WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Sep 27, 2023 – 07:20 PM EDT

PDB ID	:	8GJJ
EMDB ID	:	EMD-40091
Title	:	Multi-drug efflux pump RE-CmeB Apo form
Authors	:	Zhang, Z.
Deposited on	:	2023-03-15
Resolution	:	3.08 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1　Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.08 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		2.4%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
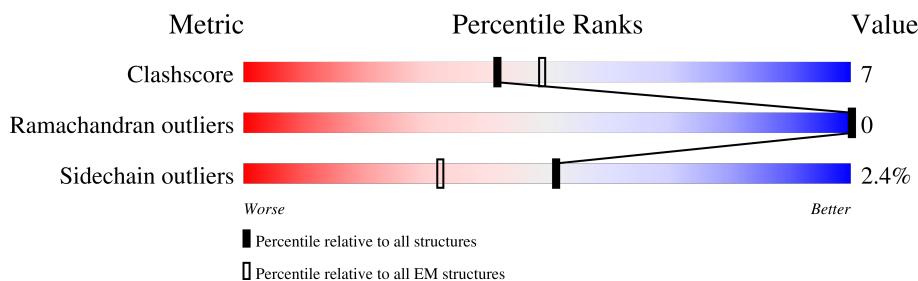
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1039	81% 18% ••
1	B	1039	79% 18% ••
1	C	1039	80% 18% ••
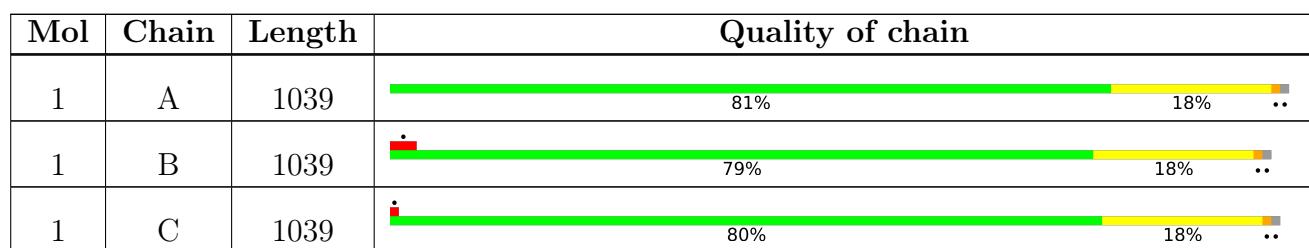
2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 23928 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 Efflux pump membrane transporter.

| Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1032	Total	C	N	O	S	0	0
			7976	5174	1285	1489	28		
1	A	1032	Total	C	N	O	S	0	0
			7982	5177	1288	1489	28		
1	C	1032	Total	C	N	O	S	0	0
			7970	5170	1287	1485	28		

3 Residue-property plots ⓘ

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: Efflux pump membrane transporter

Chain B:

• Molecule 1: Efflux pump membrane transporter

Chain A:

F455 I456 I461 I468 Q469 R470 Q471 F472 A473 L474 T475 L476 V480 T489 L490 R501 I510 Q511 K512 F524 R537 I549 L552 I555 S559 D565 Q566 S571 I581 I591 V605 L612 F613 T614 L617 N620 V624 F625

D630 W631 S632 Q633 R634 Y649 R653 P663 E675 M676 Y677 A678 Q679 N680 K681 L699 T702 R703 K704 E705 T715 Y720 I724 D725 R726 Y731 T742 T746 T749 V752 N753 P756 M757 N761 F762 R767 A768 L769 F772 T775 Q776

D777 A778 L794 N795 L798 T799 L800 V801 R802 P806 K810 R811 F812 L819 T829 L845 Y849 S850 L873 I881 L882 A883 A884 M891 P892 L893 A894 V895 I896 T897 P900 F904 G905 S906 L909 R913 G914 F915 D916 N917 D918 L927 K934

N935 A936 I937 I940 M944 K950 G951 K952 A962 K963 L964 I969 I970 M971 F976 P982 M983 I984 I1002 M1005 A1008 A1012 I1013 F1020 L1023 K1032 LYS ARG GLY LYS VAL HIS GLU

• Molecule 1: Efflux pump membrane transporter

Chain C: 80%   18%

M1 K4 E8 V15 T40 V46 Y50 T51 G52 A53 D54 A63 E67 S81 T82 L90 T91 F94 A103 A104 L125 K131 L137 E138 V139 N150 D151 I152 I162 E165 V172 G173 D174 W188 V199 I205 Q211

T217 I220 P224 V225 V226 N227 I233 T236 R240 E248 L252 R253 V254 K258 S259 F260 K264 A273 R281 L282 N283 T284 I291 I292 N293 L294 L314 F318 V341 L349 L353 S365 T366 I367 I368 P369 M370 V373 P374

L387 L396 L401 I405 D408 V413 I417 D418 R419 S425 N426 I427 S428 V429 K430 A433 A436 P443 I447 V448 L449 V450 L451 Q469 I478 S479 V480 L494 S495 A496 L497 F498 L499 T500 R501 F524 I531 T535 I549 V561

P576 S579 S580 I581 E600 S606 F610 L617 K629 Q633 D652 L660 N661 L662 P663 P664 I665 Y677 A678 Q679 N680 K681 K684 D685 Y686 D692 V693 A700 E705 L706 T711 T712 L713 Y720 Y732 Y739 N735 V739 A745 T749

V752 P756 M757 L758 R767 A768 L769 G770 D771 F772 R773 R785 N789 I792 L800 V801 R802 V809 K810 R811 F815 A825 P826 G827 I834 D835 A836 V840 L845 E848 Y849 S856 E860 V861 S862 S863 K864 G865 V878 F879 I881 L882

R888 M891 P892 I896 T897 P900 F901 A902 V903 F904 G905 S906 I907 V910 D916 N917 D918 I919 Q922 L925 L926 L927 L928 L931 K934 L938 E941 A962 K963 L964 R965 P968 T972 V980 L981 L1001 I1002 G1003 G1004 M1005 I1006 A1007

F1014 L1022 L1023 E1024 K1032 LYS ARG GLY LYS VAL HIS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31428	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 $(e^-/\text{Å}^2)$	36.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.966	Depositor
Minimum map value	-0.416	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	374.50003, 374.50003, 374.50003	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.33	0/8136	0.46	0/11051
1	B	0.30	0/8130	0.45	0/11044
1	C	0.32	0/8124	0.45	0/11037
All	All	0.32	0/24390	0.45	0/33132

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	7982	0	8165	111	0
1	B	7976	0	8154	129	0
1	C	7970	0	8146	122	0
All	All	23928	0	24465	352	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 7.

All (352) 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:A:884:ALA:HB2	1:C:15:VAL:HG21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:LYS:NZ	1:C:692:ASP:OD2	2.17	0.78
1:B:36:TYR:HH	1:B:920:TYR:HH	1.32	0.77
1:B:947:ARG:HH21	1:B:954:ILE:HG12	1.49	0.77
1:B:834:ILE:HA	1:B:837:ILE:HD12	1.71	0.73
1:A:720:TYR:HE1	1:A:802:ARG:HG2	1.54	0.71
1:A:731:TYR:HE1	1:C:258:LYS:HD2	1.55	0.71
1:A:891:MET:HE1	1:A:944:MET:HB2	1.72	0.70
1:A:179:GLY:HA2	1:A:617:LEU:HD21	1.74	0.68
1:C:700:ALA:HB2	1:C:840:VAL:HG11	1.76	0.68
1:B:73:VAL:HG22	1:B:110:ARG:HD3	1.76	0.67
1:B:205:ILE:HD11	1:B:745:ALA:HB2	1.76	0.67
1:B:405:ILE:HG21	1:B:480:VAL:HG22	1.78	0.66
1:C:405:ILE:HG21	1:C:480:VAL:HG12	1.77	0.66
1:C:449:LEU:HB3	1:C:881:ILE:HD13	1.77	0.65
1:A:37:PRO:HG3	1:A:471:GLN:HG3	1.78	0.65
1:B:535:THR:HG23	1:B:1018:LEU:HD11	1.77	0.65
1:C:205:ILE:HD11	1:C:745:ALA:HB2	1.79	0.65
1:B:680:ASN:HD21	1:B:684:LYS:HG2	1.62	0.64
1:B:706:LEU:HD22	1:B:837:ILE:HG12	1.78	0.64
1:C:720:TYR:HB3	1:C:800:LEU:HD22	1.80	0.64
1:A:681:LYS:NZ	1:A:850:SER:OG	2.28	0.63
1:B:776:GLN:NE2	1:B:800:LEU:O	2.31	0.63
1:A:240:ARG:NH2	1:A:761:ASN:OD1	2.28	0.63
1:C:693:VAL:HG11	1:C:711:THR:HG21	1.80	0.63
1:A:704:LYS:NZ	1:A:705:GLU:OE2	2.30	0.63
1:C:928:LEU:HD13	1:C:1004:GLY:HA3	1.80	0.63
1:A:248:GLU:HB3	1:A:264:LYS:HB3	1.82	0.61
1:B:406:VAL:HG12	1:B:483:SER:HB3	1.83	0.61
1:B:890:LEU:HB3	1:B:1023:LEU:HD12	1.83	0.60
1:A:565:ASP:OD2	1:A:634:ARG:NH1	2.35	0.60
1:B:330:THR:HG23	1:B:665:ILE:HG12	1.81	0.60
1:C:927:LEU:HD23	1:C:1001:LEU:HD11	1.83	0.60
1:B:345:PHE:HD1	1:B:403:ILE:HD11	1.66	0.60
1:B:928:LEU:HD13	1:B:1004:GLY:HA3	1.84	0.59
1:C:535:THR:HG23	1:C:1022:LEU:HD11	1.83	0.59
1:A:427:ILE:O	1:A:501:ARG:NH2	2.33	0.59
1:C:549:ILE:HD11	1:C:904:PHE:HB2	1.84	0.58
1:B:699:LEU:HD22	1:B:840:VAL:HG13	1.85	0.58
1:C:705:GLU:HA	1:C:825:ALA:HB2	1.85	0.58
1:A:476:LEU:HD13	1:A:927:LEU:HD13	1.85	0.58
1:C:417:ILE:HD13	1:C:436:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:LEU:HB3	1:C:927:LEU:HD22	1.85	0.58
1:B:905:GLY:HA3	1:B:1007:ALA:HB2	1.84	0.58
1:C:417:ILE:HD12	1:C:433:ALA:HA	1.86	0.58
1:B:60:SER:O	1:B:64:THR:OG1	2.21	0.57
1:C:711:THR:HG22	1:C:713:LEU:H	1.69	0.57
1:A:411:ILE:HG23	1:A:971:MET:HE2	1.86	0.57
1:A:118:LEU:HD12	1:A:122:VAL:HG21	1.87	0.57
1:A:776:GLN:OE1	1:A:795:ASN:ND2	2.37	0.57
1:C:413:VAL:O	1:C:417:ILE:HG12	2.05	0.57
1:C:469:GLN:HG3	1:C:919:ILE:HD11	1.87	0.57
1:B:401:LEU:HD13	1:B:927:LEU:HD22	1.86	0.56
1:C:680:ASN:HD21	1:C:684:LYS:HD3	1.71	0.56
1:C:888:ARG:NH1	1:C:1024:GLU:OE1	2.37	0.56
1:C:152:ILE:HG12	1:C:273:ALA:HB2	1.87	0.56
1:A:70:ILE:O	1:A:73:VAL:HG23	2.05	0.56
1:B:143:TYR:HB3	1:B:287:ALA:HB2	1.87	0.56
1:B:456:ILE:O	1:B:459:SER:OG	2.19	0.56
1:B:864:LYS:HE2	1:B:866:ALA:H	1.70	0.56
1:A:720:TYR:CE1	1:A:802:ARG:HG2	2.38	0.56
1:C:341:VAL:HG21	1:C:396:LEU:HB3	1.88	0.56
1:A:677:TYR:HE2	1:A:810:LYS:HD3	1.71	0.56
1:B:885:GLN:NE2	1:B:941:GLU:OE1	2.39	0.55
1:A:446:SER:HB3	1:A:937:ILE:HD13	1.87	0.55
1:C:451:LEU:HD12	1:C:480:VAL:HG11	1.87	0.55
1:B:882:LEU:HB2	1:B:892:PRO:HB3	1.88	0.55
1:C:917:ASN:HD21	1:C:922:GLN:HE21	1.54	0.55
1:A:461:ILE:O	1:A:470:ARG:NH2	2.39	0.55
1:B:516:PHE:HA	1:B:519:TRP:CD1	2.41	0.55
1:C:353:LEU:HD21	1:C:370:MET:HG3	1.89	0.55
1:B:893:LEU:HA	1:B:896:ILE:HG12	1.89	0.55
1:B:829:THR:HB	1:B:832:GLN:HG2	1.89	0.55
1:C:67:GLU:OE1	1:C:811:ARG:NH1	2.40	0.55
1:A:451:LEU:HD13	1:A:480:VAL:HG21	1.88	0.55
1:A:559:SER:HB3	1:A:829:THR:HB	1.88	0.55
1:C:419:ARG:HD2	1:C:964:LEU:HD22	1.89	0.55
1:B:680:ASN:HD21	1:B:684:LYS:H	1.54	0.54
1:A:769:LEU:HD12	1:C:225:VAL:HG12	1.88	0.54
1:C:8:GLU:HG2	1:C:430:LYS:HE2	1.89	0.54
1:B:409:ASP:N	1:B:409:ASP:OD1	2.40	0.54
1:A:1:MET:SD	1:A:1:MET:N	2.76	0.54
1:C:4:LYS:NZ	1:C:8:GLU:OE2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HG13	1:B:878:VAL:HG22	1.90	0.54
1:B:139:VAL:HG22	1:B:291:ILE:HG22	1.88	0.54
1:B:570:MET:HE3	1:B:662:LEU:HD13	1.90	0.54
1:B:674:PHE:CE1	1:B:837:ILE:HD13	2.42	0.54
1:B:704:LYS:HD2	1:B:836:ALA:HB1	1.89	0.54
1:B:749:THR:HG22	1:B:767:ARG:HD2	1.91	0.53
1:B:950:LYS:HD2	1:B:952:LYS:HZ2	1.74	0.53
1:C:281:ARG:HB2	1:C:606:SER:HB2	1.91	0.53
1:B:140:VAL:HG11	1:B:311:MET:SD	2.49	0.53
1:C:447:ILE:HG21	1:C:934:LYS:HG3	1.91	0.53
1:A:172:VAL:HG21	1:A:307:ILE:HD11	1.91	0.53
1:C:443:PRO:HG3	1:C:941:GLU:HG2	1.90	0.52
1:C:720:TYR:HE1	1:C:802:ARG:HG2	1.75	0.52
1:B:24:GLY:HA2	1:B:382:ALA:HB2	1.92	0.52
1:C:629:LYS:HE2	1:C:633:GLN:HB3	1.91	0.52
1:C:561:VAL:HG21	1:C:665:ILE:HD12	1.92	0.52
1:C:199:VAL:HG11	1:C:252:LEU:HD13	1.91	0.51
1:C:892:PRO:O	1:C:896:ILE:HG12	2.10	0.51
1:C:139:VAL:HG22	1:C:291:ILE:HG12	1.92	0.51
1:C:902:ALA:HB1	1:C:928:LEU:HB3	1.93	0.51
1:B:101:ASP:OD1	1:B:131:LYS:NZ	2.38	0.51
1:C:248:GLU:HB3	1:C:264:LYS:HB3	1.93	0.51
1:B:222:GLU:O	1:C:773:ARG:NH1	2.40	0.50
1:B:401:LEU:HD12	1:B:472:PHE:HZ	1.76	0.50
1:A:566:GLN:NE2	1:A:663:PRO:O	2.44	0.50
1:B:531:ILE:HG12	1:B:538:PHE:CZ	2.46	0.50
1:B:50:TYR:O	1:B:86:GLY:HA2	2.11	0.50
1:B:460:PHE:H	1:B:470:ARG:HB2	1.77	0.50
1:A:436:ALA:O	1:A:440:VAL:HG22	2.11	0.50
1:C:732:TYR:HB3	1:C:792:ILE:HD13	1.93	0.50
1:C:172:VAL:HG13	1:C:292:ILE:HG23	1.94	0.50
1:C:368:ILE:HB	1:C:369:PRO:HD3	1.94	0.50
1:C:662:LEU:HG	1:C:663:PRO:HD2	1.93	0.50
1:C:706:LEU:HD21	1:C:836:ALA:HB3	1.92	0.50
1:C:931:LEU:HD12	1:C:1005:MET:HE1	1.94	0.50
1:A:731:TYR:CE1	1:C:258:LYS:HD2	2.42	0.50
1:C:494:LEU:HD22	1:C:498:PHE:HE2	1.76	0.50
1:B:680:ASN:ND2	1:B:684:LYS:HG2	2.24	0.49
1:A:829:THR:HG21	1:A:916:ASP:HB3	1.95	0.49
1:C:600:GLU:OE1	1:C:600:GLU:N	2.41	0.49
1:A:895:VAL:HG13	1:A:936:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:ILE:HD12	1:C:1014:PHE:HB3	1.94	0.49
1:B:352:VAL:HG22	1:B:975:ALA:HB1	1.95	0.49
1:A:94:PHE:CE2	1:A:103:ALA:HB1	2.47	0.49
1:C:427:ILE:O	1:C:501:ARG:NH2	2.45	0.49
1:B:34:GLU:O	1:B:392:ASN:HA	2.13	0.49
1:A:101:ASP:O	1:A:105:ILE:HG12	2.13	0.49
1:A:794:LEU:HB3	1:A:798:LEU:HD12	1.95	0.49
1:B:467:GLU:OE1	1:B:470:ARG:NE	2.42	0.49
1:B:257:ASP:OD1	1:B:257:ASP:N	2.43	0.49
1:B:465:VAL:HG13	1:B:919:ILE:HD11	1.95	0.49
1:A:845:LEU:HB3	1:A:849:TYR:HB2	1.95	0.49
1:B:552:LEU:HA	1:B:555:ILE:HG12	1.95	0.48
1:B:972:THR:HB	1:B:976:PHE:CZ	2.48	0.48
1:A:757:MET:HB3	1:A:762:PHE:HD2	1.77	0.48
1:C:679:GLN:HE21	1:C:815:PHE:HB2	1.78	0.48
1:B:903:VAL:HG22	1:B:925:LEU:HD11	1.96	0.48
1:B:707:ALA:HB2	1:B:825:ALA:HA	1.95	0.48
1:A:677:TYR:CZ	1:A:819:LEU:HD13	2.48	0.48
1:B:248:GLU:HB3	1:B:264:LYS:HB3	1.94	0.48
1:C:165:GLU:HG3	1:C:314:LEU:HD21	1.94	0.48
1:C:217:THR:HG22	1:C:236:THR:HA	1.94	0.48
1:C:387:LEU:HD12	1:C:478:ILE:HD11	1.95	0.48
1:C:938:LEU:HB3	1:C:965:ARG:HD2	1.96	0.48
1:C:981:LEU:HA	1:C:1002:ILE:HD11	1.95	0.48
1:B:158:VAL:HG12	1:B:162:ILE:HD12	1.95	0.48
1:B:192:ASP:OD1	1:B:192:ASP:N	2.46	0.48
1:B:561:VAL:HG23	1:B:670:LEU:HD23	1.96	0.47
1:A:67:GLU:HA	1:A:79:MET:HE1	1.96	0.47
1:B:401:LEU:HB3	1:B:927:LEU:HD22	1.95	0.47
1:A:882:LEU:HD21	1:A:937:ILE:HD11	1.96	0.47
1:C:845:LEU:HB3	1:C:849:TYR:HB2	1.96	0.47
1:B:64:THR:OG1	1:B:65:PRO:HD3	2.14	0.47
1:B:653:ARG:HE	1:B:654:ASN:N	2.11	0.47
1:B:864:LYS:HD3	1:B:865:GLY:H	1.79	0.47
1:B:531:ILE:HA	1:B:538:PHE:CE2	2.49	0.47
1:A:419:ARG:HH11	1:A:964:LEU:HD12	1.79	0.47
1:A:679:GLN:HE21	1:A:812:PHE:HD2	1.61	0.47
1:A:772:PHE:CG	1:A:778:ALA:HB2	2.49	0.47
1:C:882:LEU:HB2	1:C:892:PRO:HB3	1.95	0.47
1:A:380:THR:HG21	1:A:475:THR:HG23	1.96	0.47
1:A:873:LEU:HD12	1:A:873:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ARG:HD2	1:C:756:PRO:HD3	1.96	0.47
1:B:80:ASP:HB3	1:B:812:PHE:HD1	1.78	0.47
1:A:82:THR:HG21	1:A:614:THR:HG23	1.97	0.47
1:A:277:ASN:OD1	1:A:277:ASN:N	2.45	0.47
1:A:1008:ALA:O	1:A:1012:ALA:HB3	2.14	0.47
1:C:757:MET:HG2	1:C:758:LEU:HG	1.97	0.47
1:B:77:ILE:HG23	1:B:78:TYR:CD2	2.49	0.46
1:B:577:SER:OG	1:B:714:ASP:OD2	2.33	0.46
1:A:397:PHE:O	1:A:401:LEU:HG	2.15	0.46
1:B:569:ILE:HG13	1:B:626:PHE:HB2	1.96	0.46
1:C:917:ASN:ND2	1:C:917:ASN:O	2.48	0.46
1:A:894:ALA:HB2	1:A:1023:LEU:HD12	1.97	0.46
1:A:909:LEU:HD12	1:A:909:LEU:HA	1.76	0.46
1:B:965:ARG:HD2	1:B:965:ARG:HA	1.69	0.46
1:A:24:GLY:HA3	1:A:378:LEU:HB3	1.98	0.46
1:A:212:ASN:O	1:A:753:ASN:ND2	2.49	0.46
1:A:605:VAL:HG13	1:A:625:PHE:HB2	1.97	0.46
1:B:189:LEU:HD23	1:B:267:ALA:HB2	1.98	0.46
1:B:733:ASN:OD1	1:B:733:ASN:N	2.49	0.46
1:A:984:ILE:HD12	1:A:1002:ILE:HD12	1.98	0.46
1:C:150:ASN:OD1	1:C:150:ASN:N	2.48	0.46
1:A:341:VAL:HG11	1:A:396:LEU:HB3	1.99	0.45
1:C:907:ILE:HA	1:C:910:VAL:HG22	1.98	0.45
1:C:980:VAL:HG11	1:C:1001:LEU:HD23	1.98	0.45
1:B:31:LEU:HD21	1:B:385:TYR:HA	1.98	0.45
1:B:217:THR:N	1:C:52:GLY:O	2.49	0.45
1:B:447:ILE:HD13	1:B:934:LYS:HG3	1.97	0.45
1:B:674:PHE:CZ	1:B:837:ILE:HG21	2.52	0.45
1:C:685:ASP:OD1	1:C:686:TYR:N	2.50	0.45
1:B:421:LEU:HD13	1:B:501:ARG:HA	1.98	0.45
1:B:938:LEU:HD22	1:B:965:ARG:NH2	2.31	0.45
1:A:240:ARG:HB3	1:A:756:PRO:HD3	1.98	0.45
1:A:453:ALA:HB2	1:A:881:ILE:HG13	1.98	0.45
1:A:591:ILE:HA	1:A:649:TYR:OH	2.17	0.45
1:B:838:ALA:HB2	1:B:853:TRP:HZ2	1.81	0.45
1:A:279:THR:HG22	1:A:280:GLY:H	1.82	0.45
1:B:585:ILE:HG12	1:B:608:ILE:HG21	1.98	0.45
1:A:456:ILE:HD13	1:A:456:ILE:HA	1.76	0.45
1:C:917:ASN:HD21	1:C:922:GLN:NE2	2.15	0.45
1:A:950:LYS:HB3	1:A:952:LYS:HE2	1.99	0.45
1:C:576:PRO:O	1:C:579:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:O	1:A:361:LYS:HG2	2.16	0.44
1:A:630:ASP:OD2	1:A:632:SER:OG	2.33	0.44
1:A:675:GLU:HB3	1:A:819:LEU:HD11	1.99	0.44
1:C:137:LEU:HD22	1:C:294:LEU:HD13	2.00	0.44
1:C:897:THR:O	1:C:900:PRO:HD2	2.17	0.44
1:A:394:LEU:HD13	1:A:468:ILE:HG23	1.99	0.44
1:C:905:GLY:HA3	1:C:1007:ALA:HB2	1.98	0.44
1:B:15:VAL:HG13	1:C:880:LEU:HB3	1.99	0.44
1:A:620:ASN:HD22	1:A:620:ASN:H	1.66	0.44
1:A:720:TYR:HB3	1:A:800:LEU:HD11	1.99	0.44
1:A:976:PHE:HD2	1:A:1005:MET:HG2	1.82	0.44
1:C:429:VAL:HG12	1:C:496:ALA:HA	2.00	0.44
1:B:835:ASP:O	1:B:839:GLU:HG2	2.16	0.44
1:A:726:ARG:NH1	1:C:211:GLN:O	2.46	0.44
1:C:425:SER:HA	1:C:501:ARG:HH12	1.83	0.44
1:A:373:VAL:HB	1:A:374:PRO:HD3	2.00	0.44
1:A:699:LEU:HD23	1:A:699:LEU:HA	1.83	0.44
1:B:232:VAL:HG23	1:C:580:SER:HA	1.99	0.43
1:B:518:ASP:O	1:B:521:THR:HG22	2.18	0.43
1:B:662:LEU:HB3	1:B:665:ILE:HG13	2.00	0.43
1:C:54:ASP:OD1	1:C:54:ASP:N	2.38	0.43
1:C:692:ASP:OD2	1:C:849:TYR:OH	2.27	0.43
1:A:58:ILE:HG22	1:A:83:SER:HB3	2.00	0.43
1:C:174:ASP:N	1:C:174:ASP:OD1	2.51	0.43
1:C:692:ASP:CG	1:C:849:TYR:HH	2.21	0.43
1:B:31:LEU:HB3	1:B:391:ILE:HG13	1.99	0.43
1:B:506:PRO:HB2	1:B:511:GLN:HE21	1.83	0.43
1:B:949:LYS:HD2	1:B:950:LYS:N	2.33	0.43
1:B:967:ARG:HB3	1:B:968:PRO:HD3	2.00	0.43
1:A:749:THR:HG22	1:A:767:ARG:HD2	1.99	0.43
1:B:39:LEU:HB3	1:B:464:PHE:HE1	1.83	0.43
1:B:443:PRO:HG3	1:B:941:GLU:CD	2.39	0.43
1:A:277:ASN:O	1:A:581:ILE:HG12	2.18	0.43
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.74	0.43
1:B:363:PHE:O	1:B:367:ILE:HG13	2.18	0.43
1:C:610:PHE:HD1	1:C:617:LEU:HD23	1.83	0.43
1:C:856:SER:O	1:C:860:GLU:HG2	2.18	0.43
1:B:516:PHE:HA	1:B:519:TRP:HD1	1.84	0.43
1:B:517:PHE:CZ	1:B:967:ARG:HA	2.54	0.43
1:A:303:THR:O	1:A:307:ILE:HG12	2.18	0.43
1:A:549:ILE:HD11	1:A:904:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG21	1:B:785:ARG:H	1.83	0.43
1:B:674:PHE:CZ	1:B:837:ILE:HD13	2.54	0.43
1:A:53:ALA:HB3	1:A:58:ILE:HG13	2.01	0.43
1:C:94:PHE:CE1	1:C:103:ALA:HB1	2.53	0.43
1:B:253:ARG:HG2	1:B:254:VAL:N	2.34	0.42
1:B:653:ARG:HE	1:B:654:ASN:H	1.66	0.42
1:A:54:ASP:OD1	1:A:54:ASP:N	2.41	0.42
1:C:220:ILE:HG23	1:C:233:ILE:HB	2.01	0.42
1:B:476:LEU:HD23	1:B:476:LEU:HA	1.91	0.42
1:B:531:ILE:HD12	1:B:1014:PHE:HB3	2.01	0.42
1:C:254:VAL:HG22	1:C:260:PHE:HD1	1.84	0.42
1:C:681:LYS:HD3	1:C:848:GLU:O	2.20	0.42
1:C:882:LEU:CB	1:C:892:PRO:HB3	2.50	0.42
1:B:666:PRO:O	1:B:668:LEU:HG	2.19	0.42
1:B:715:THR:HG23	1:B:806:PRO:HD3	2.00	0.42
1:B:757:MET:HB3	1:B:762:PHE:HD2	1.83	0.42
1:B:954:ILE:HG23	1:B:1024:GLU:HB3	2.01	0.42
1:C:82:THR:OG1	1:C:810:LYS:NZ	2.53	0.42
1:C:968:PRO:O	1:C:972:THR:HG22	2.19	0.42
1:B:733:ASN:HB2	1:B:787:SER:HB3	2.01	0.42
1:B:897:THR:O	1:B:900:PRO:HD2	2.20	0.42
1:A:165:GLU:HG3	1:A:314:LEU:HD21	2.02	0.42
1:C:769:LEU:HB3	1:C:772:PHE:HD2	1.84	0.42
1:B:545:MET:O	1:B:549:ILE:HG13	2.19	0.42
1:B:779:LEU:HD22	1:B:800:LEU:HG	2.01	0.42
1:B:882:LEU:HD13	1:B:895:VAL:HG11	2.01	0.42
1:C:925:LEU:HD23	1:C:925:LEU:HA	1.86	0.42
1:A:449:LEU:HB3	1:A:881:ILE:HG21	2.01	0.42
1:C:524:PHE:CZ	1:C:962:ALA:HB1	2.55	0.42
1:C:907:ILE:HA	1:C:907:ILE:HD12	1.95	0.42
1:A:524:PHE:CE2	1:A:962:ALA:HB1	2.55	0.42
1:A:742:THR:O	1:A:746:THR:OG1	2.29	0.42
1:C:46:VAL:HB	1:C:90:LEU:HB3	2.02	0.42
1:C:365:SER:HB3	1:C:499:LEU:HD13	2.01	0.42
1:C:450:VAL:HG13	1:C:878:VAL:HG22	2.02	0.42
1:B:596:THR:OG1	1:B:597:GLN:NE2	2.52	0.41
1:A:883:ALA:HB2	1:A:892:PRO:HG3	2.01	0.41
1:C:677:TYR:HE2	1:C:810:LYS:HD3	1.86	0.41
1:B:399:LEU:O	1:B:403:ILE:HG13	2.20	0.41
1:A:344:THR:HG23	1:A:982:PRO:HB2	2.02	0.41
1:A:489:THR:OG1	1:A:490:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:O	1:A:702:THR:OG1	2.31	0.41
1:C:125:LEU:HD23	1:C:125:LEU:HA	1.89	0.41
1:C:162:ILE:HD11	1:C:318:PHE:HE1	1.85	0.41
1:A:357:TYR:CE2	1:A:510:ILE:HD11	2.55	0.41
1:A:620:ASN:H	1:A:620:ASN:ND2	2.19	0.41
1:C:353:LEU:HD22	1:C:366:THR:HB	2.02	0.41
1:B:125:LEU:HD13	1:B:125:LEU:HA	1.88	0.41
1:B:468:ILE:H	1:B:468:ILE:HG13	1.52	0.41
1:B:684:LYS:HE2	1:B:688:ALA:HB1	2.03	0.41
1:B:780:LYS:HB3	1:B:780:LYS:HE2	1.79	0.41
1:A:934:LYS:NZ	1:A:935:ASN:OD1	2.54	0.41
1:A:70:ILE:HD11	1:A:111:ILE:HD11	2.02	0.41
1:A:212:ASN:O	1:A:212:ASN:ND2	2.54	0.41
1:A:188:TRP:HB3	1:A:769:LEU:HB2	2.02	0.41
1:A:897:THR:O	1:A:900:PRO:HD2	2.21	0.41
1:C:104:ALA:HB2	1:C:131:LYS:HG2	2.02	0.41
1:C:240:ARG:HD3	1:C:240:ARG:HA	1.87	0.41
1:B:460:PHE:HB3	1:B:470:ARG:CZ	2.51	0.41
1:A:345:PHE:CE2	1:A:403:ILE:HD11	2.56	0.41
1:A:552:LEU:HA	1:A:555:ILE:HG12	2.03	0.41
1:A:571:SER:HB3	1:A:624:VAL:HB	2.03	0.41
1:A:634:ARG:H	1:A:634:ARG:HG3	1.61	0.41
1:A:969:ILE:HG21	1:A:1013:ILE:HG21	2.02	0.41
1:C:81:SER:HB2	1:C:90:LEU:HG	2.03	0.41
1:C:283:ASN:O	1:C:284:THR:OG1	2.31	0.41
1:C:785:ARG:NH1	1:C:789:ASN:OD1	2.54	0.41
1:B:700:ALA:HB2	1:B:840:VAL:HG11	2.03	0.41
1:A:559:SER:O	1:A:918:ASP:HA	2.20	0.41
1:A:882:LEU:HD23	1:A:882:LEU:HA	1.89	0.41
1:A:913:ARG:HH11	1:A:915:PHE:HE2	1.69	0.41
1:C:373:VAL:HB	1:C:374:PRO:HD3	2.02	0.41
1:B:105:ILE:HG21	1:A:105:ILE:CD1	2.52	0.40
1:B:368:ILE:HB	1:B:369:PRO:HD3	2.03	0.40
1:B:405:ILE:HD11	1:B:927:LEU:HD12	2.03	0.40
1:A:455:PHE:HB3	1:A:473:ALA:HB1	2.01	0.40
1:C:137:LEU:HB2	1:C:294:LEU:HB2	2.03	0.40
1:C:188:TRP:HA	1:C:767:ARG:O	2.22	0.40
1:C:735:ASN:O	1:C:739:VAL:HG13	2.20	0.40
1:A:724:ILE:H	1:A:724:ILE:HG12	1.55	0.40
1:A:940:ILE:CD1	1:A:1020:PHE:HB2	2.52	0.40
1:B:459:SER:HB2	1:B:470:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:GLN:O	1:B:648:GLN:HG2	2.20	0.40
1:B:665:ILE:HB	1:B:666:PRO:HD3	2.03	0.40
1:B:697:LEU:HD21	1:B:710:ARG:HA	2.04	0.40
1:B:699:LEU:HD13	1:B:844:SER:HB3	2.02	0.40
1:A:80:ASP:HB3	1:A:812:PHE:CD1	2.57	0.40
1:C:63:ALA:O	1:C:67:GLU:HB2	2.21	0.40
1:C:349:LEU:O	1:C:353:LEU:HG	2.21	0.40
1:C:749:THR:HG22	1:C:767:ARG:HD2	2.03	0.40
1:B:244:PRO:HG3	1:B:271:ILE:HG13	2.02	0.40
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.92	0.40
1:B:842:LYS:HE2	1:B:842:LYS:HB3	1.92	0.40
1:B:997:LEU:O	1:B:1001:LEU:HG	2.21	0.40
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.87	0.40
1:A:715:THR:HG22	1:A:806:PRO:HG3	2.04	0.40
1:A:891:MET:HE3	1:A:891:MET:HB2	1.89	0.40
1:A:896:ILE:HD13	1:A:896:ILE:HA	1.95	0.40
1:C:408:ASP:OD2	1:C:934:LYS:HD3	2.21	0.40
1:C:686:TYR:CZ	1:C:809:VAL:HG13	2.56	0.40
1:C:891:MET:N	1:C:892:PRO:HD2	2.37	0.40
1:B:640:GLN:HE21	1:B:640:GLN:HB2	1.66	0.40
1:A:73:VAL:HG22	1:A:110:ARG:HD3	2.03	0.40
1:C:224:PRO:O	1:C:227:ASN:ND2	2.54	0.40
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1030/1039 (99%)	1007 (98%)	23 (2%)	0	100	100
1	B	1030/1039 (99%)	1005 (98%)	25 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1030/1039 (99%)	1011 (98%)	19 (2%)	0	100	100
All	All	3090/3117 (99%)	3023 (98%)	67 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	877/883 (99%)	858 (98%)	19 (2%)	52	76
1	B	876/883 (99%)	847 (97%)	29 (3%)	38	68
1	C	874/883 (99%)	859 (98%)	15 (2%)	60	82
All	All	2627/2649 (99%)	2564 (98%)	63 (2%)	51	74

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	50	TYR
1	B	54	ASP
1	B	111	ILE
1	B	178	ILE
1	B	257	ASP
1	B	311	MET
1	B	345	PHE
1	B	409	ASP
1	B	468	ILE
1	B	471	GLN
1	B	548	PHE
1	B	561	VAL
1	B	653	ARG
1	B	658	TYR
1	B	668	LEU
1	B	701	ARG
1	B	705	GLU

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Mol	Chain	Res	Type
1	B	709	VAL
1	B	715	THR
1	B	733	ASN
1	B	860	GLU
1	B	864	LYS
1	B	895	VAL
1	B	909	LEU
1	B	913	ARG
1	B	949	LYS
1	B	955	PHE
1	B	965	ARG
1	B	1005	MET
1	A	43	THR
1	A	50	TYR
1	A	81	SER
1	A	91	THR
1	A	210	ASP
1	A	279	THR
1	A	284	THR
1	A	512	LYS
1	A	537	ARG
1	A	605	VAL
1	A	612	LEU
1	A	699	LEU
1	A	724	ILE
1	A	752	VAL
1	A	772	PHE
1	A	775	THR
1	A	906	SER
1	A	916	ASP
1	A	917	ASN
1	C	40	THR
1	C	50	TYR
1	C	54	ASP
1	C	91	THR
1	C	150	ASN
1	C	151	ASP
1	C	318	PHE
1	C	451	LEU
1	C	581	ILE
1	C	660	LEU
1	C	662	LEU

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Mol	Chain	Res	Type
1	C	739	VAL
1	C	752	VAL
1	C	771	ASP
1	C	916	ASP

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

Mol	Chain	Res	Type
1	B	511	GLN
1	B	597	GLN
1	B	640	GLN
1	B	648	GLN
1	B	680	ASN
1	B	885	GLN
1	B	960	ASN
1	A	87	GLN
1	A	202	ASN
1	A	255	ASN
1	A	325	GLN
1	A	582	HIS
1	A	620	ASN
1	A	737	GLN
1	A	741	ASN
1	A	765	ASN
1	A	776	GLN
1	A	795	ASN
1	A	917	ASN
1	C	45	GLN
1	C	238	GLN
1	C	245	GLN
1	C	277	ASN
1	C	312	GLN
1	C	325	GLN
1	C	511	GLN
1	C	679	GLN
1	C	691	GLN
1	C	917	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-40091. 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 ⓘ
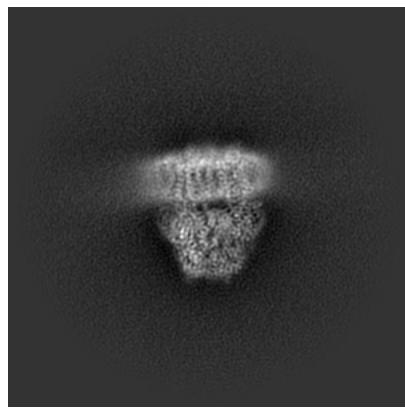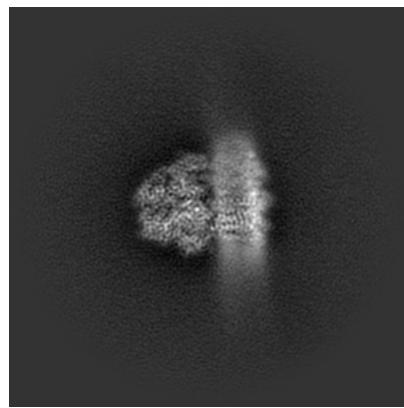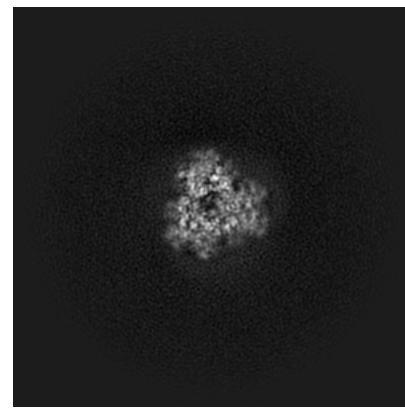
6.1.1 Primary map

X Y Z

6.1.2 Raw map

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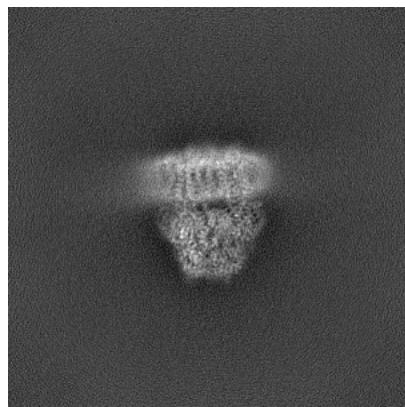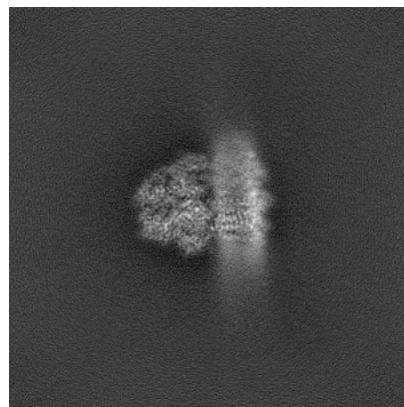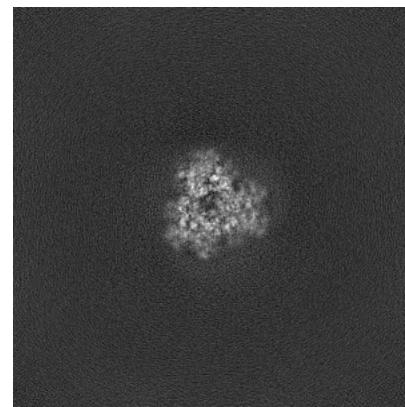
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
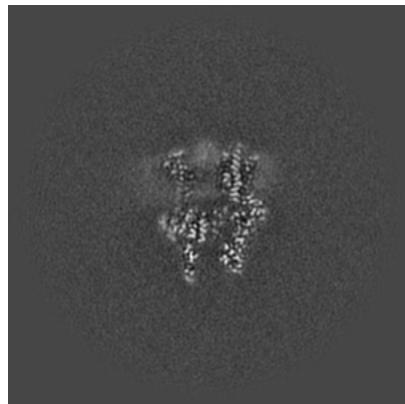
6.2.1 Primary map
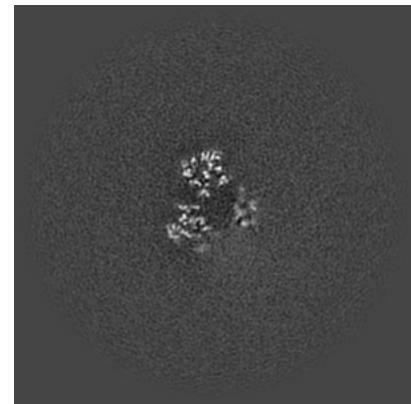
X Index: 175   Y Index: 175   Z Index: 175

6.2.2 Raw map
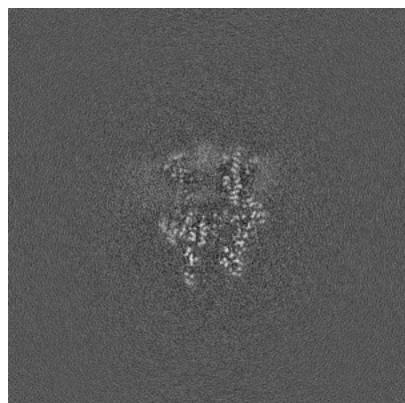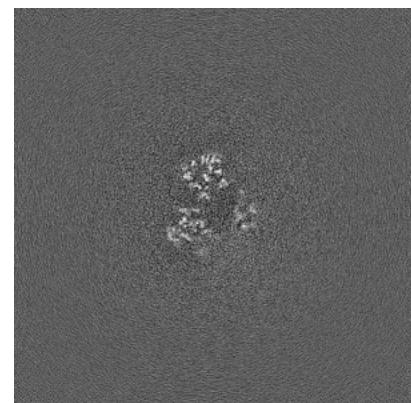
X Index: 175   Y Index: 175   Z Index: 175

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
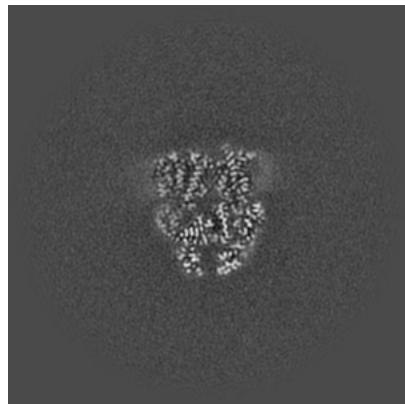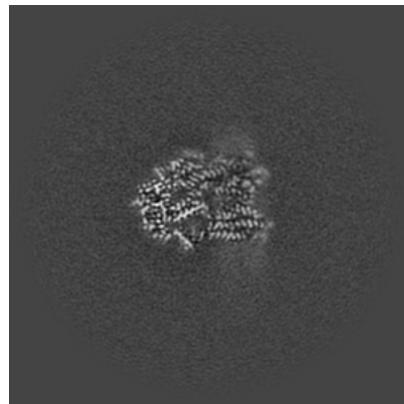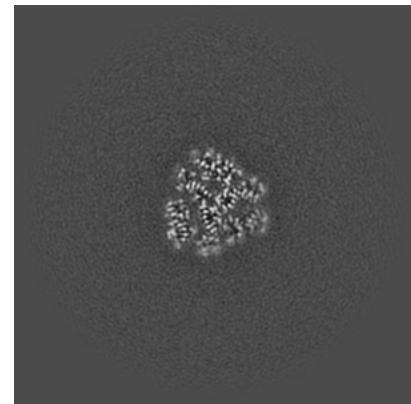
X Index: 165   Y Index: 160   Z Index: 157

6.3.2 Raw map
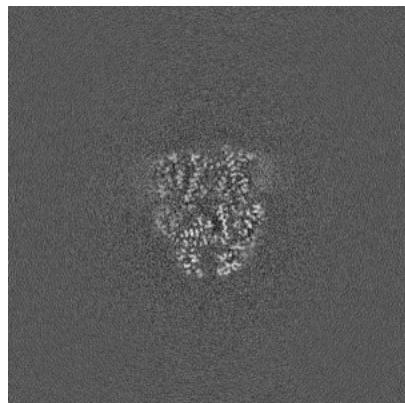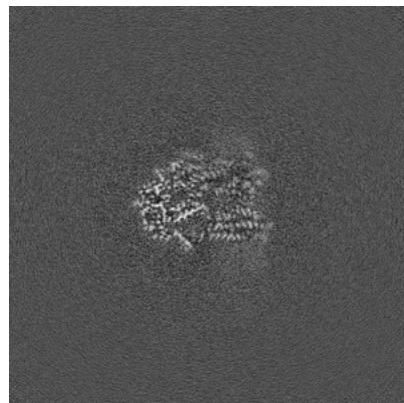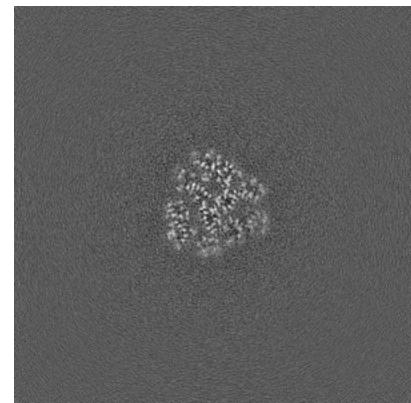
X Index: 165   Y Index: 160   Z Index: 157

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

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

6.4.1 Primary map
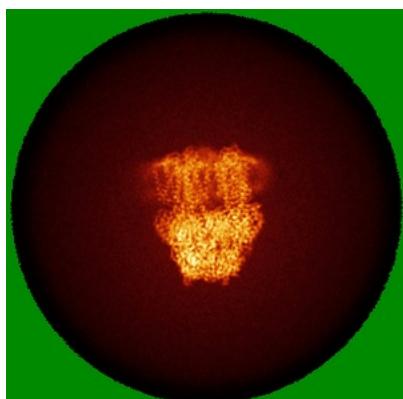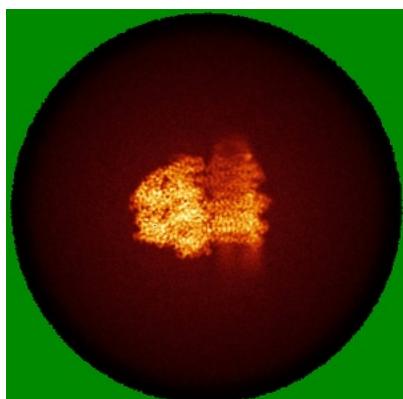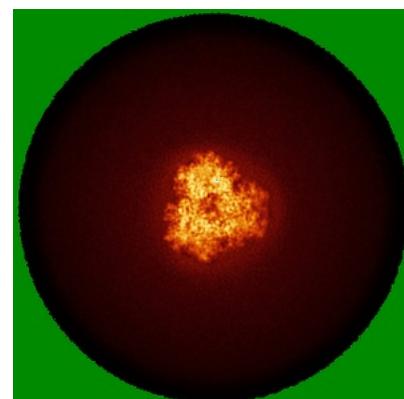
| X | Y | Z |

6.4.2 Raw map

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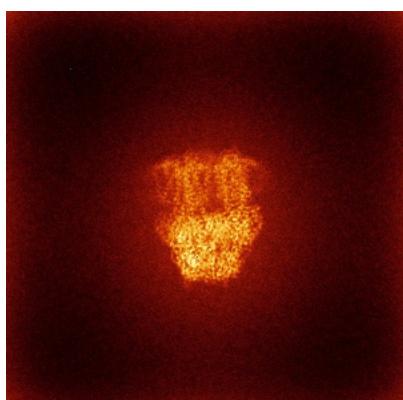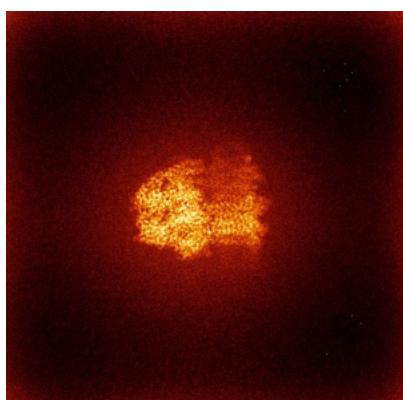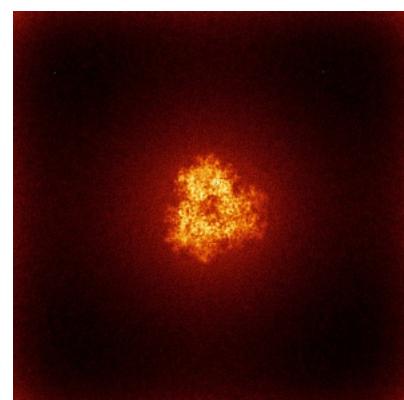
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
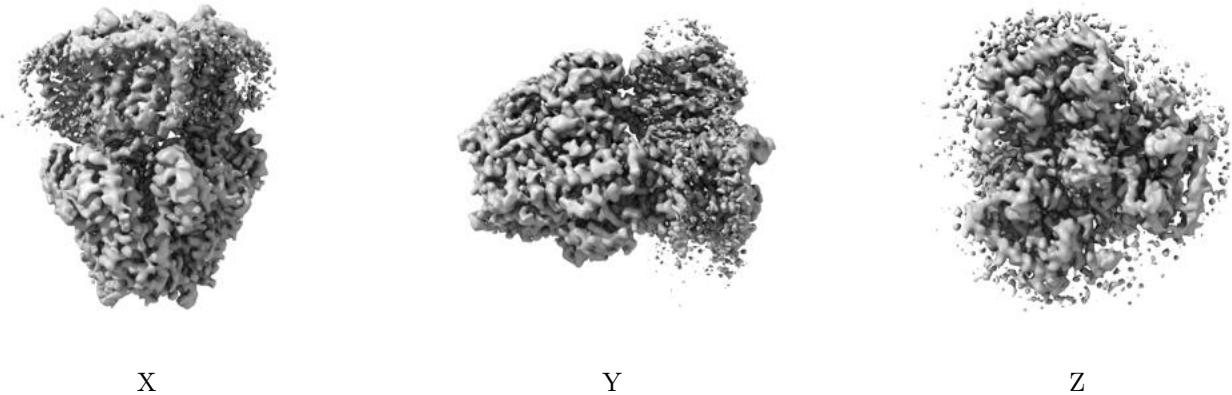
The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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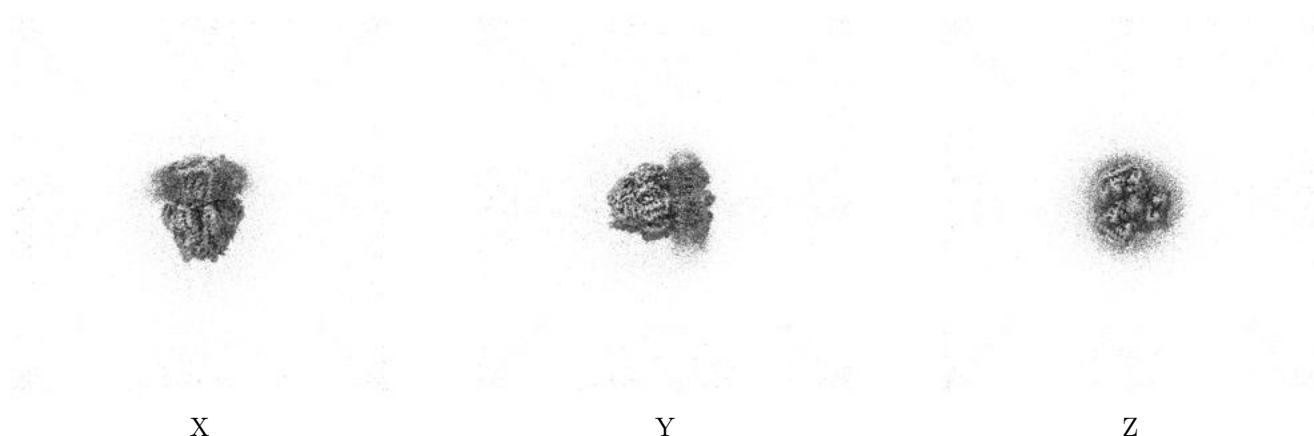
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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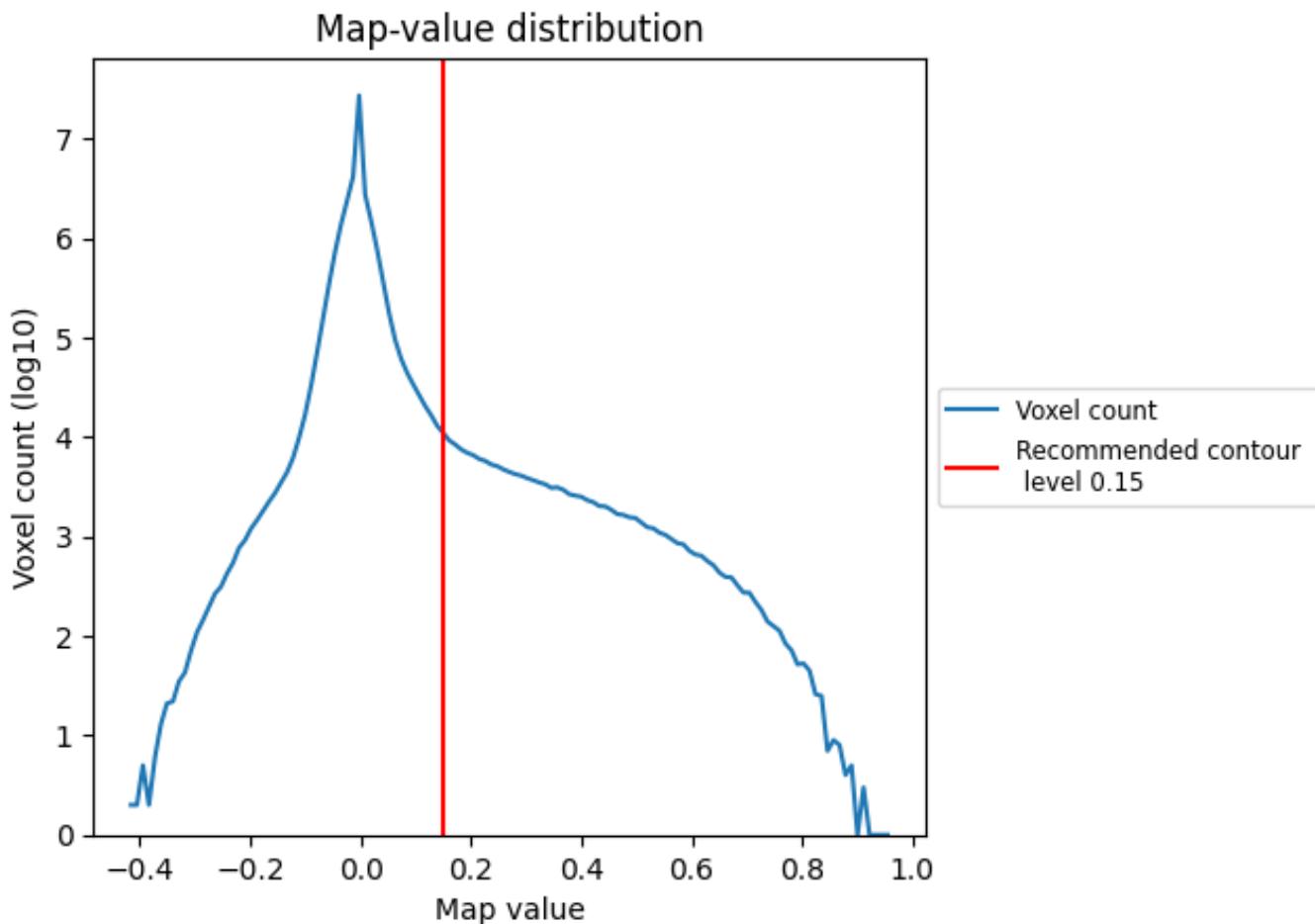
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
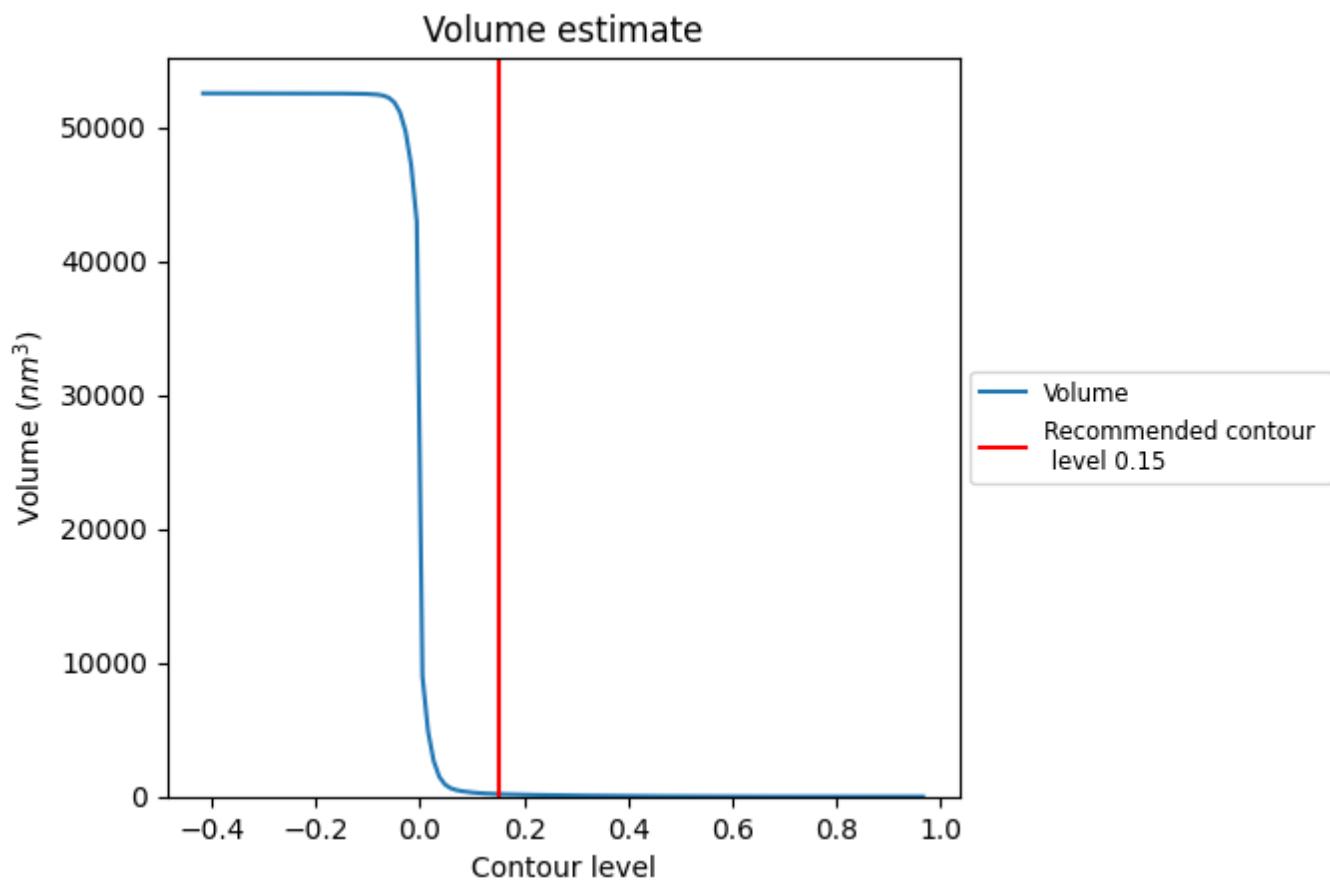
The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
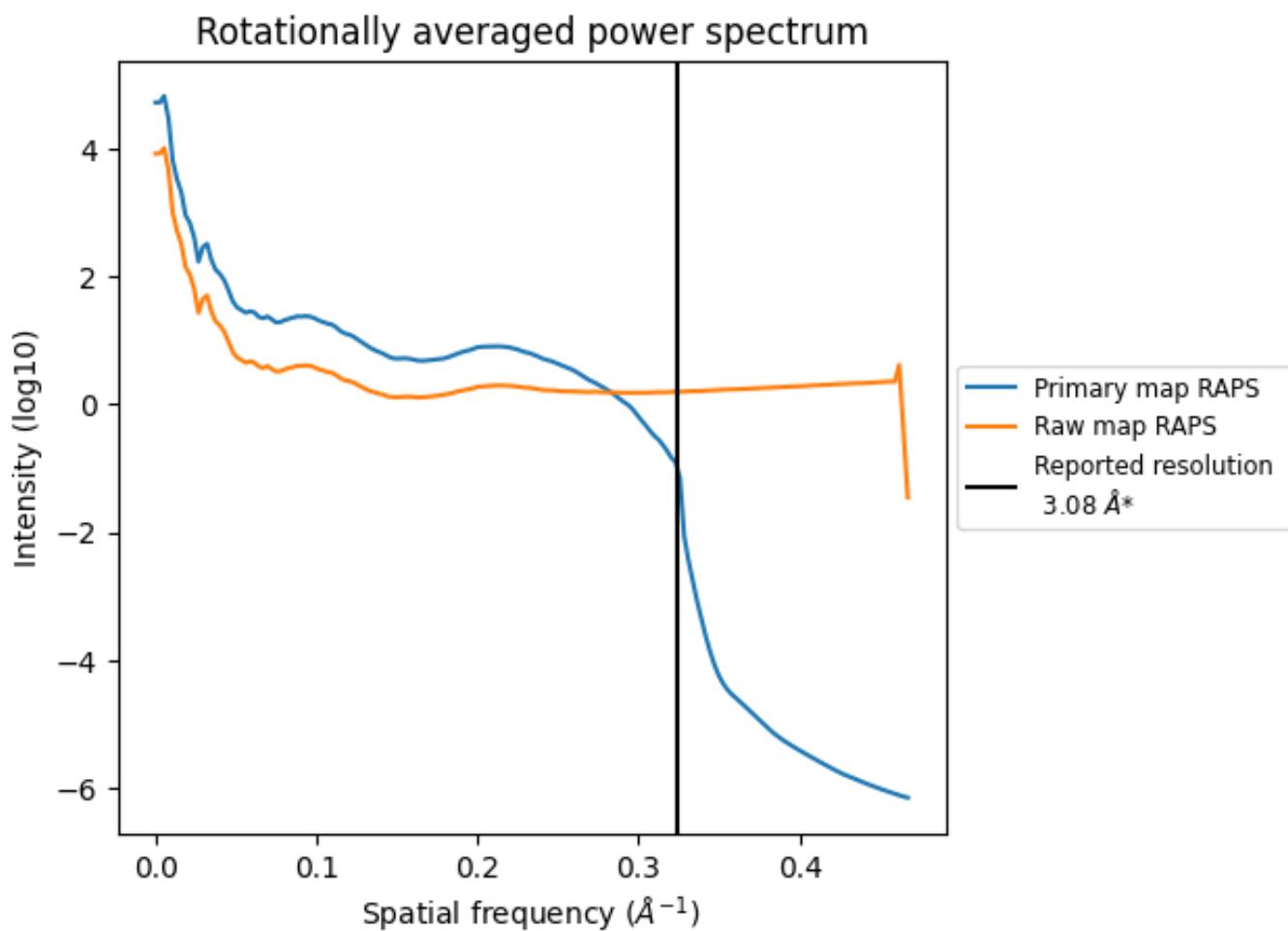
*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

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)
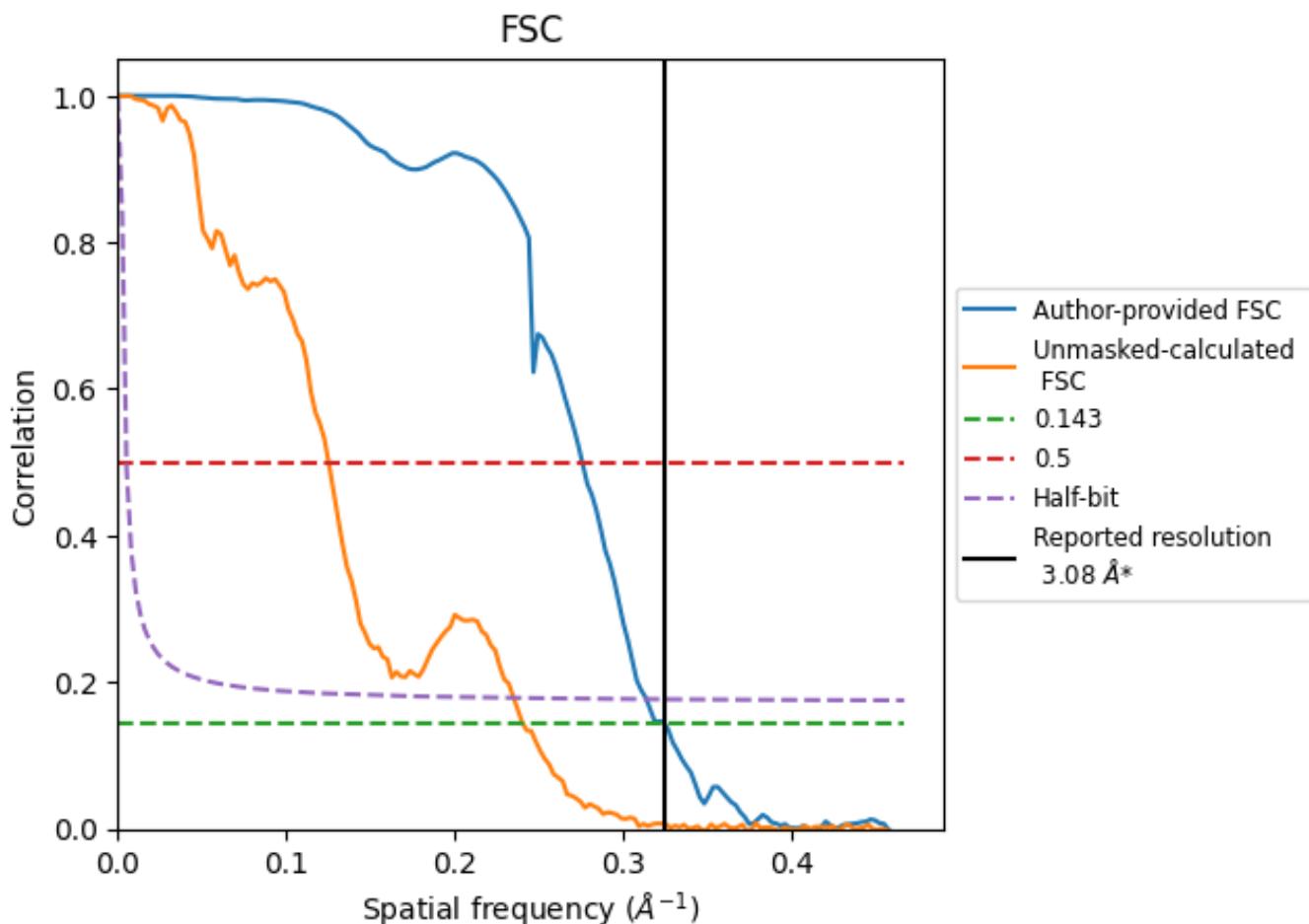
*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.62	3.18
Unmasked-calculated*	4.15	7.98	4.25

*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 4.15 differs from the reported value 3.08 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-40091 and PDB model 8GJJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1　Map-model overlay ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
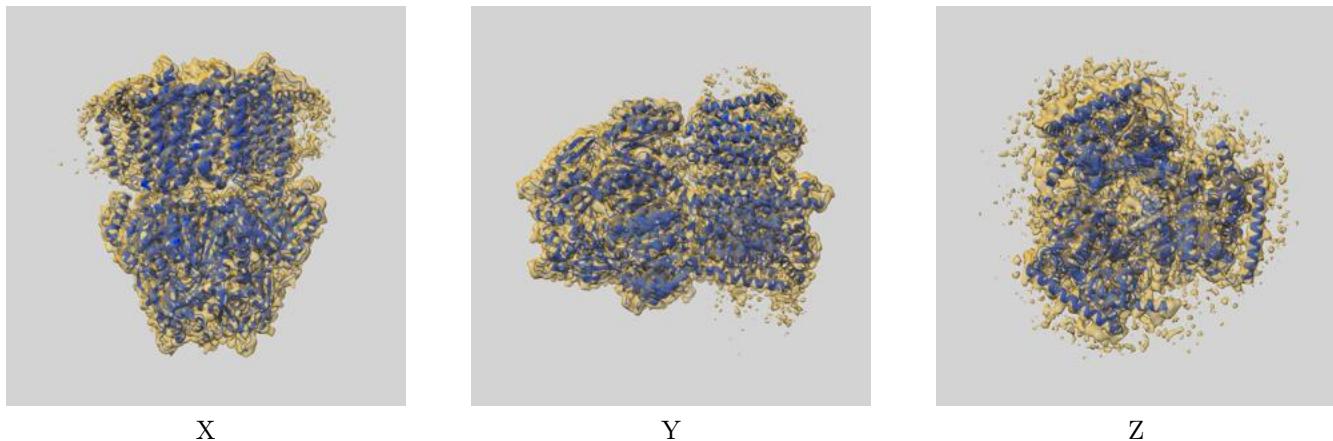
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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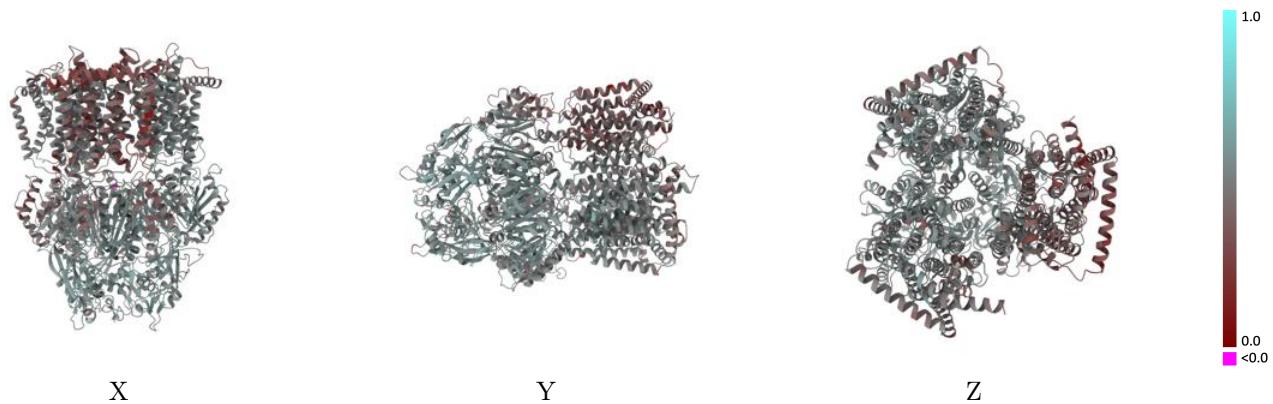
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
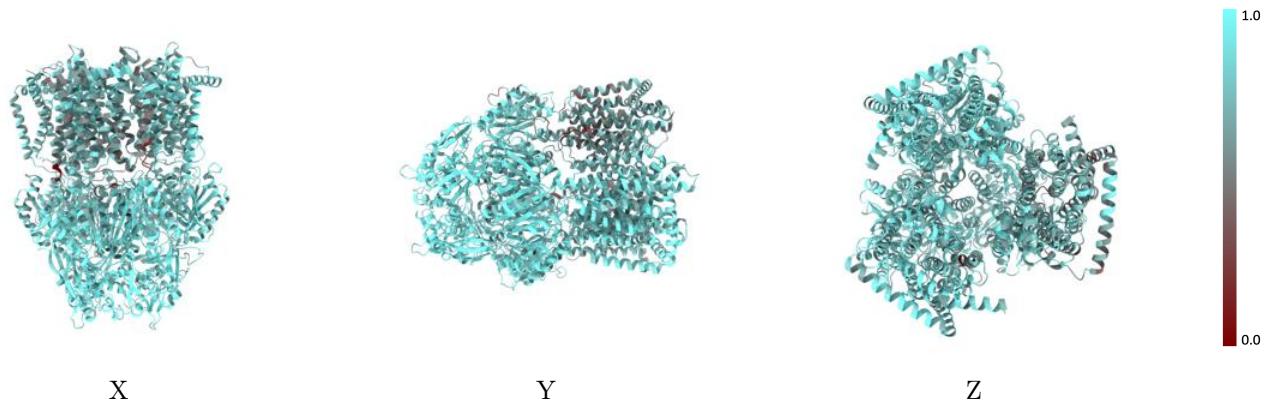
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ
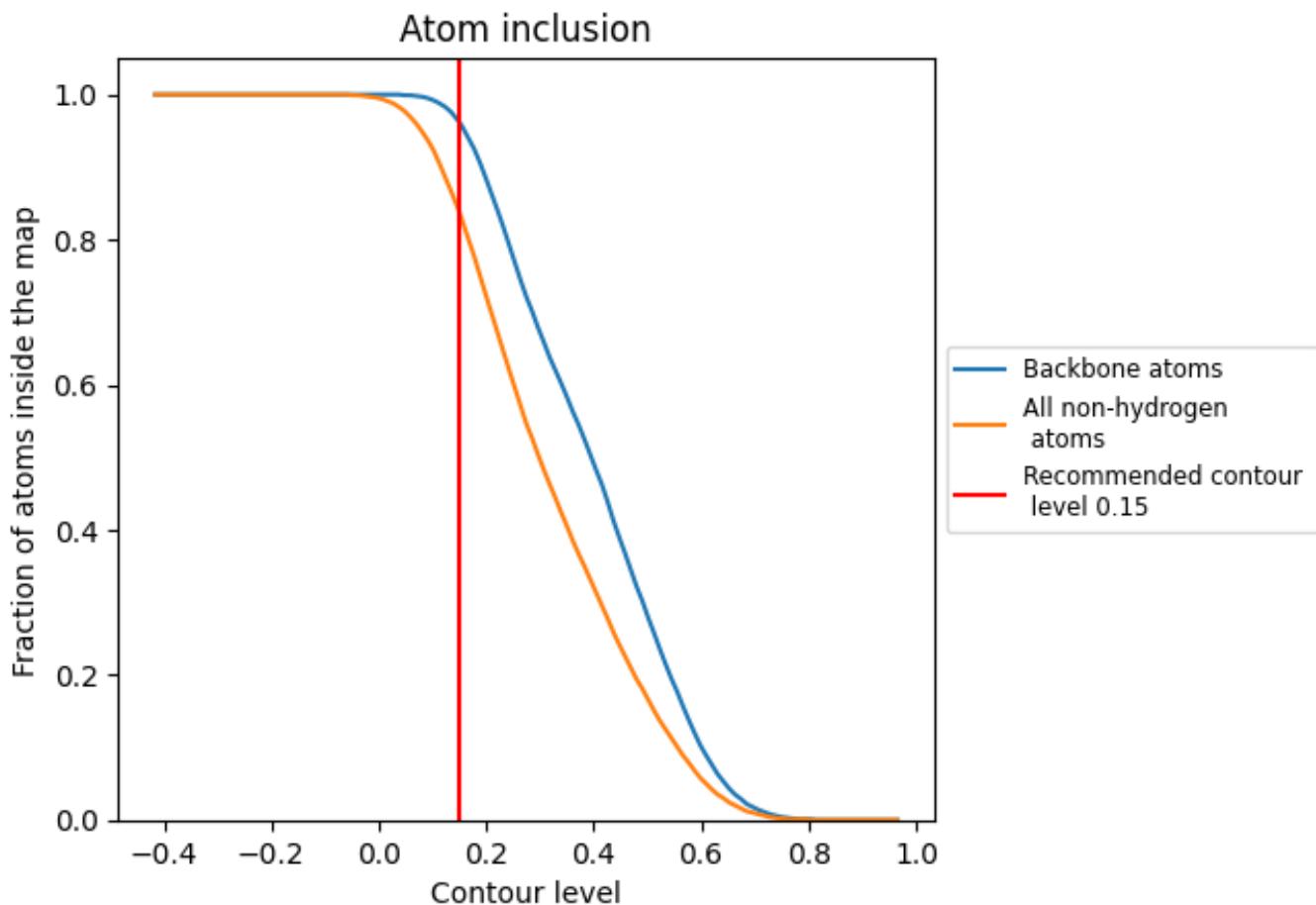
At the recommended contour level, 96% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.4870
A	0.8750	0.5130
B	0.7860	0.4500
C	0.8510	0.4980

1.0

0.0
<0.0