Full wwPDB EM Validation Report (i)

Feb 27, 2024 – 12:08 PM EST

PDB ID	:	6V9Y
EMDB ID	:	EMD-21130
Title	:	Structure of TRPA1 bound with A-967079, PMAL-C8
Authors	:	Zhao, J.; Lin King, J.V.; Paulsen, C.E.; Cheng, Y.; Julius, D.
Deposited on	:	2019-12-16
Resolution	:	3.60 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:

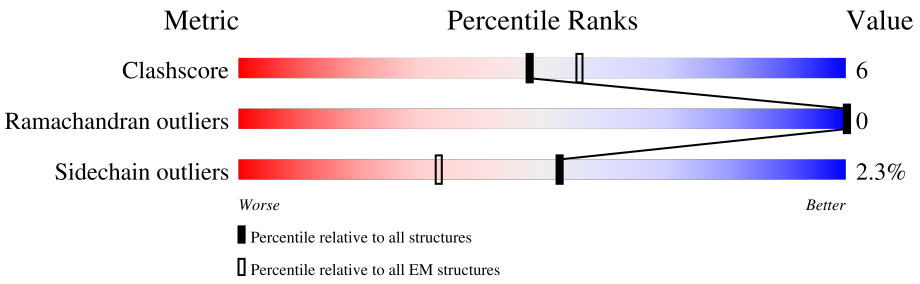
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1119	41% 9% 50%
1	B	1119	42% 8% 50%
1	C	1119	41% 8% 50%
1	D	1119	41% 9% 50%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17716 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 Transient receptor potential cation channel subfamily A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	562	4429	2907	738	753	31	0	0
1	B	562	4429	2907	738	753	31	0	0
1	D	562	4429	2907	738	753	31	0	0
1	C	562	4429	2907	738	753	31	0	0

There are 4 discrepancies between the modelled and reference sequences:

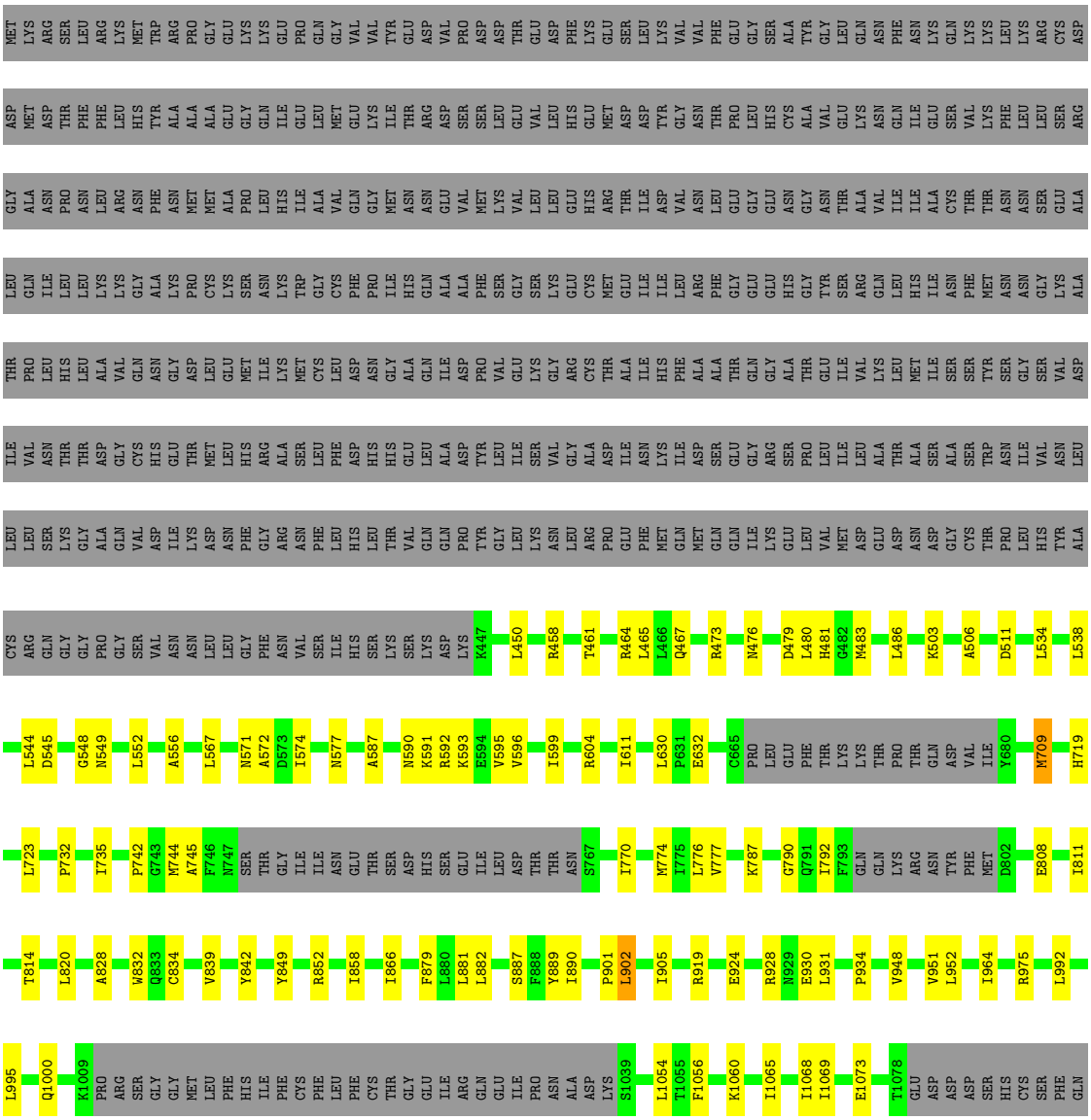
Chain	Residue	Modelled	Actual	Comment	Reference
A	966	ASP	GLU	engineered mutation	UNP O75762
B	966	ASP	GLU	engineered mutation	UNP O75762
D	966	ASP	GLU	engineered mutation	UNP O75762
C	966	ASP	GLU	engineered mutation	UNP O75762

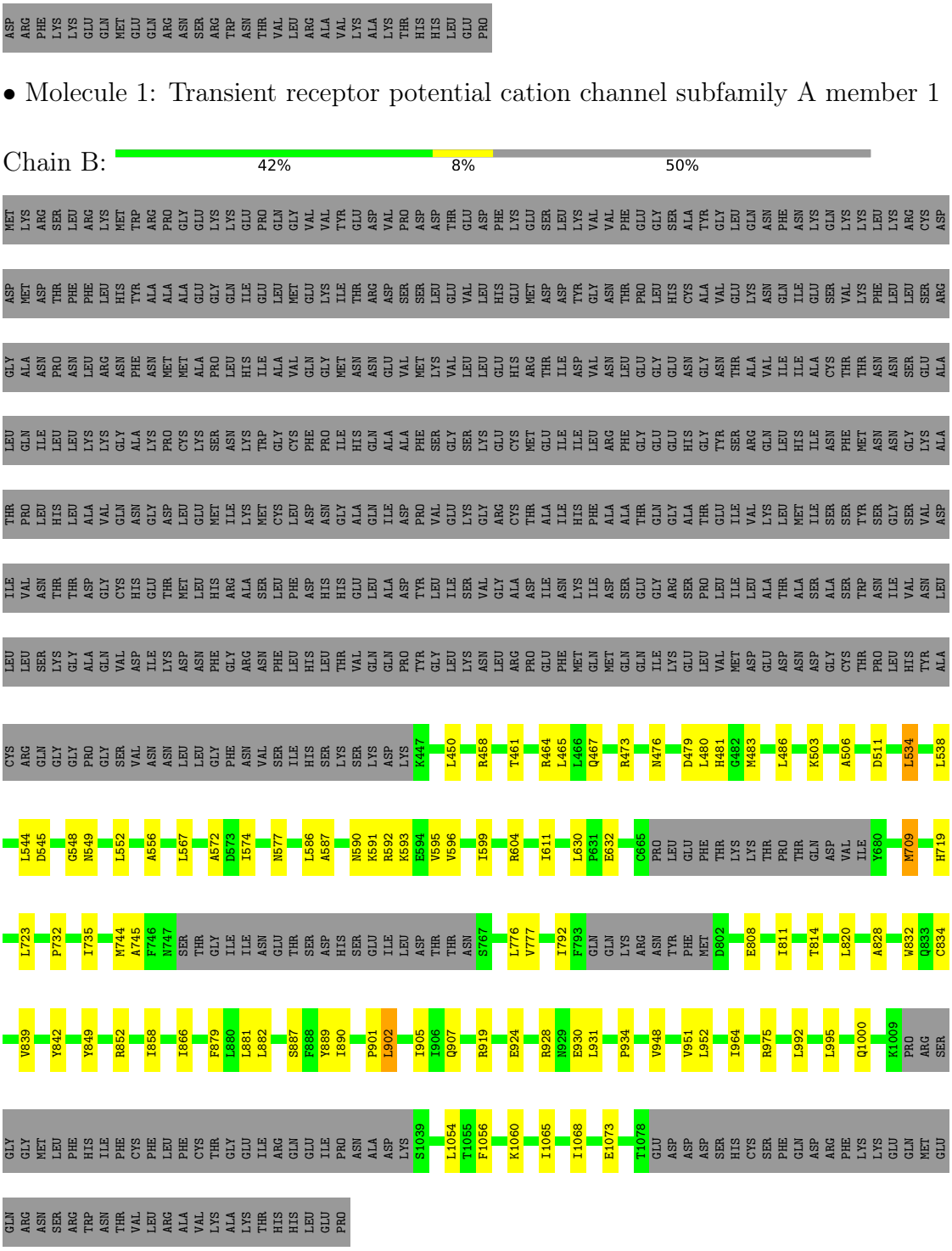
3 Residue-property plots (i)

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: Transient receptor potential cation channel subfamily A member 1

Chain A: 41% 9% 50%



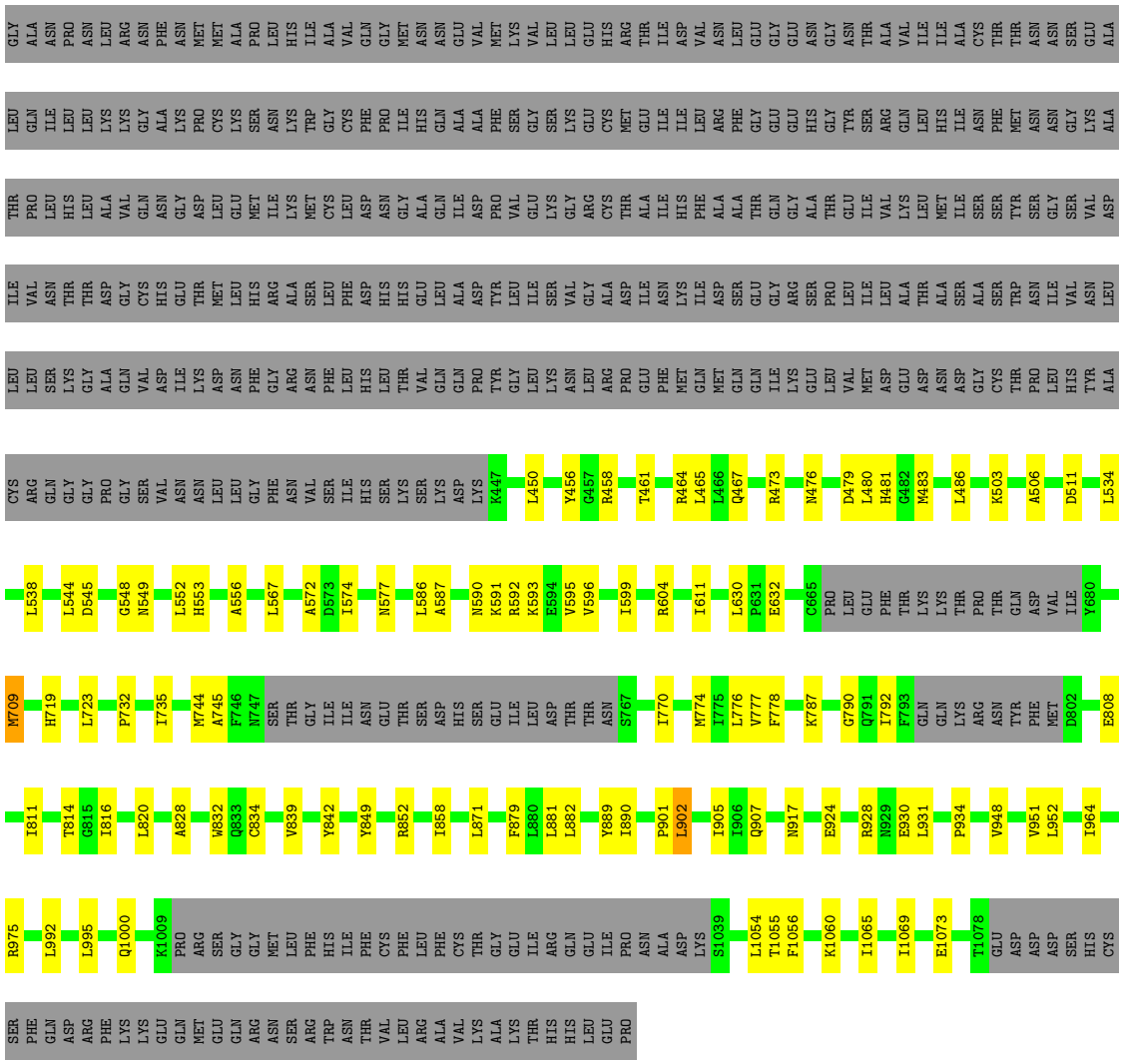


• Molecule 1: Transient receptor potential cation channel subfamily A member 1

Chain B: 42% 8% 50%

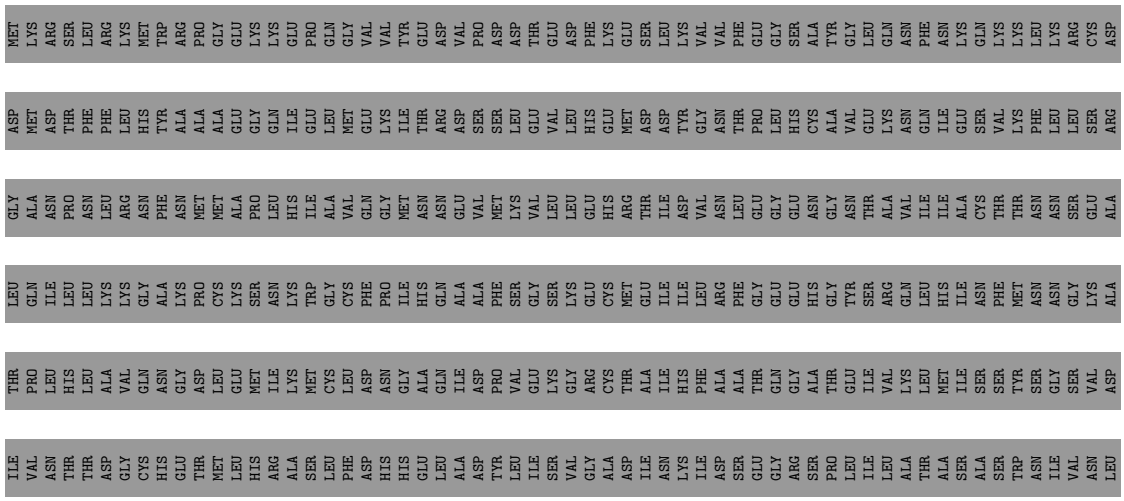
• Molecule 1: Transient receptor potential cation channel subfamily A member 1

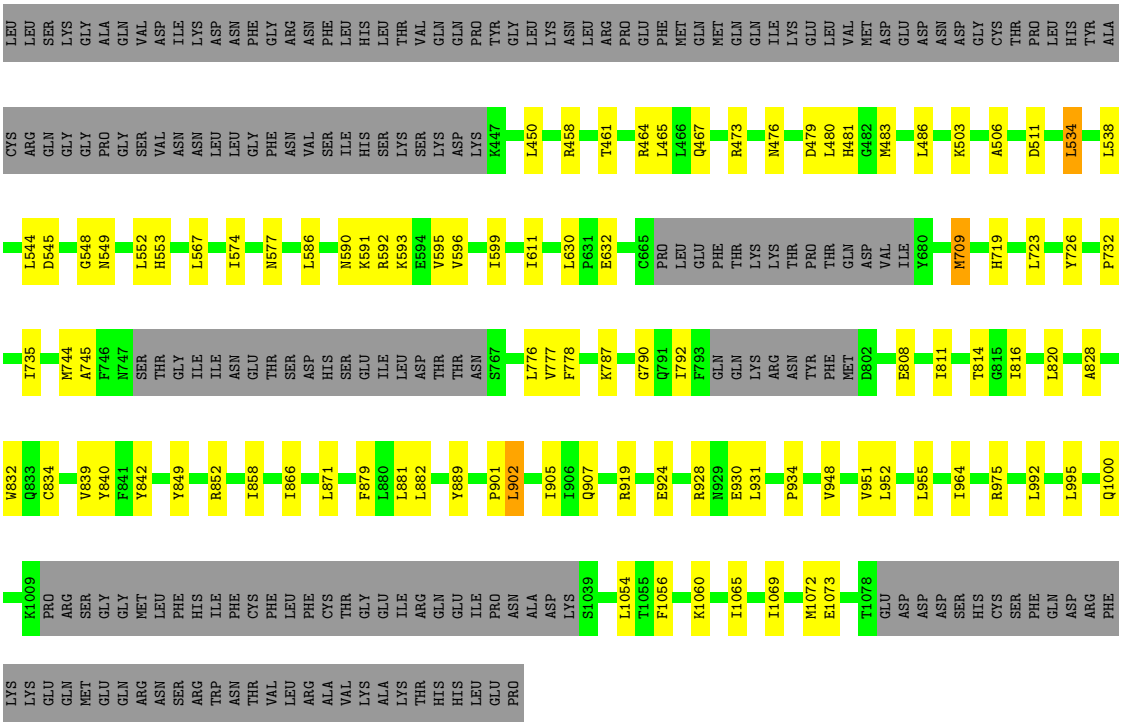
Chain D: 41% 9% 50%



• Molecule 1: Transient receptor potential cation channel subfamily A member 1

Chain C: 41% 8% 50%




LYS LYS GLU GLN MET GLU GLN ARG ASN SER ARG TRP ASN THR VAL LEU ARG ALA VAL LYS ALA LYS THR HIS HIS LEU GLU PRO
K1009 PRO ARG SER GLY GLY MET LEU PHE HIS ILE PHE CYS PHE LEU PHE CYS THR GLY GLU ILE ARG GLN GLU ILE PRO ASN ALA ASP LYS S1039 L1054 T1055 F1056 K1060 I1065 I1069 M1072 E1073 T1078 GLU ASP ASP ASP SER HIS CYS SER PHE GLN ASP ARG PHE
W832 Q833 C834 V839 Y840 F841 Y842 Y849 R852 I858 I866 L871 F879 L880 L881 L882 Y889 P901 L902 I905 I906 Q907 R919 E924 R928 N929 E930 L931 P934 V948 V951 L952 L955 I964 R975 L992 L995 Q1000
I735 M744 A745 F746 N747 SER THR GLY ILE ILE ASN GLU THR SER ASP HIS SER GLU ILE LEU ASP THR THR ASN S767 L776 V777 F778 K787 G790 Q791 I792 F793 GLN GLN LYS ARG ASN TYR PHE MET D802 E808 I811 T814 G815 I816 L820 A828
L544 D545 G548 N549 L552 H553 L567 I574 N577 L586 N590 K591 R592 K593 E594 V595 V596 I599 I611 L630 P631 E632 C665 PRO LEU GLU PHE THR LYS LYS THR PRO THR GLN ASP VAL ILE Y680 M709 H719 L723 Y726 P732
CYS ARG GLN GLY GLY PRO GLY SER VAL ASN ASN LEU LEU GLY PHE ASN VAL SER ILE HIS SER LYS SER LYS ASP LYS K447 L450 R458 T461 R464 L465 L466 Q467 R473 N476 D479 L480 H481 G482 M483 L486 K503 A506 D511 L534 L538
LEU LEU SER LYS GLY ALA GLN VAL ASP ILE LYS ASP ASN PHE LEU HIS LEU THR VAL GLN GLN PRO TYR GLY LEU LYS ASN LEU ARG PRO GLU PHE MET GLN MET GLN GLN ILE LYS GLU LEU VAL MET ASP GLU ASP ASN ASP GLY CYS THR PRO LEU HIS TYR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	30321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.620	Depositor
Minimum map value	-18.891	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.44	0/4524	0.64	3/6130 (0.0%)
1	B	0.44	0/4524	0.64	3/6130 (0.0%)
1	C	0.44	0/4524	0.64	3/6130 (0.0%)
1	D	0.44	0/4524	0.64	3/6130 (0.0%)
All	All	0.44	0/18096	0.64	12/24520 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	902	LEU	CA-CB-CG	7.88	133.43	115.30
1	A	902	LEU	CA-CB-CG	7.87	133.41	115.30
1	C	902	LEU	CA-CB-CG	7.87	133.40	115.30
1	D	902	LEU	CA-CB-CG	7.86	133.37	115.30
1	B	503	LYS	CD-CE-NZ	7.27	128.42	111.70
1	C	503	LYS	CD-CE-NZ	7.27	128.42	111.70
1	A	503	LYS	CD-CE-NZ	7.27	128.42	111.70
1	D	503	LYS	CD-CE-NZ	7.27	128.42	111.70
1	D	538	LEU	CA-CB-CG	6.16	129.46	115.30
1	A	538	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	538	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	538	LEU	CA-CB-CG	6.14	129.43	115.30

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	4429	0	4494	60	0
1	B	4429	0	4494	59	0
1	C	4429	0	4494	61	0
1	D	4429	0	4494	61	0
All	All	17716	0	17976	224	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 (224) 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:D:1056:PHE:CZ	1:D:1060:LYS:HE2	1.99	0.97
1:C:1056:PHE:CZ	1:C:1060:LYS:HE2	1.99	0.97
1:B:1056:PHE:CZ	1:B:1060:LYS:HE2	1.99	0.97
1:A:1056:PHE:CZ	1:A:1060:LYS:HE2	1.99	0.96
1:B:732:PRO:HG2	1:B:776:LEU:HD22	1.77	0.67
1:A:732:PRO:HG2	1:A:776:LEU:HD22	1.76	0.67
1:D:732:PRO:HG2	1:D:776:LEU:HD22	1.76	0.67
1:C:732:PRO:HG2	1:C:776:LEU:HD22	1.77	0.66
1:A:1068:ILE:HB	1:D:1069:ILE:HD11	1.78	0.65
1:C:545:ASP:OD1	1:C:549:ASN:N	2.32	0.61
1:A:545:ASP:OD1	1:A:549:ASN:N	2.32	0.61
1:D:545:ASP:OD1	1:D:549:ASN:N	2.32	0.61
1:B:858:ILE:HD11	1:B:975:ARG:HB3	1.83	0.60
1:D:858:ILE:HD11	1:D:975:ARG:HB3	1.83	0.59
1:C:858:ILE:HD11	1:C:975:ARG:HB3	1.83	0.59
1:A:858:ILE:HD11	1:A:975:ARG:HB3	1.83	0.59
1:B:545:ASP:OD1	1:B:549:ASN:N	2.32	0.58
1:B:919:ARG:HE	1:C:907:GLN:HE22	1.52	0.57
1:D:458:ARG:NH1	1:C:1072:MET:O	2.26	0.57
1:A:590:ASN:O	1:A:592:ARG:NH1	2.38	0.57
1:B:590:ASN:O	1:B:592:ARG:NH1	2.38	0.56
1:D:590:ASN:O	1:D:592:ARG:NH1	2.38	0.56
1:D:917:ASN:OD1	1:C:919:ARG:NH2	2.38	0.56
1:C:590:ASN:O	1:C:592:ARG:NH1	2.38	0.56
1:D:907:GLN:HE22	1:C:919:ARG:HE	1.54	0.56
1:D:552:LEU:HD22	1:D:567:LEU:HD13	1.88	0.56
1:A:552:LEU:HD22	1:A:567:LEU:HD13	1.88	0.55
1:B:552:LEU:HD22	1:B:567:LEU:HD13	1.88	0.55
1:C:552:LEU:HD22	1:C:567:LEU:HD13	1.88	0.55
1:A:742:PRO:HB3	1:D:890:ILE:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:HA	1:A:630:LEU:HD11	1.91	0.53
1:D:476:ASN:ND2	1:D:506:ALA:O	2.42	0.53
1:A:476:ASN:ND2	1:A:506:ALA:O	2.42	0.53
1:D:591:LYS:HA	1:D:630:LEU:HD11	1.91	0.53
1:C:591:LYS:HA	1:C:630:LEU:HD11	1.91	0.53
1:B:544:LEU:HB3	1:B:548:GLY:HA2	1.91	0.53
1:C:476:ASN:ND2	1:C:506:ALA:O	2.42	0.53
1:C:902:LEU:HA	1:C:905:ILE:HG22	1.91	0.53
1:B:902:LEU:HA	1:B:905:ILE:HG22	1.90	0.53
1:A:919:ARG:HE	1:B:907:GLN:HE22	1.57	0.53
1:D:544:LEU:HB3	1:D:548:GLY:HA2	1.91	0.52
1:A:544:LEU:HB3	1:A:548:GLY:HA2	1.91	0.52
1:B:591:LYS:HA	1:B:630:LEU:HD11	1.91	0.52
1:B:732:PRO:HB2	1:B:777:VAL:HG13	1.91	0.52
1:D:902:LEU:HA	1:D:905:ILE:HG22	1.91	0.52
1:D:709:MET:HE3	1:D:1000:GLN:H	1.75	0.52
1:C:544:LEU:HB3	1:C:548:GLY:HA2	1.91	0.52
1:C:709:MET:HE3	1:C:1000:GLN:H	1.75	0.52
1:D:745:ALA:HB2	1:D:828:ALA:HB2	1.92	0.52
1:D:811:ILE:HG23	1:D:842:TYR:HE1	1.75	0.52
1:C:745:ALA:HB2	1:C:828:ALA:HB2	1.92	0.52
1:A:811:ILE:HG23	1:A:842:TYR:HE1	1.75	0.52
1:A:902:LEU:HA	1:A:905:ILE:HG22	1.91	0.52
1:D:732:PRO:HB2	1:D:777:VAL:HG13	1.92	0.51
1:C:732:PRO:HB2	1:C:777:VAL:HG13	1.91	0.51
1:A:732:PRO:HA	1:A:735:ILE:HG12	1.93	0.51
1:A:745:ALA:HB2	1:A:828:ALA:HB2	1.92	0.51
1:B:948:VAL:HG12	1:B:952:LEU:HD12	1.93	0.51
1:B:1056:PHE:CZ	1:B:1060:LYS:CE	2.86	0.51
1:C:811:ILE:HG23	1:C:842:TYR:HE1	1.75	0.51
1:B:476:ASN:ND2	1:B:506:ALA:O	2.42	0.51
1:B:811:ILE:HG23	1:B:842:TYR:HE1	1.75	0.51
1:D:732:PRO:HA	1:D:735:ILE:HG12	1.93	0.51
1:A:709:MET:HE3	1:A:1000:GLN:H	1.75	0.50
1:A:732:PRO:HB2	1:A:777:VAL:HG13	1.92	0.50
1:A:948:VAL:HG12	1:A:952:LEU:HD12	1.93	0.50
1:D:479:ASP:N	1:D:483:MET:O	2.43	0.50
1:B:745:ALA:HB2	1:B:828:ALA:HB2	1.92	0.50
1:B:709:MET:HE3	1:B:1000:GLN:H	1.75	0.50
1:B:732:PRO:HA	1:B:735:ILE:HG12	1.93	0.50
1:A:479:ASP:N	1:A:483:MET:O	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:792:ILE:HD13	1:D:852:ARG:HH22	1.77	0.50
1:C:948:VAL:HG12	1:C:952:LEU:HD12	1.93	0.50
1:B:723:LEU:HD12	1:B:849:TYR:HB3	1.94	0.49
1:A:792:ILE:HD13	1:A:852:ARG:HH22	1.78	0.49
1:C:723:LEU:HD12	1:C:849:TYR:HB3	1.94	0.49
1:C:732:PRO:HA	1:C:735:ILE:HG12	1.93	0.49
1:A:723:LEU:HD12	1:A:849:TYR:HB3	1.94	0.49
1:D:948:VAL:HG12	1:D:952:LEU:HD12	1.93	0.49
1:D:450:LEU:HB2	1:D:465:LEU:HD13	1.95	0.49
1:B:792:ILE:HD13	1:B:852:ARG:HH22	1.77	0.49
1:B:596:VAL:HA	1:B:599:ILE:HD12	1.95	0.49
1:C:450:LEU:HB2	1:C:465:LEU:HD13	1.95	0.49
1:C:792:ILE:HD13	1:C:852:ARG:HH22	1.78	0.49
1:C:1056:PHE:CZ	1:C:1060:LYS:CE	2.86	0.49
1:A:890:ILE:HD11	1:B:832:TRP:CE3	2.47	0.49
1:D:596:VAL:HA	1:D:599:ILE:HD12	1.95	0.48
1:C:596:VAL:HA	1:C:599:ILE:HD12	1.95	0.48
1:B:890:ILE:HD11	1:C:832:TRP:CE3	2.48	0.48
1:C:574:ILE:HB	1:C:611:ILE:HD13	1.95	0.48
1:B:879:PHE:HA	1:B:882:LEU:HB2	1.95	0.48
1:A:596:VAL:HA	1:A:599:ILE:HD12	1.95	0.48
1:B:450:LEU:HB2	1:B:465:LEU:HD13	1.95	0.48
1:C:480:LEU:HD12	1:C:481:HIS:N	2.29	0.48
1:A:450:LEU:HB2	1:A:465:LEU:HD13	1.95	0.48
1:A:574:ILE:HB	1:A:611:ILE:HD13	1.95	0.48
1:B:480:LEU:HD12	1:B:481:HIS:N	2.29	0.48
1:D:574:ILE:HB	1:D:611:ILE:HD13	1.95	0.48
1:A:1056:PHE:CZ	1:A:1060:LYS:CE	2.86	0.48
1:A:879:PHE:HA	1:A:882:LEU:HB2	1.95	0.48
1:B:574:ILE:HB	1:B:611:ILE:HD13	1.95	0.48
1:A:480:LEU:HD12	1:A:481:HIS:N	2.29	0.48
1:D:879:PHE:HA	1:D:882:LEU:HB2	1.95	0.48
1:C:479:ASP:N	1:C:483:MET:O	2.43	0.48
1:C:931:LEU:HD23	1:C:934:PRO:HA	1.96	0.48
1:B:808:GLU:HA	1:B:811:ILE:HB	1.96	0.48
1:D:931:LEU:HD23	1:D:934:PRO:HA	1.96	0.47
1:D:723:LEU:HD12	1:D:849:TYR:HB3	1.94	0.47
1:D:808:GLU:HA	1:D:811:ILE:HB	1.96	0.47
1:C:879:PHE:HA	1:C:882:LEU:HB2	1.95	0.47
1:A:931:LEU:HD23	1:A:934:PRO:HA	1.96	0.47
1:D:480:LEU:HD12	1:D:481:HIS:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:THR:OG1	1:C:834:CYS:O	2.32	0.47
1:A:808:GLU:HA	1:A:811:ILE:HB	1.96	0.47
1:B:577:ASN:OD1	1:B:577:ASN:N	2.48	0.47
1:C:808:GLU:HA	1:C:811:ILE:HB	1.96	0.47
1:B:931:LEU:HD23	1:B:934:PRO:HA	1.96	0.47
1:A:577:ASN:OD1	1:A:577:ASN:N	2.48	0.47
1:B:479:ASP:N	1:B:483:MET:O	2.43	0.47
1:D:744:MET:O	1:D:832:TRP:NE1	2.45	0.46
1:A:464:ARG:HA	1:A:467:GLN:HG2	1.97	0.46
1:D:577:ASN:OD1	1:D:577:ASN:N	2.48	0.46
1:A:1054:LEU:HD12	1:D:1055:THR:HB	1.97	0.46
1:C:480:LEU:HD11	1:C:481:HIS:CE1	2.51	0.46
1:A:832:TRP:CE3	1:D:890:ILE:HD11	2.51	0.46
1:B:464:ARG:HA	1:B:467:GLN:HG2	1.97	0.46
1:C:577:ASN:OD1	1:C:577:ASN:N	2.48	0.46
1:D:593:LYS:HE2	1:D:632:GLU:HG3	1.98	0.46
1:C:744:MET:O	1:C:832:TRP:NE1	2.45	0.46
1:A:889:TYR:CZ	1:A:901:PRO:HD3	2.51	0.46
1:B:480:LEU:HD11	1:B:481:HIS:CE1	2.51	0.46
1:B:719:HIS:HE1	1:B:852:ARG:HG3	1.81	0.46
1:D:464:ARG:HA	1:D:467:GLN:HG2	1.97	0.46
1:C:464:ARG:HA	1:C:467:GLN:HG2	1.97	0.45
1:B:572:ALA:O	1:B:604:ARG:NH2	2.41	0.45
1:B:814:THR:OG1	1:B:834:CYS:O	2.32	0.45
1:C:889:TYR:CZ	1:C:901:PRO:HD3	2.51	0.45
1:A:480:LEU:HD11	1:A:481:HIS:CE1	2.51	0.45
1:A:719:HIS:HE1	1:A:852:ARG:HG3	1.81	0.45
1:D:456:TYR:HB3	1:C:1069:ILE:HG22	1.99	0.45
1:D:480:LEU:HD11	1:D:481:HIS:CE1	2.51	0.45
1:D:889:TYR:CZ	1:D:901:PRO:HD3	2.51	0.45
1:D:964:ILE:HD11	1:C:955:LEU:HA	1.98	0.45
1:A:572:ALA:O	1:A:604:ARG:NH2	2.41	0.45
1:A:593:LYS:HE2	1:A:632:GLU:HG3	1.98	0.45
1:B:889:TYR:CZ	1:B:901:PRO:HD3	2.51	0.45
1:A:814:THR:OG1	1:A:834:CYS:O	2.32	0.45
1:D:511:ASP:OD1	1:D:511:ASP:N	2.50	0.45
1:D:719:HIS:HE1	1:D:852:ARG:HG3	1.82	0.45
1:D:1056:PHE:CZ	1:D:1060:LYS:CE	2.86	0.45
1:D:814:THR:OG1	1:D:834:CYS:O	2.32	0.45
1:B:458:ARG:O	1:B:461:THR:OG1	2.35	0.44
1:B:593:LYS:HE2	1:B:632:GLU:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LEU:HD12	1:B:480:LEU:C	2.38	0.44
1:C:719:HIS:HE1	1:C:852:ARG:HG3	1.81	0.44
1:D:480:LEU:HD12	1:D:480:LEU:C	2.38	0.44
1:A:480:LEU:HD12	1:A:480:LEU:C	2.38	0.44
1:C:480:LEU:HD12	1:C:480:LEU:C	2.38	0.44
1:B:511:ASP:OD1	1:B:511:ASP:N	2.50	0.44
1:C:593:LYS:HE2	1:C:632:GLU:HG3	1.98	0.44
1:A:744:MET:O	1:A:832:TRP:NE1	2.45	0.44
1:C:458:ARG:O	1:C:461:THR:OG1	2.35	0.43
1:B:744:MET:O	1:B:832:TRP:NE1	2.45	0.43
1:C:992:LEU:HA	1:C:995:LEU:HD22	2.01	0.43
1:B:887:SER:HB2	1:C:840:TYR:HB2	2.01	0.43
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.89	0.43
1:A:511:ASP:OD1	1:A:511:ASP:N	2.50	0.43
1:A:719:HIS:CE1	1:A:852:ARG:HE	2.37	0.43
1:A:458:ARG:O	1:A:461:THR:OG1	2.35	0.42
1:B:461:THR:HA	1:B:464:ARG:HH11	1.84	0.42
1:B:924:GLU:O	1:B:928:ARG:NE	2.52	0.42
1:D:770:ILE:O	1:D:774:MET:N	2.51	0.42
1:C:871:LEU:HD23	1:C:871:LEU:HA	1.88	0.42
1:C:461:THR:HA	1:C:464:ARG:HH11	1.84	0.42
1:C:719:HIS:CE1	1:C:852:ARG:HE	2.37	0.42
1:C:924:GLU:O	1:C:928:ARG:NE	2.52	0.42
1:A:461:THR:HA	1:A:464:ARG:HH11	1.84	0.42
1:D:992:LEU:HA	1:D:995:LEU:HD22	2.01	0.42
1:A:1054:LEU:HD22	1:B:1054:LEU:HD11	2.00	0.42
1:B:719:HIS:CE1	1:B:852:ARG:HE	2.37	0.42
1:B:992:LEU:HA	1:B:995:LEU:HD22	2.01	0.42
1:A:992:LEU:HA	1:A:995:LEU:HD22	2.01	0.42
1:C:726:TYR:OH	1:C:842:TYR:O	2.38	0.42
1:A:770:ILE:O	1:A:774:MET:N	2.51	0.42
1:D:719:HIS:CE1	1:D:852:ARG:HE	2.37	0.42
1:B:852:ARG:H	1:B:852:ARG:HG2	1.59	0.42
1:A:924:GLU:O	1:A:928:ARG:NE	2.52	0.41
1:A:1069:ILE:HD11	1:B:1068:ILE:HB	2.02	0.41
1:D:924:GLU:O	1:D:928:ARG:NE	2.52	0.41
1:A:571:ASN:OD1	1:A:571:ASN:N	2.54	0.41
1:D:461:THR:HA	1:D:464:ARG:HH11	1.84	0.41
1:D:458:ARG:O	1:D:461:THR:OG1	2.35	0.41
1:B:556:ALA:HB1	1:B:587:ALA:HB2	2.02	0.41
1:B:866:ILE:HD11	1:B:964:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ALA:HB1	1:A:587:ALA:HB2	2.02	0.41
1:B:719:HIS:O	1:B:723:LEU:N	2.53	0.41
1:D:852:ARG:H	1:D:852:ARG:HG2	1.59	0.41
1:D:1054:LEU:HD11	1:C:1054:LEU:HD22	2.02	0.41
1:C:928:ARG:HG3	1:C:930:GLU:HG3	2.03	0.41
1:A:787:LYS:HD2	1:A:790:GLY:HA2	2.03	0.41
1:A:928:ARG:HG3	1:A:930:GLU:HG3	2.03	0.41
1:B:928:ARG:HG3	1:B:930:GLU:HG3	2.03	0.41
1:D:572:ALA:O	1:D:604:ARG:NH2	2.41	0.41
1:D:787:LYS:HD2	1:D:790:GLY:HA2	2.03	0.41
1:D:928:ARG:HG3	1:D:930:GLU:HG3	2.03	0.41
1:C:534:LEU:HD13	1:C:534:LEU:HA	1.90	0.41
1:C:719:HIS:O	1:C:723:LEU:N	2.53	0.41
1:C:866:ILE:HD11	1:C:964:ILE:HD11	2.02	0.41
1:C:952:LEU:HD23	1:C:952:LEU:HA	1.89	0.41
1:B:465:LEU:HD23	1:B:465:LEU:HA	1.90	0.41
1:B:534:LEU:HD13	1:B:534:LEU:HA	1.90	0.41
1:C:787:LYS:HD2	1:C:790:GLY:HA2	2.03	0.41
1:D:553:HIS:HB3	1:D:586:LEU:HD23	2.03	0.40
1:D:556:ALA:HB1	1:D:587:ALA:HB2	2.02	0.40
1:A:866:ILE:HD11	1:A:964:ILE:HD11	2.03	0.40
1:B:586:LEU:HD12	1:B:586:LEU:HA	1.92	0.40
1:C:511:ASP:N	1:C:511:ASP:OD1	2.50	0.40
1:C:553:HIS:HB3	1:C:586:LEU:HD23	2.03	0.40
1:C:778:PHE:HE1	1:C:816:ILE:HG23	1.87	0.40
1:A:887:SER:HA	1:A:890:ILE:HG22	2.03	0.40
1:D:871:LEU:HD23	1:D:871:LEU:HA	1.88	0.40
1:D:778:PHE:HE1	1:D:816:ILE:HG23	1.86	0.40
1:A:465:LEU:HA	1:A:465:LEU:HD23	1.90	0.40
1:B:952:LEU:HD23	1:B:952:LEU:HA	1.90	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	552/1119 (49%)	521 (94%)	31 (6%)	0	100	100
1	B	552/1119 (49%)	521 (94%)	31 (6%)	0	100	100
1	C	552/1119 (49%)	521 (94%)	31 (6%)	0	100	100
1	D	552/1119 (49%)	521 (94%)	31 (6%)	0	100	100
All	All	2208/4476 (49%)	2084 (94%)	124 (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	469/995 (47%)	458 (98%)	11 (2%)	50	76
1	B	469/995 (47%)	458 (98%)	11 (2%)	50	76
1	C	469/995 (47%)	458 (98%)	11 (2%)	50	76
1	D	469/995 (47%)	458 (98%)	11 (2%)	50	76
All	All	1876/3980 (47%)	1832 (98%)	44 (2%)	53	76

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	ARG
1	A	486	LEU
1	A	534	LEU
1	A	595	VAL
1	A	709	MET
1	A	820	LEU
1	A	839	VAL
1	A	881	LEU
1	A	951	VAL
1	A	1065	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1073	GLU
1	B	473	ARG
1	B	486	LEU
1	B	534	LEU
1	B	595	VAL
1	B	709	MET
1	B	820	LEU
1	B	839	VAL
1	B	881	LEU
1	B	951	VAL
1	B	1065	ILE
1	B	1073	GLU
1	D	473	ARG
1	D	486	LEU
1	D	534	LEU
1	D	595	VAL
1	D	709	MET
1	D	820	LEU
1	D	839	VAL
1	D	881	LEU
1	D	951	VAL
1	D	1065	ILE
1	D	1073	GLU
1	C	473	ARG
1	C	486	LEU
1	C	534	LEU
1	C	595	VAL
1	C	709	MET
1	C	820	LEU
1	C	839	VAL
1	C	881	LEU
1	C	951	VAL
1	C	1065	ILE
1	C	1073	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	HIS
1	A	585	HIS
1	A	644	HIS
1	A	700	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	719	HIS
1	A	933	HIS
1	A	954	ASN
1	B	519	HIS
1	B	585	HIS
1	B	644	HIS
1	B	700	HIS
1	B	719	HIS
1	B	829	HIS
1	B	933	HIS
1	B	954	ASN
1	D	519	HIS
1	D	644	HIS
1	D	700	HIS
1	D	719	HIS
1	D	907	GLN
1	D	954	ASN
1	C	519	HIS
1	C	644	HIS
1	C	700	HIS
1	C	719	HIS
1	C	829	HIS
1	C	907	GLN
1	C	933	HIS
1	C	954	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

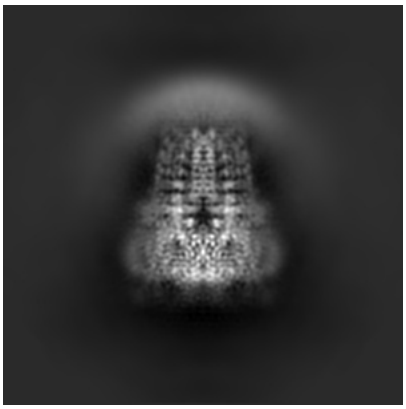
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21130. These allow visual inspection of the internal detail of the map and identification of artifacts.

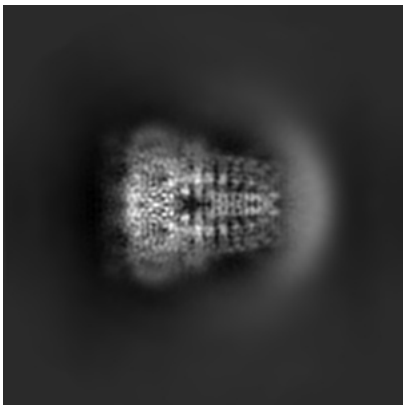
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

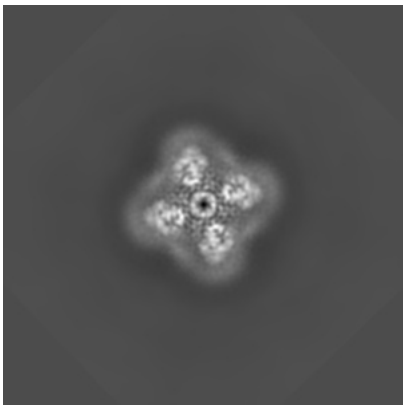
6.1.1 Primary map



X

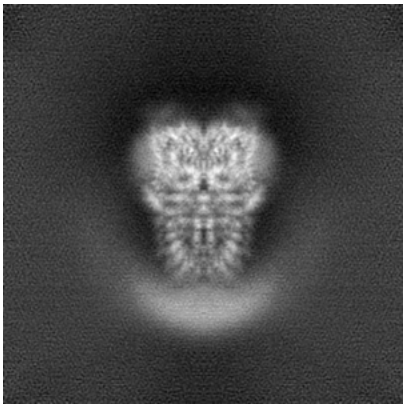


Y

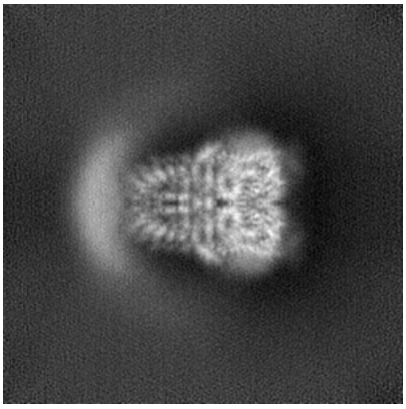


Z

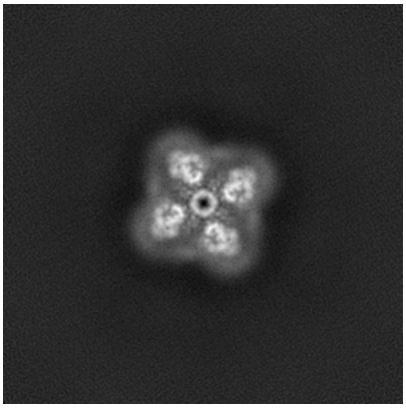
6.1.2 Raw map



X



Y

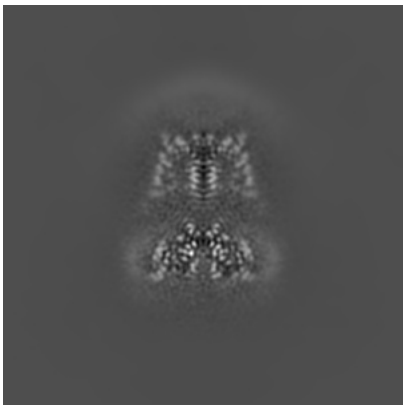


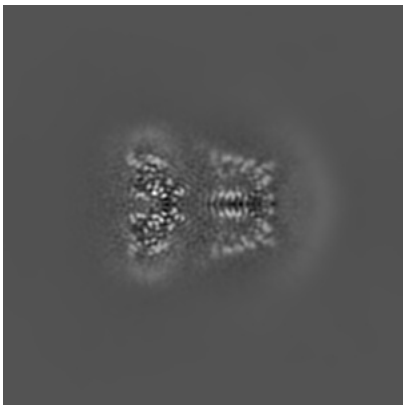
Z

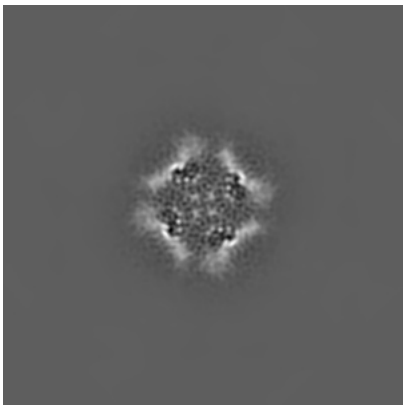
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

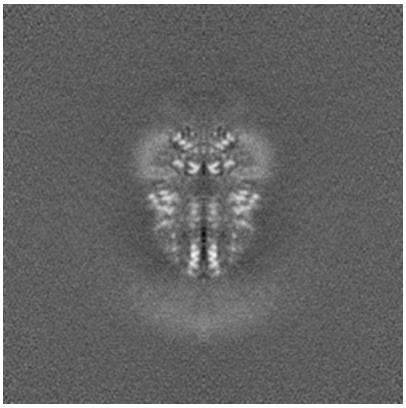
6.2.1 Primary map

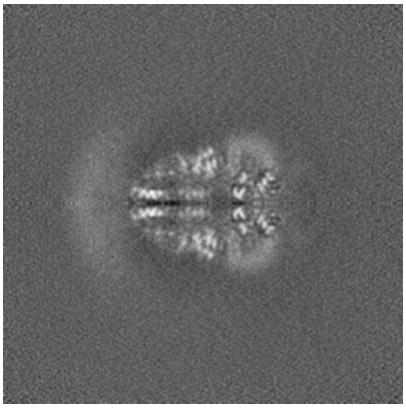

X Index: 128

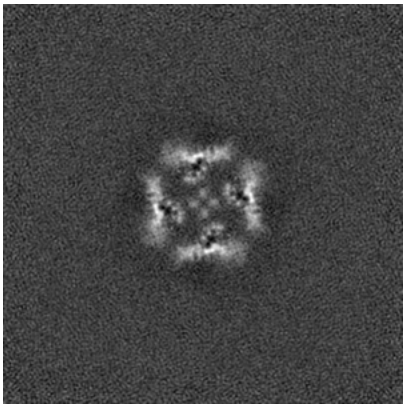

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

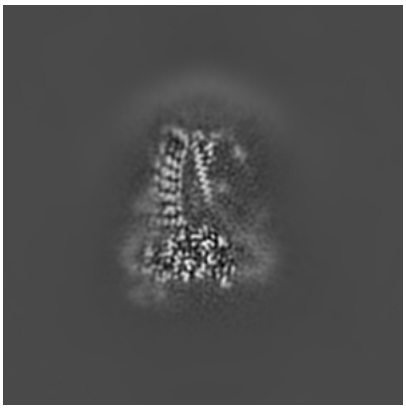

Y Index: 128

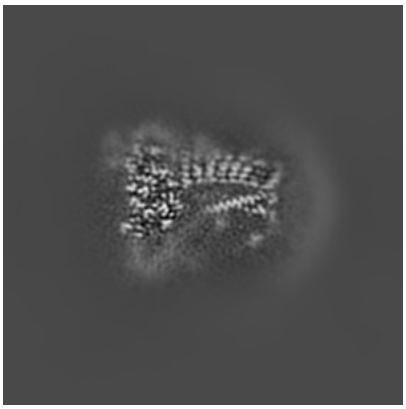

Z Index: 128

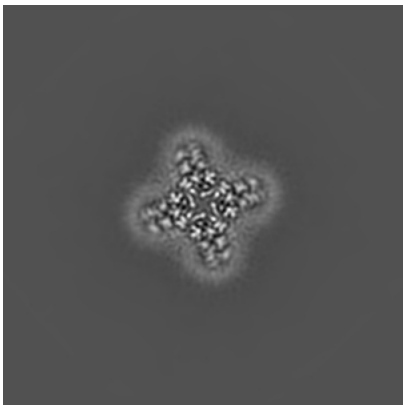
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

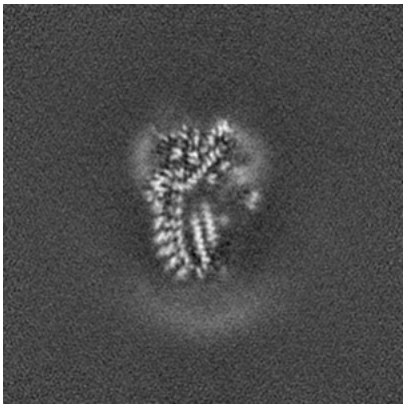
6.3.1 Primary map

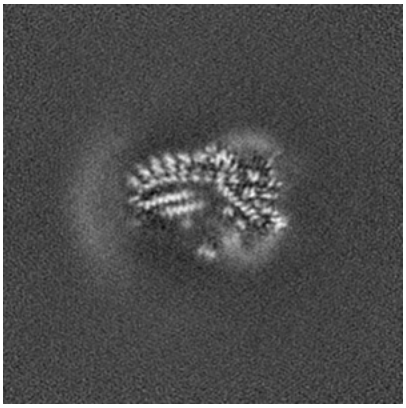

X Index: 134

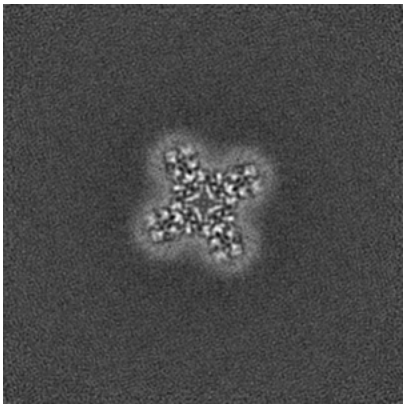

Y Index: 134


Z Index: 87

6.3.2 Raw map


X Index: 133

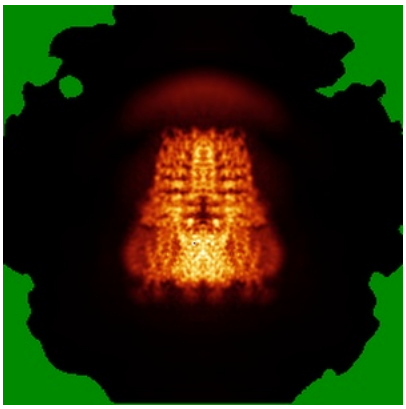

Y Index: 133

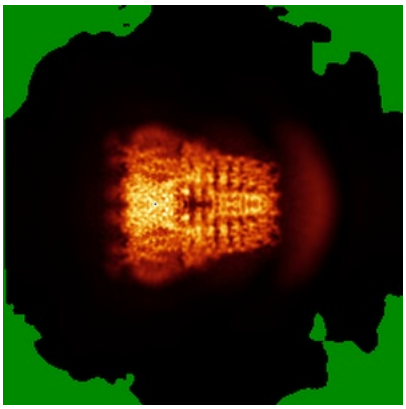

Z Index: 170

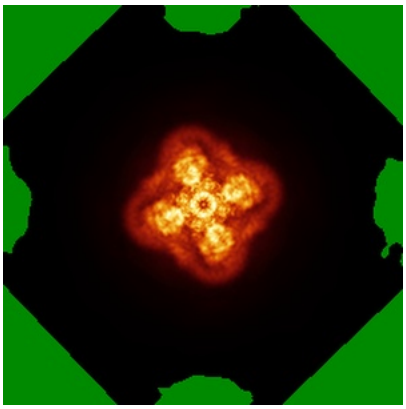
The images above show the largest variance slices of the map in three orthogonal directions.

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

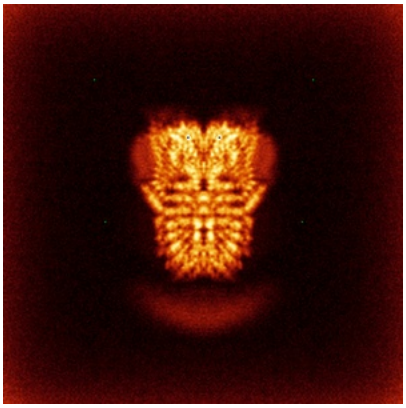
6.4.1 Primary map

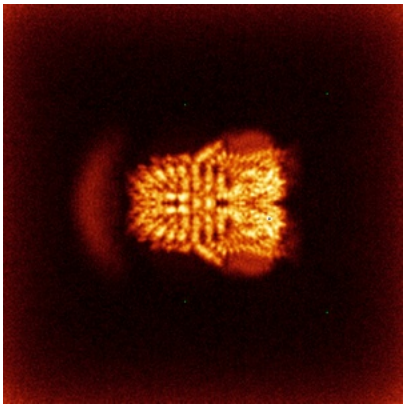

X

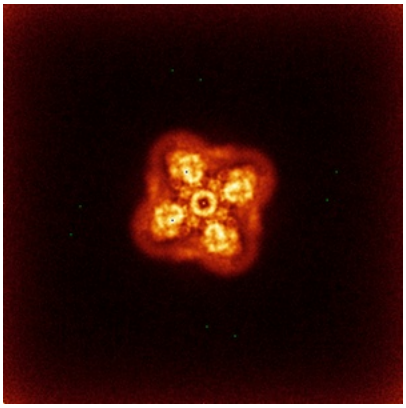

Y


Z

6.4.2 Raw map


X

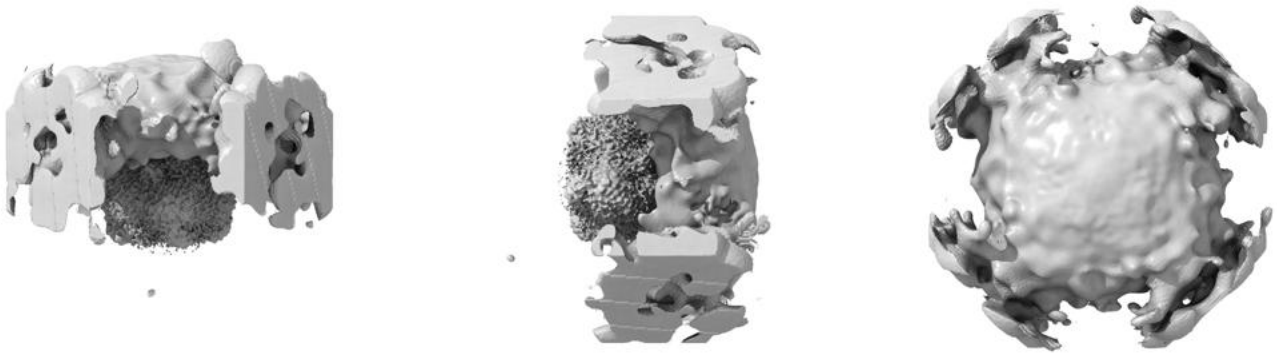

Y


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)

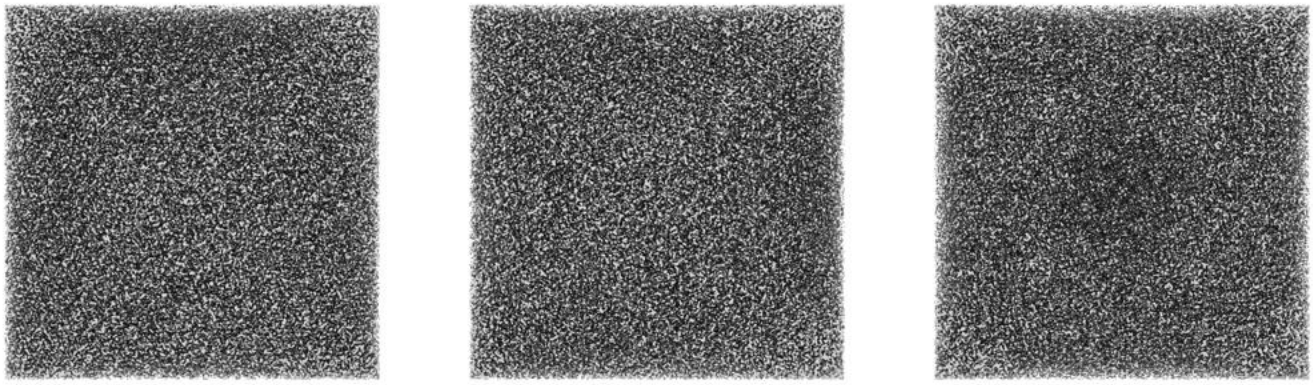
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

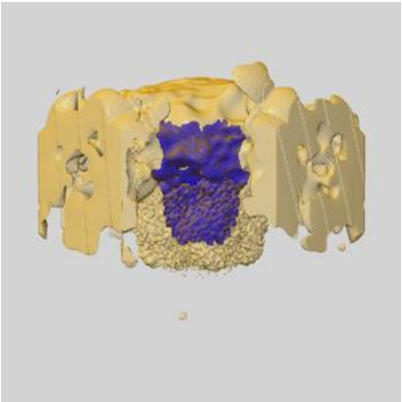
6.6 Mask visualisation (i)

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

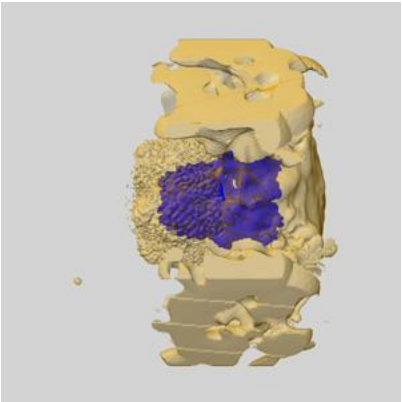
A mask typically either:

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

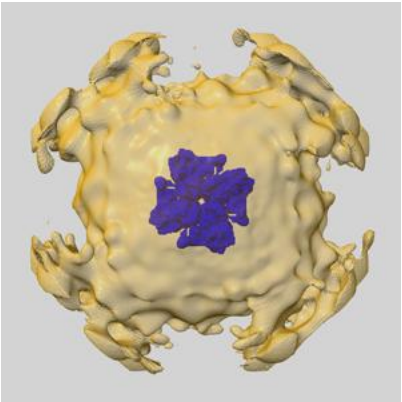
6.6.1 emd_21130_msk_1.map (i)



X



Y

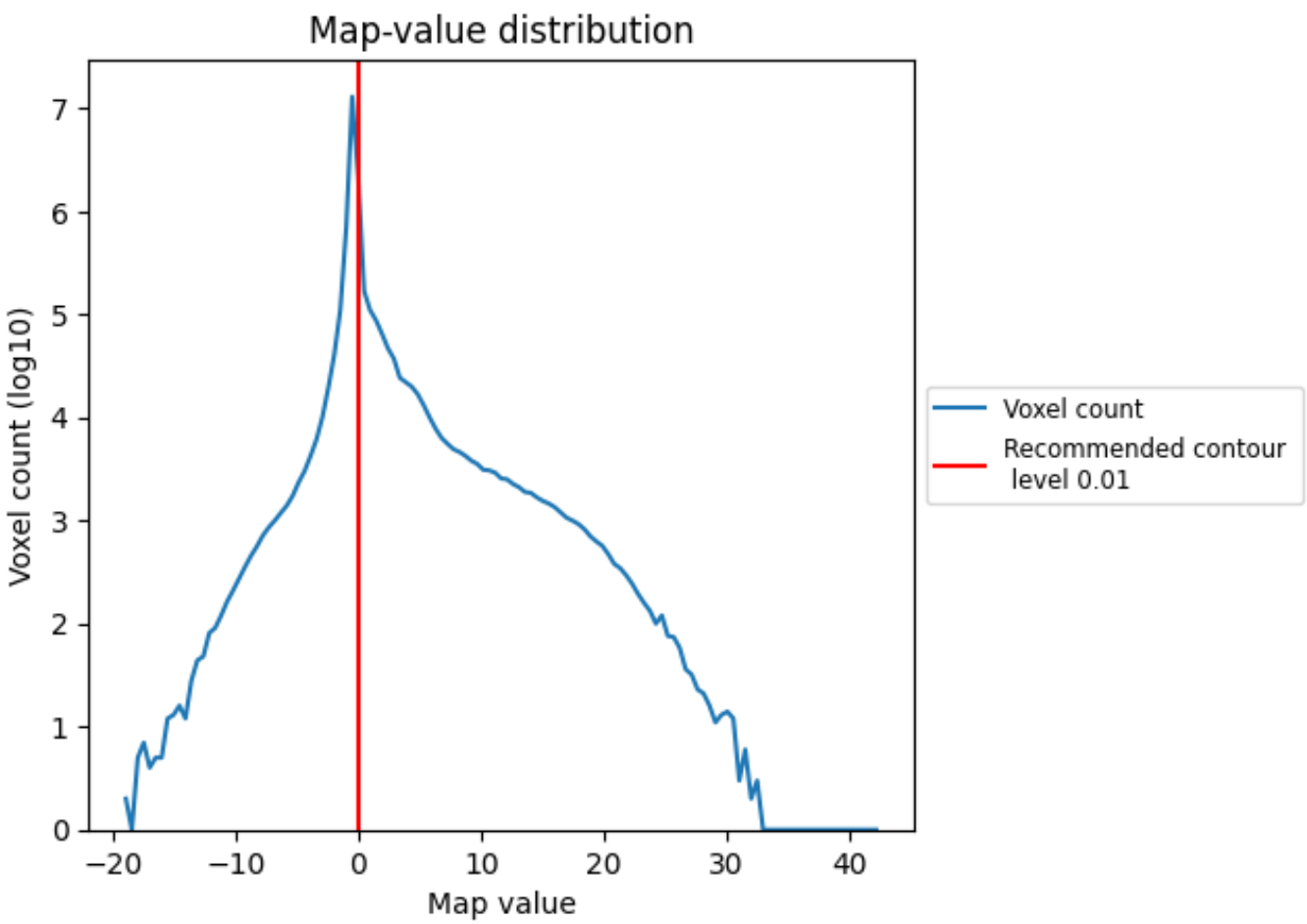


Z

7 Map analysis (i)

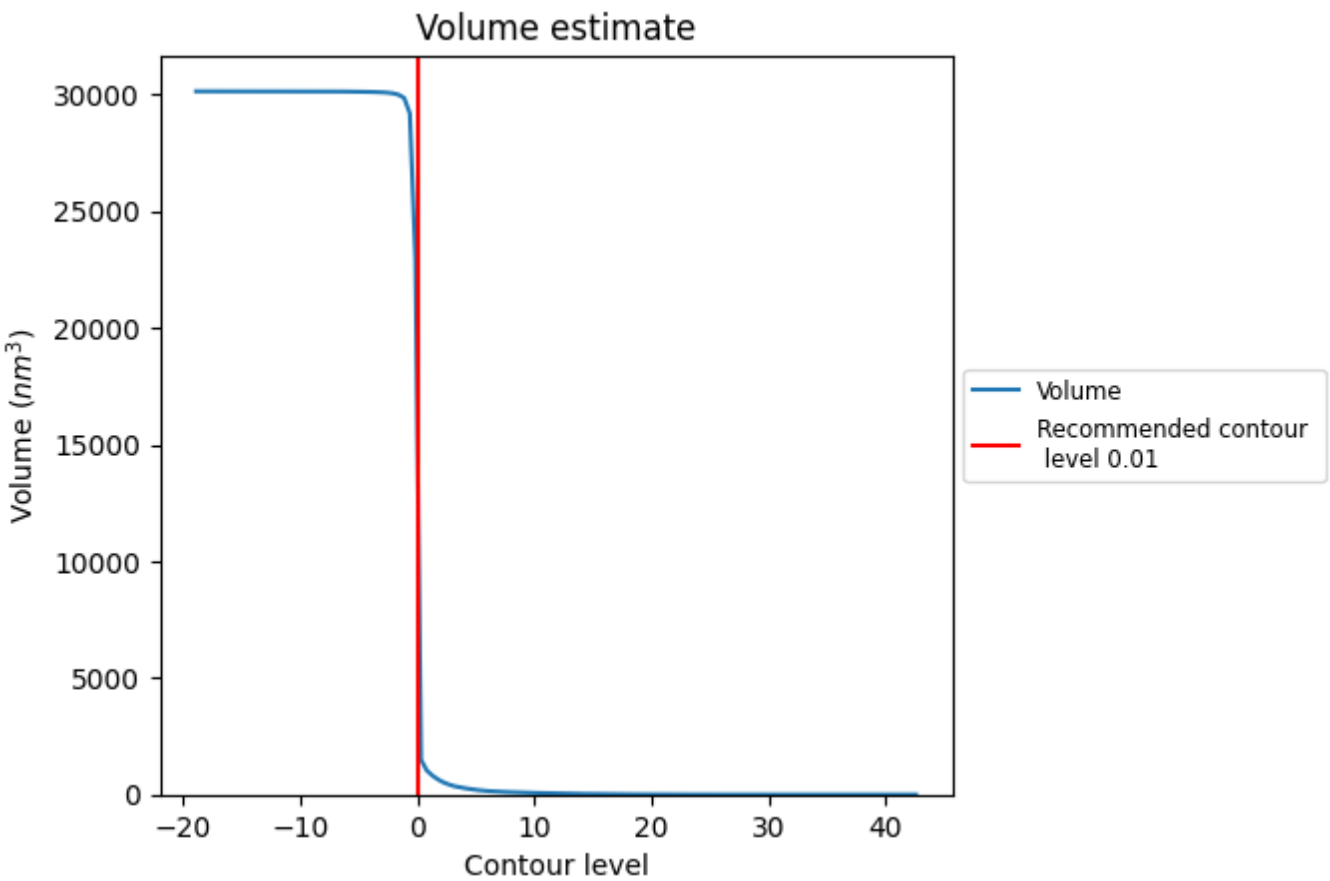
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

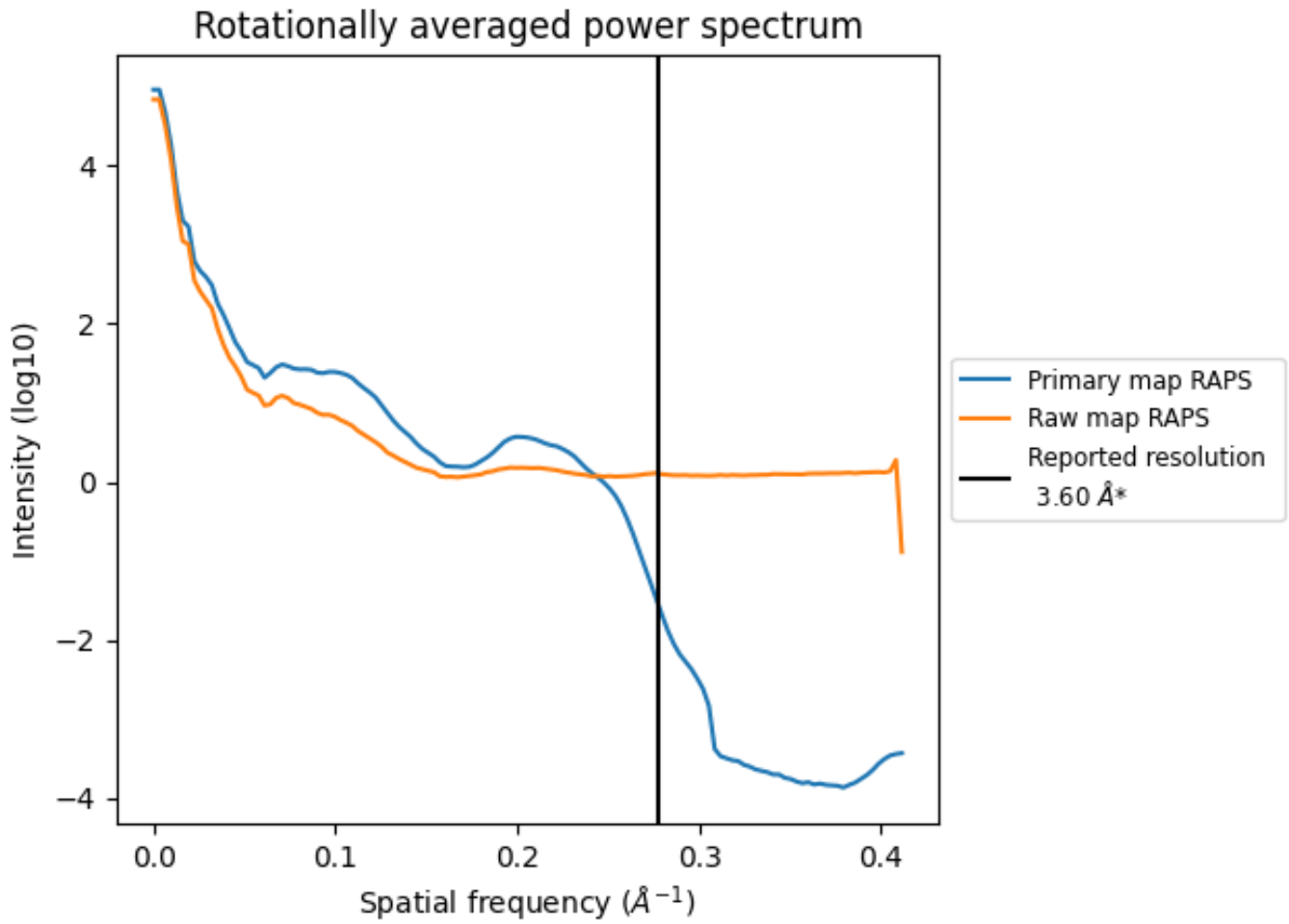
7.2 Volume estimate (i)



The volume at the recommended contour level is 15828 nm^3; this corresponds to an approximate mass of 14298 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)

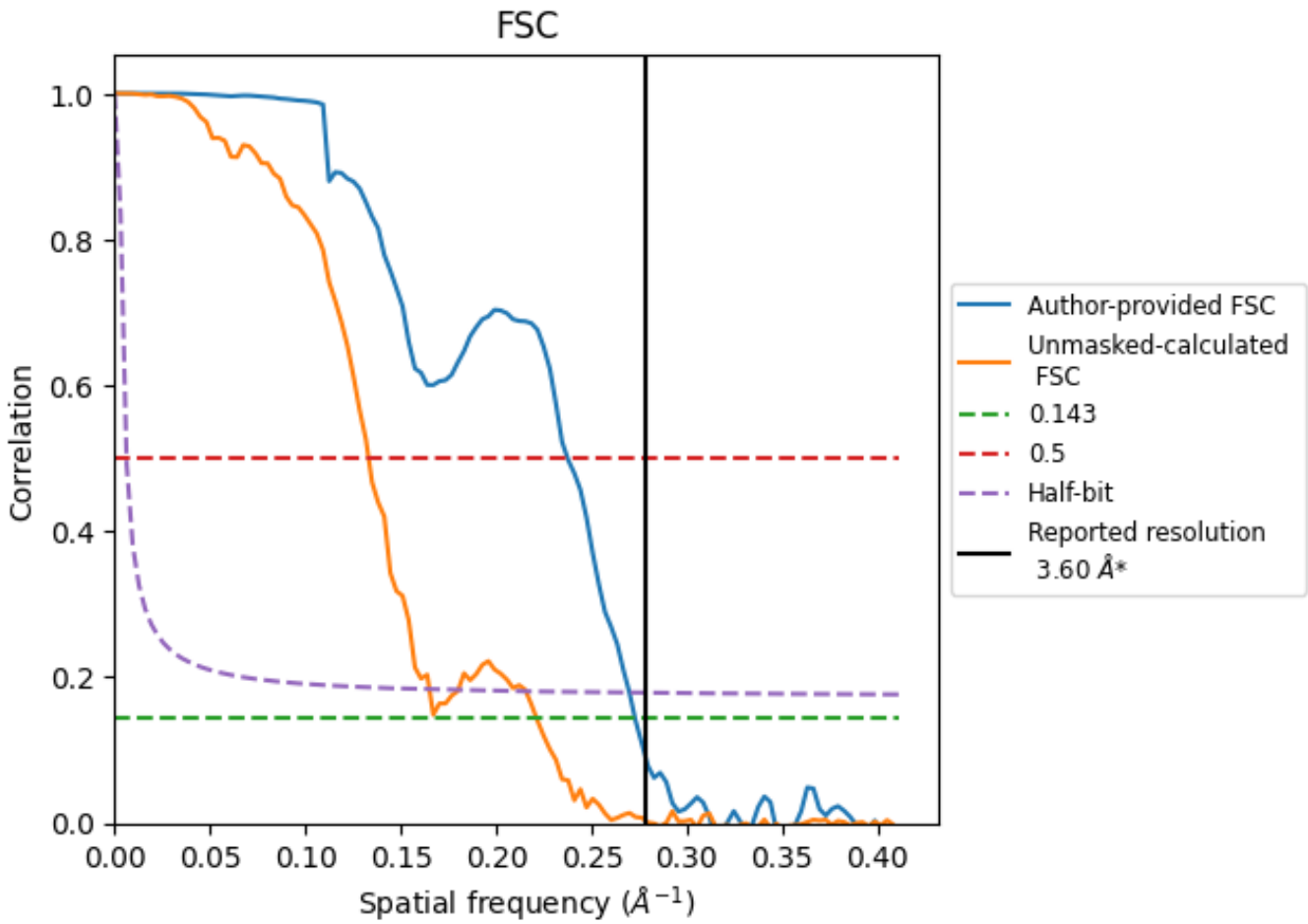


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.66	4.21	3.71
Unmasked-calculated*	4.52	7.51	6.06

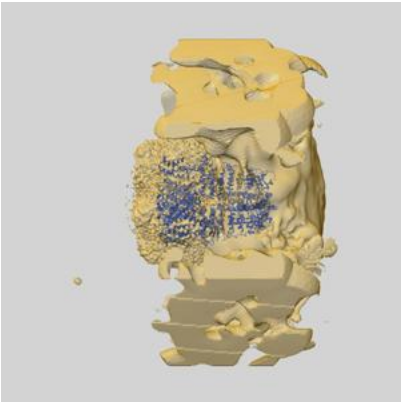
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.6 by more than 10 %

9 Map-model fit (i)

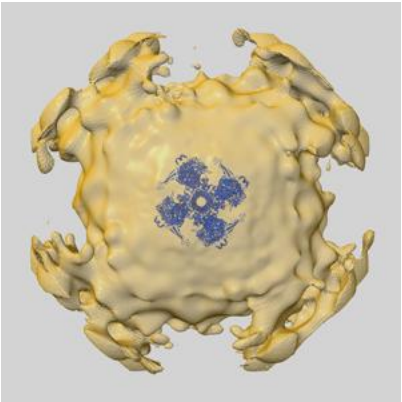
This section contains information regarding the fit between EMDB map EMD-21130 and PDB model 6V9Y. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)

X



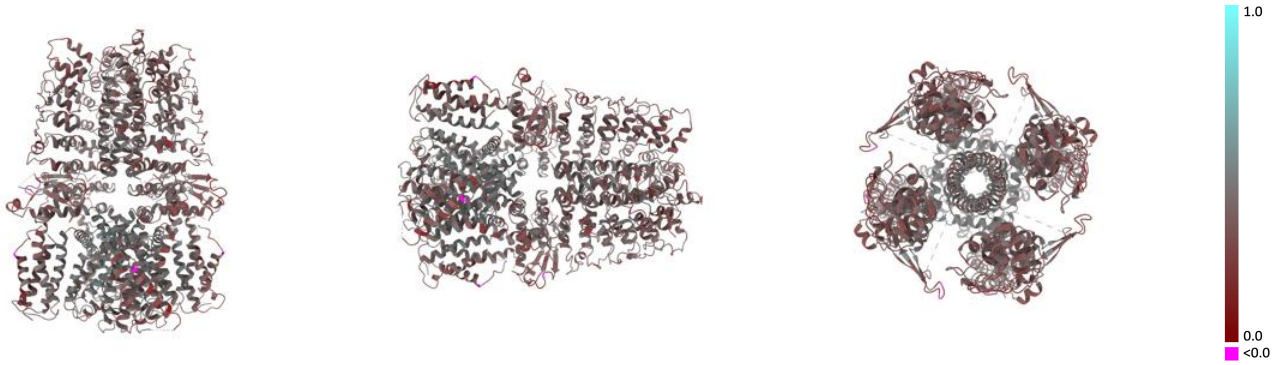
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

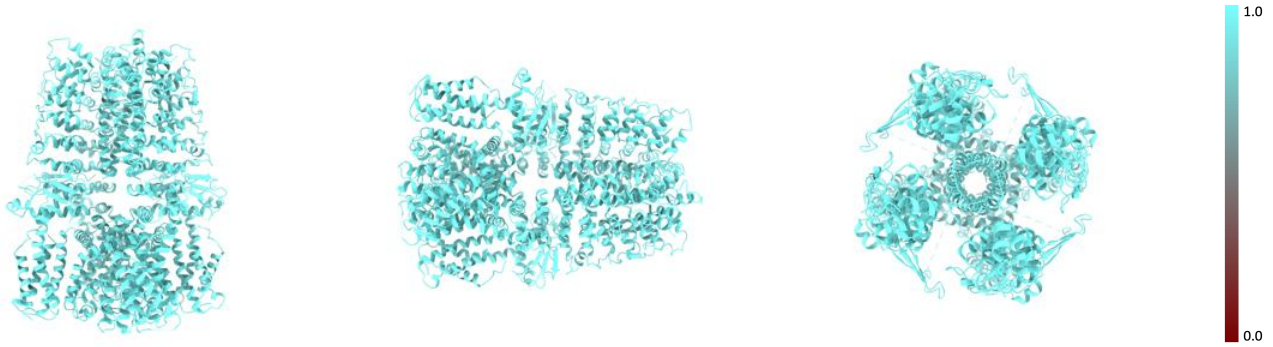
9.2 Q-score mapped to coordinate model (i)



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.

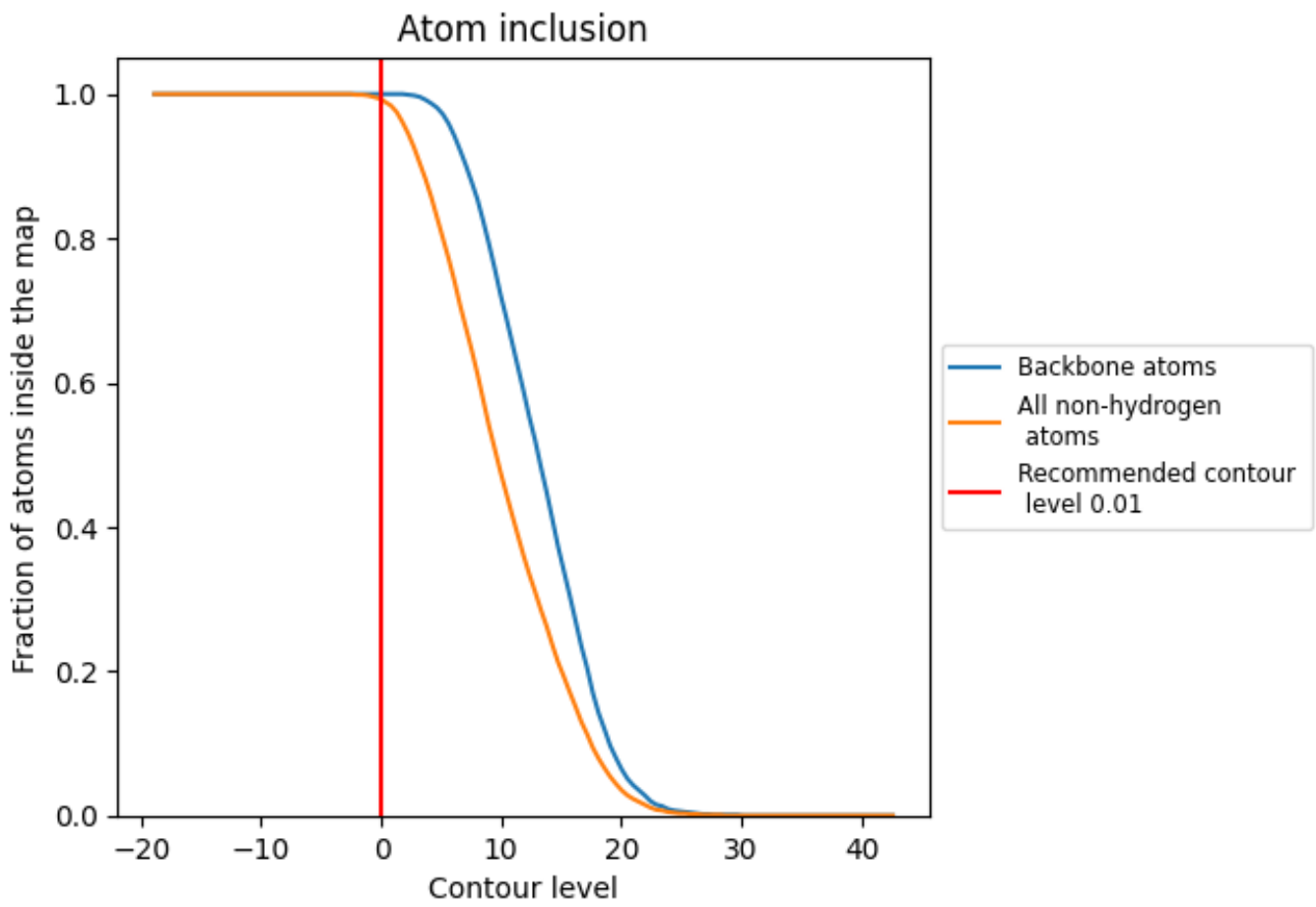
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.3900
A	0.9940	0.3950
B	0.9930	0.3930
C	0.9930	0.3880
D	0.9930	0.3860