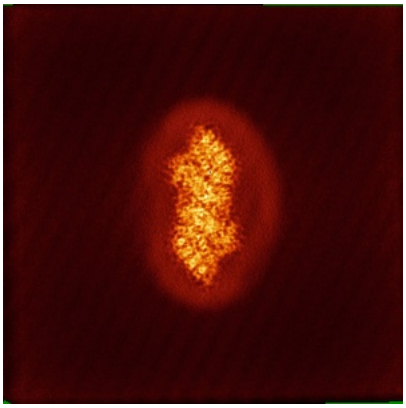
6.4.1 Primary map

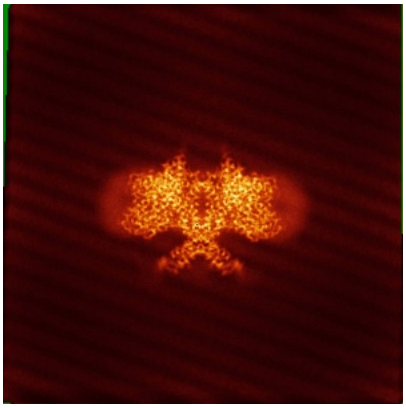

X

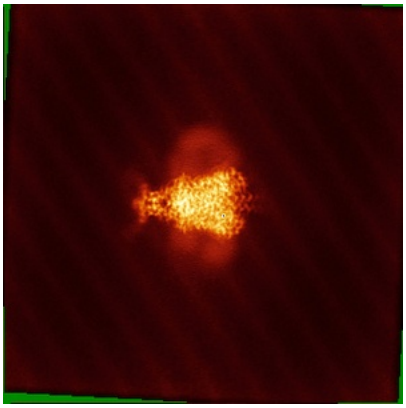

Y


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.

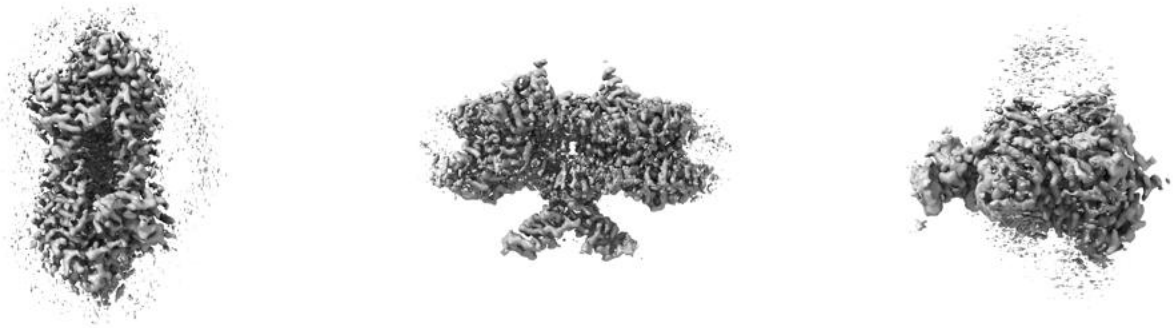
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.114. 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.

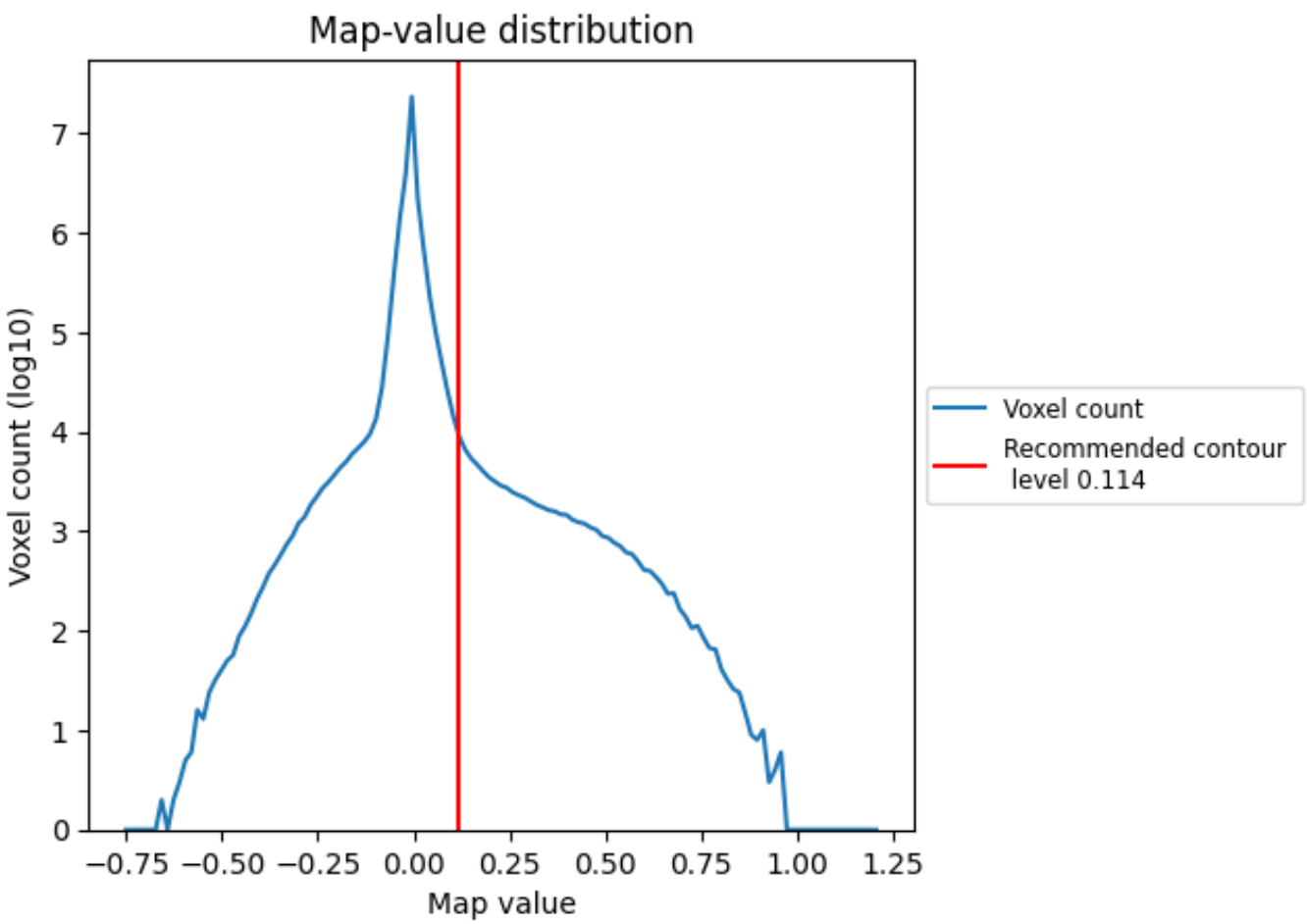
6.6 Mask visualisation (i)

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

7 Map analysis (i)

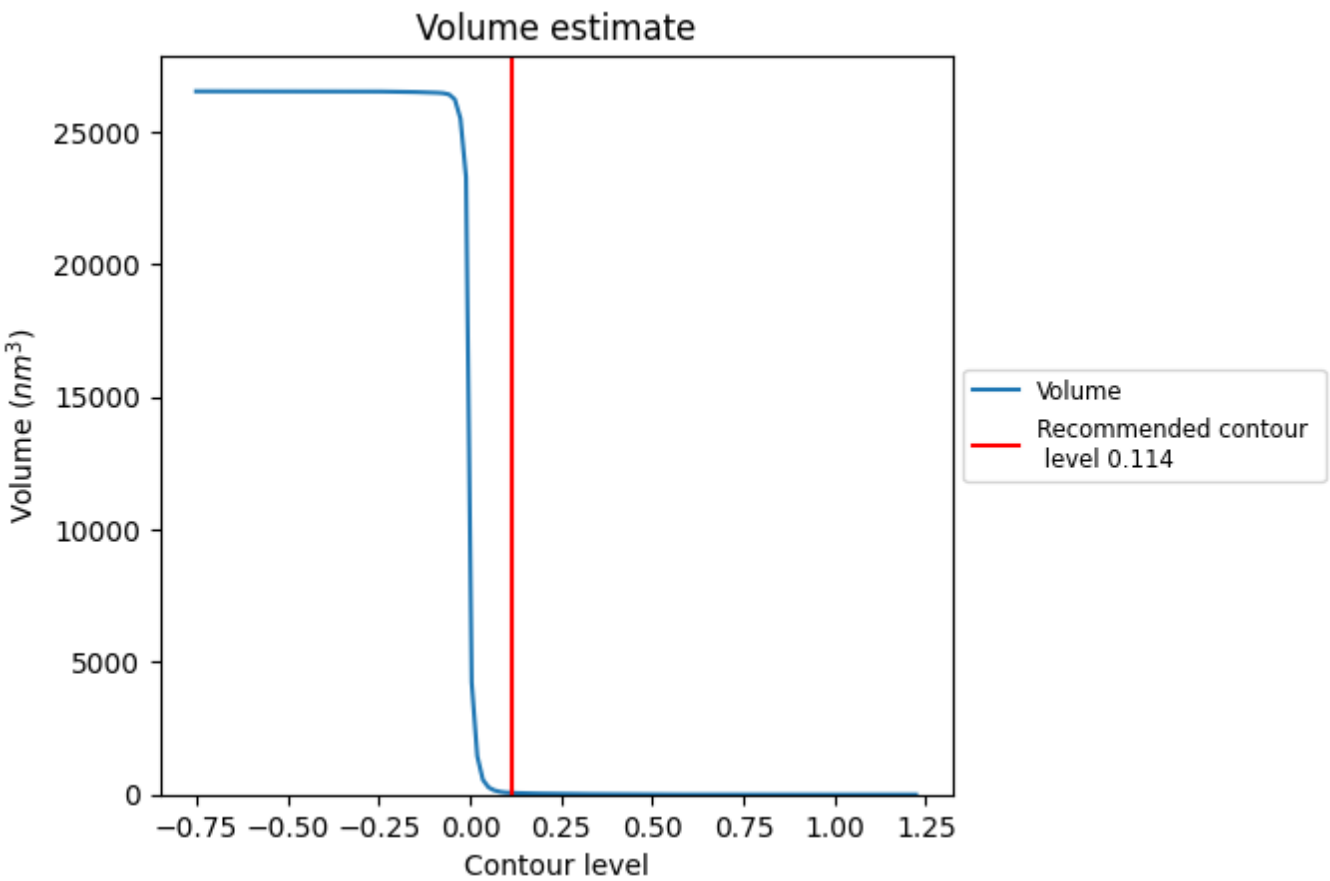
This section contains the results of statistical analysis of the map.

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.

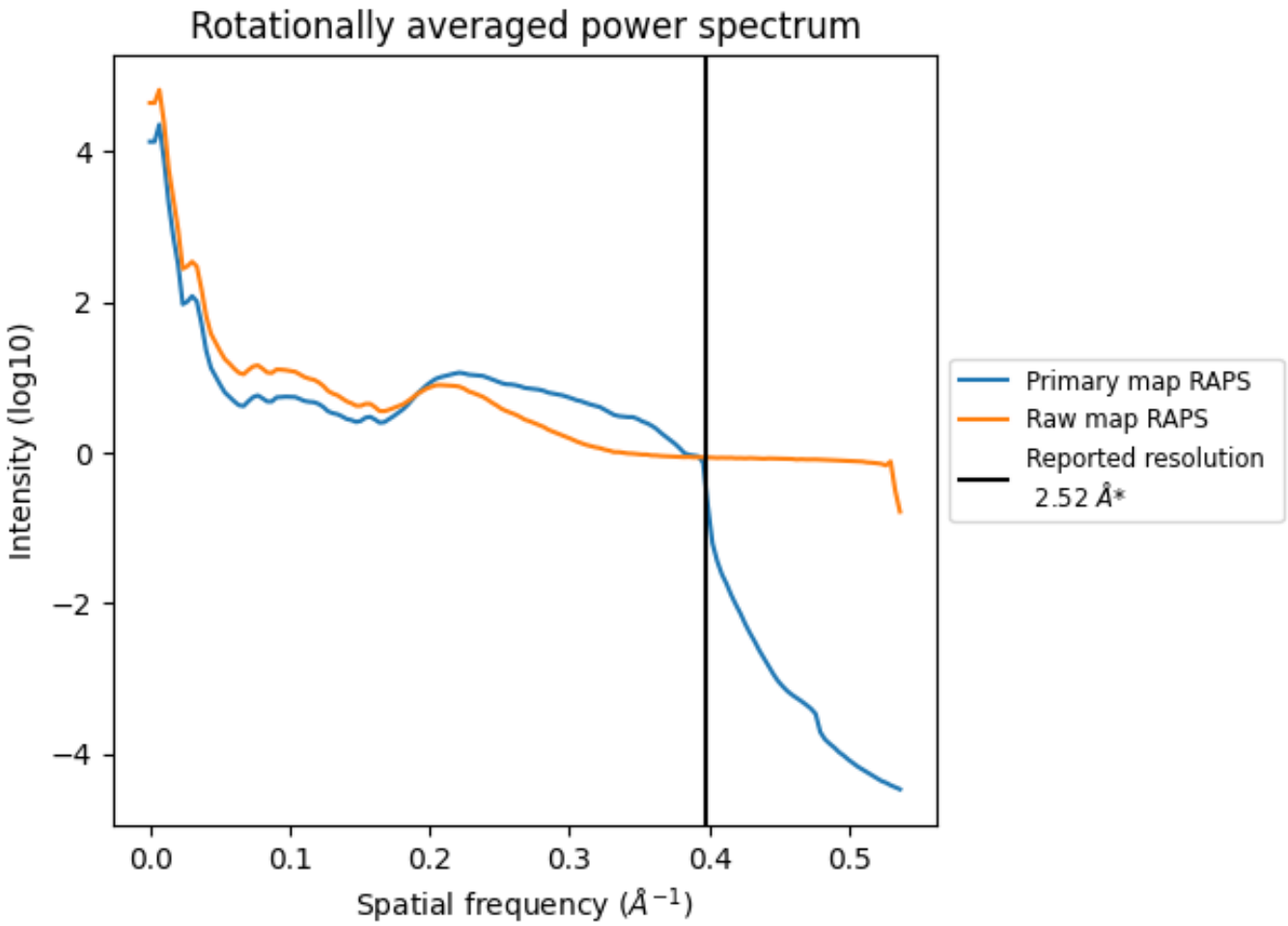
7.2 Volume estimate (i)



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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)

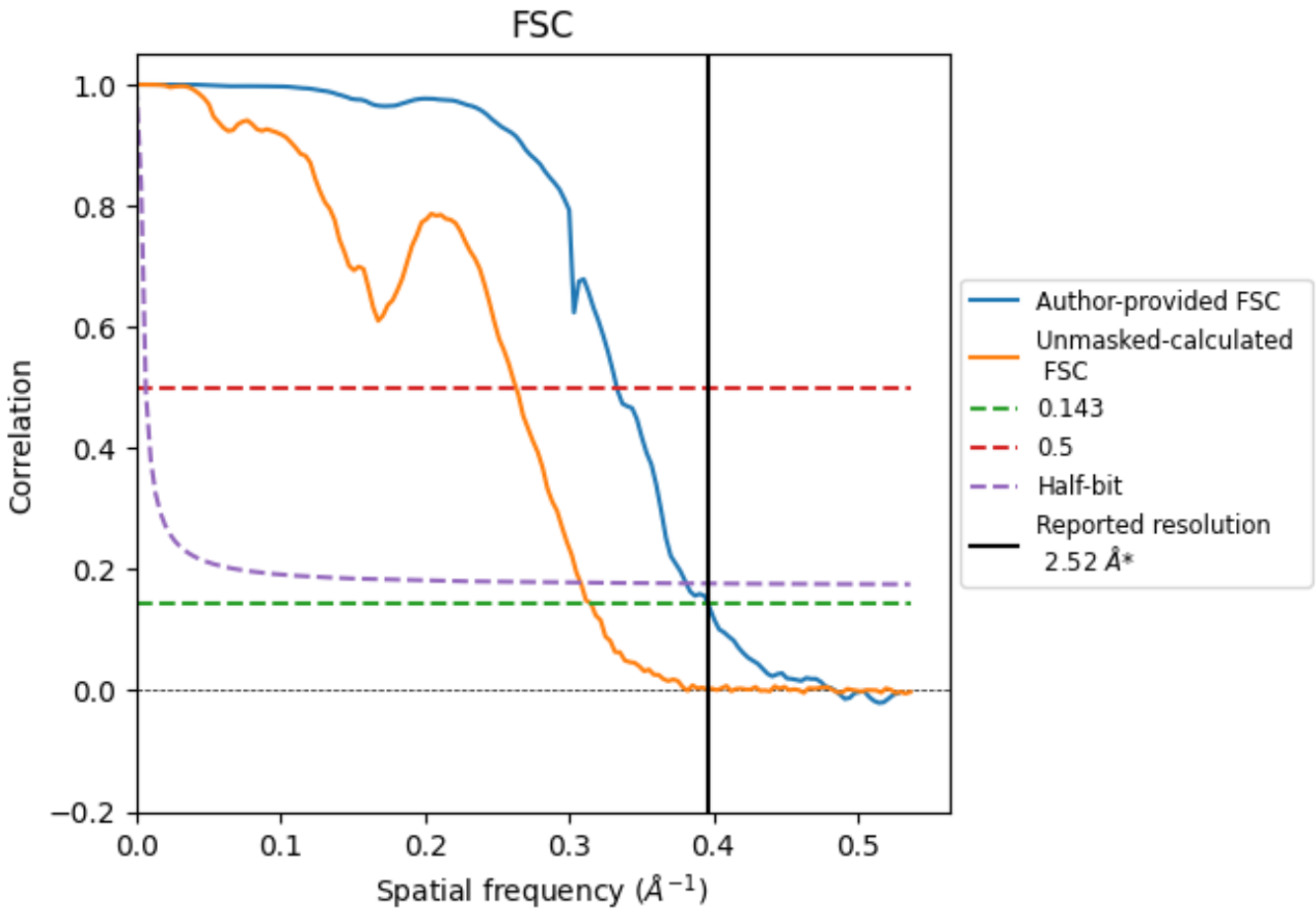


*Reported resolution corresponds to spatial frequency of 0.397 Å^{-1}

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 0.397 Å^{-1}

8.2 Resolution estimates (i)

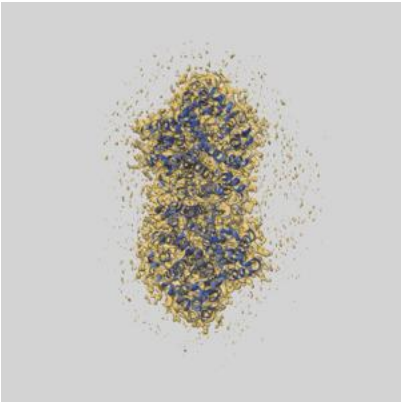
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.52	3.00	2.62
Unmasked-calculated*	3.17	3.80	3.25

*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 3.17 differs from the reported value 2.52 by more than 10 %

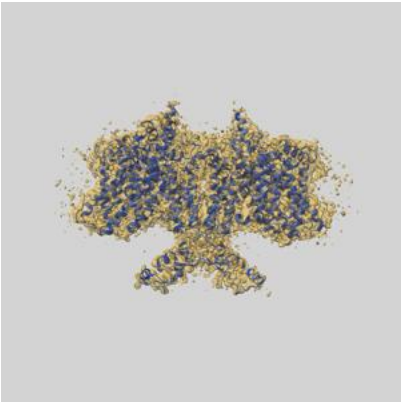
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-66591 and PDB model 9X5N. Per-residue inclusion information can be found in section 3 on page 5.

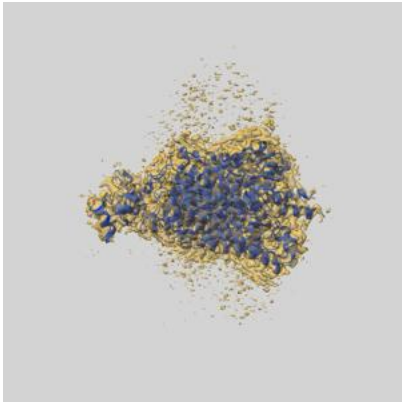
9.1 Map-model overlay (i)



X



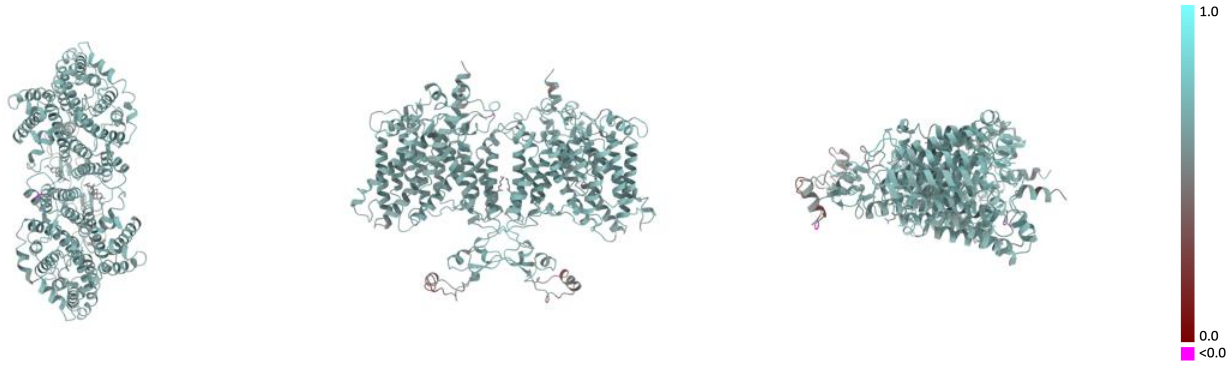
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.114 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.

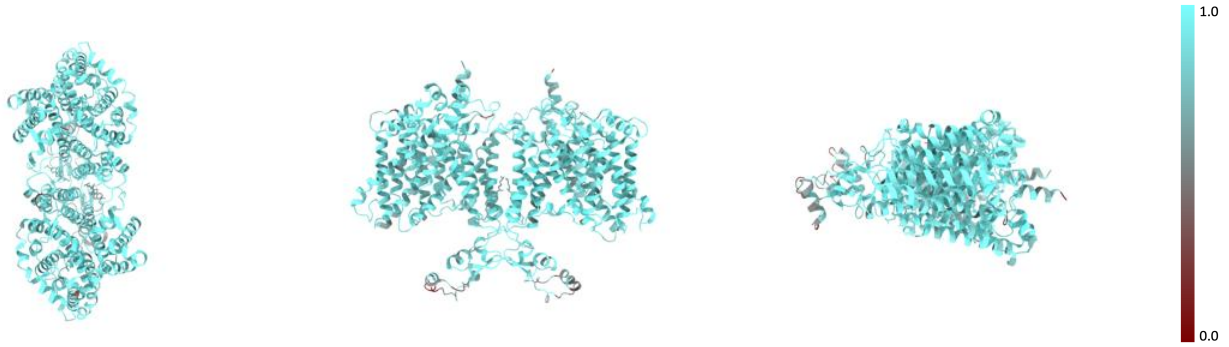
9.2 Q-score mapped to coordinate model (i)



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.

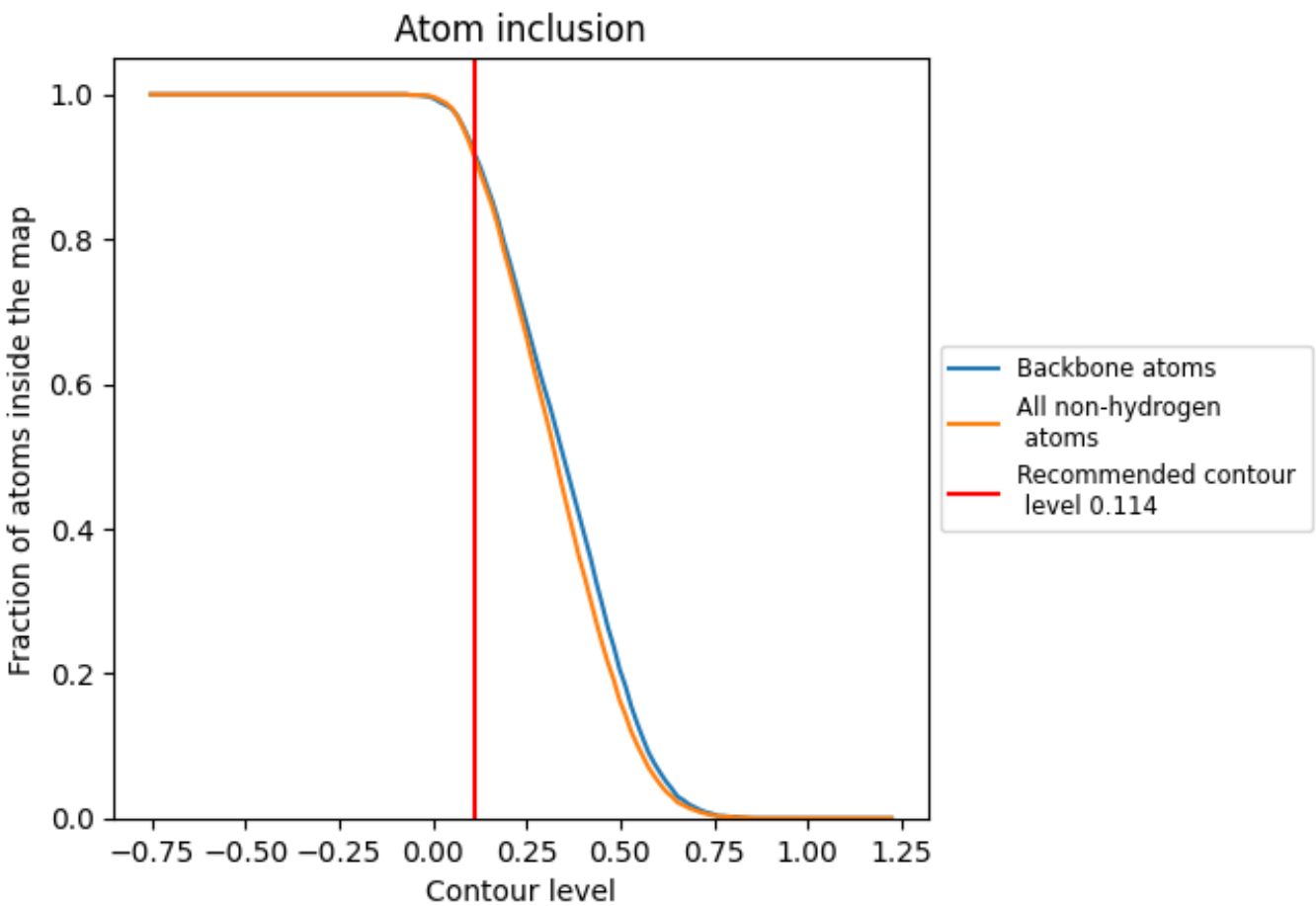
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.114).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.6200
A	0.9190	0.6240
B	0.9030	0.6160