



Full wwPDB EM Validation Report ⓘ

Sep 19, 2026 – 01:40 PM EDT

PDB ID : 9PLR / pdb_00009plr
EMDB ID : EMD-71721
Title : CryoEM reconstruction of HUWE1-USP7 complex in the closed state
Authors : Yatskevich, S.; Juskiewicz, S.
Deposited on : 2025-07-16
Resolution : 2.88 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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

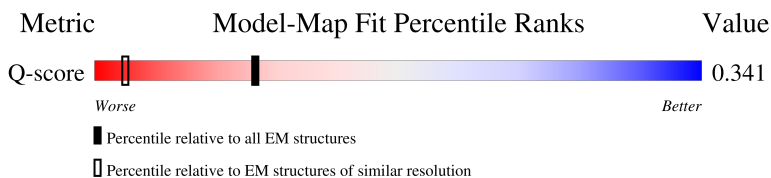
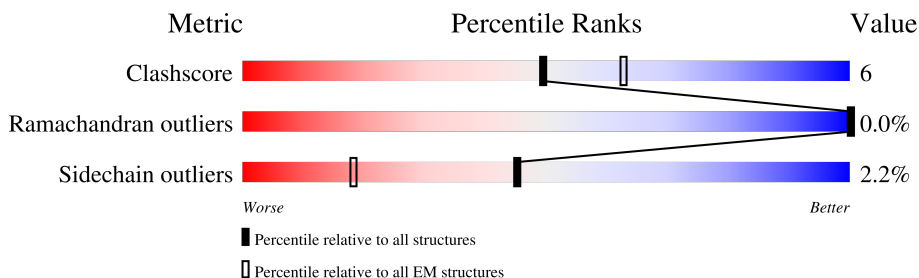
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4374	 47% 9% 44%
2	C	1102	 74% 14% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27348 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2445	Total	C	N	O	S	0	0
			19304	12313	3314	3555	122		

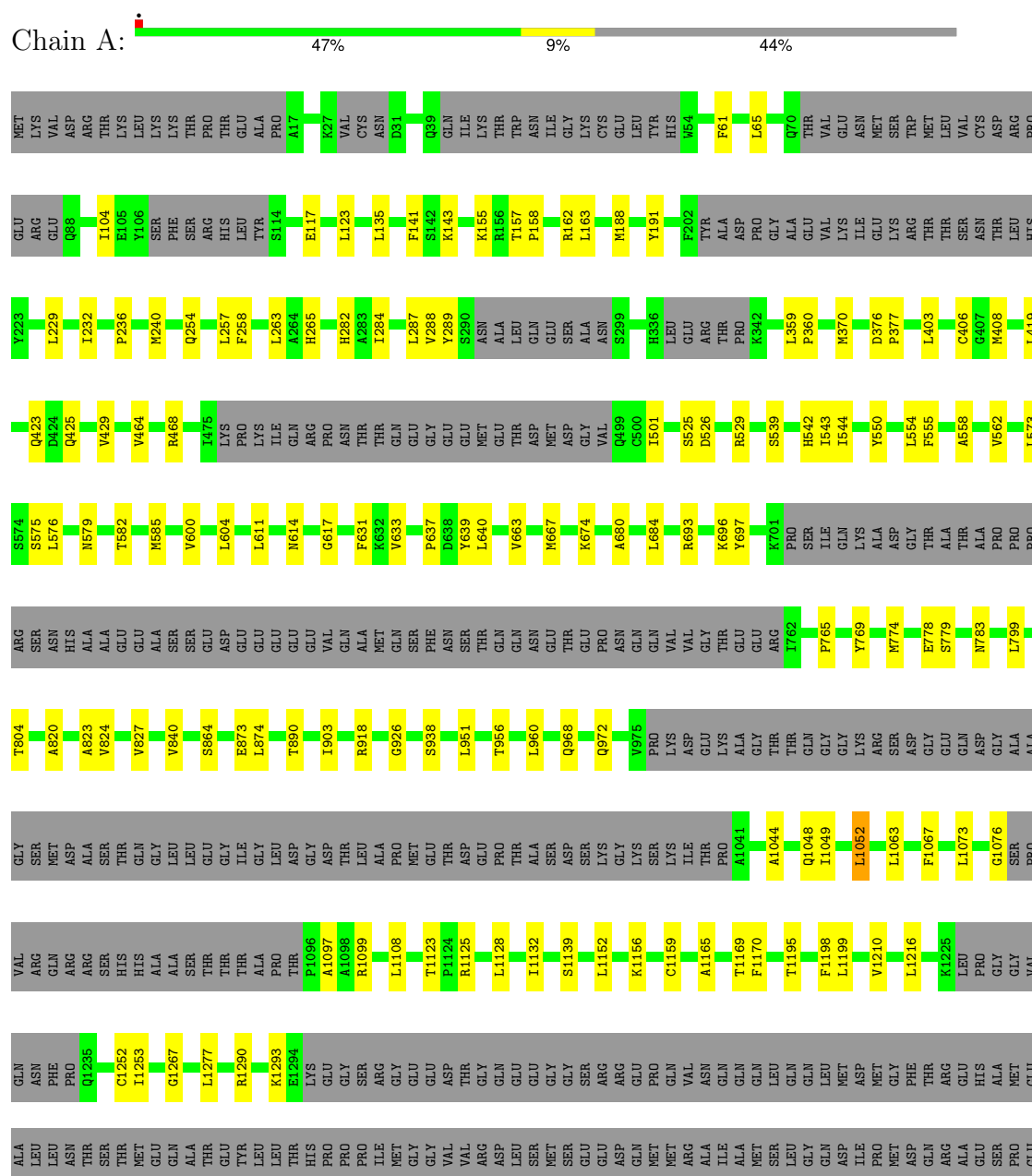
- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	977	Total	C	N	O	S	0	0
			8044	5123	1367	1505	49		

3 Residue-property plots

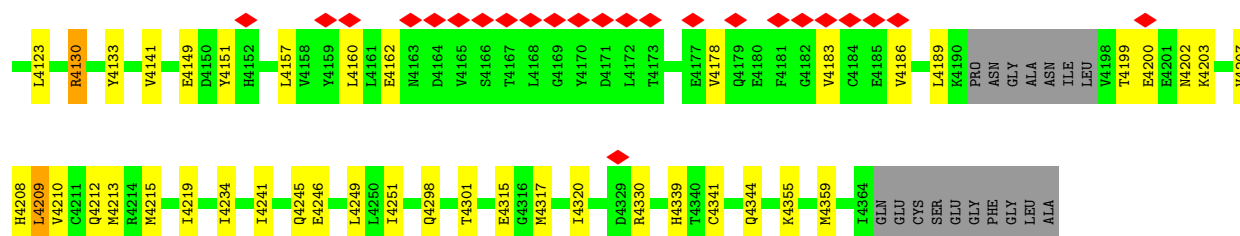
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase HUWE1



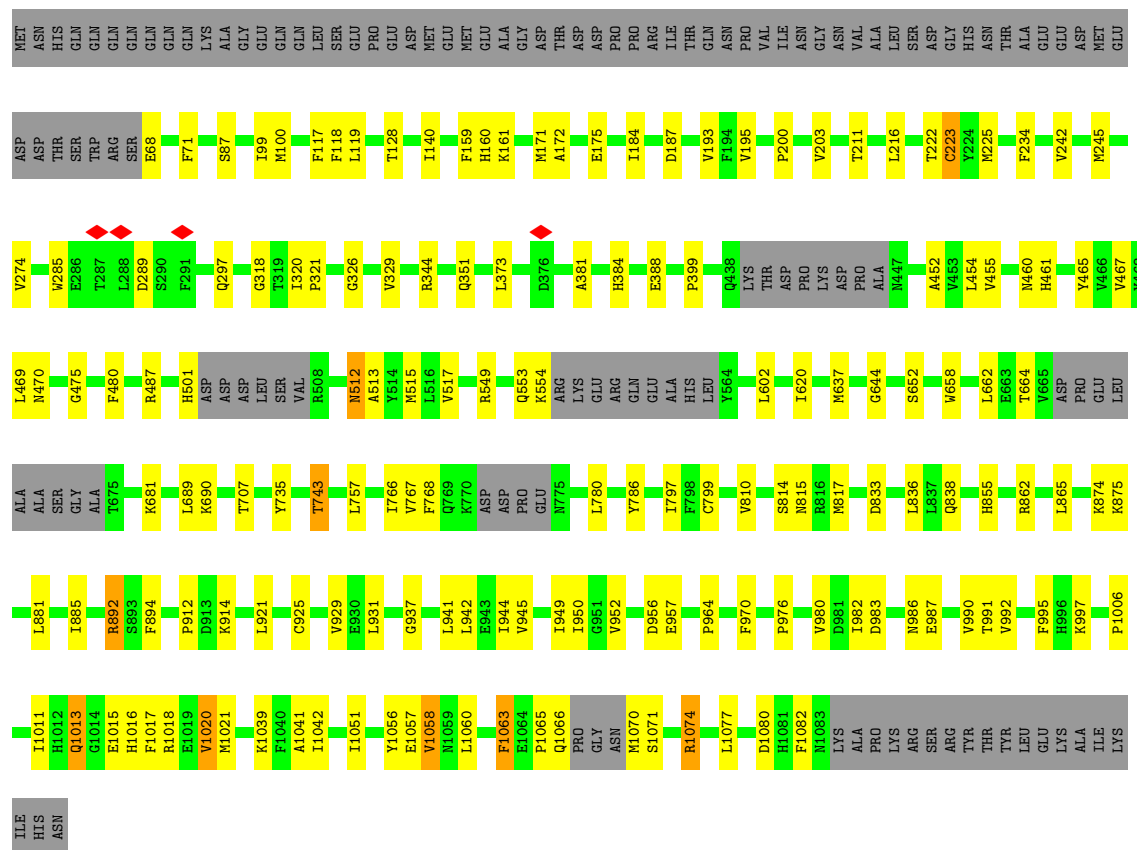






• Molecule 2: Ubiquitin carboxyl-terminal hydrolase 7

Chain C: 74% 14% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118192	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.516	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	277.78, 277.78, 277.78	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	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	0.19	0/19649	0.51	3/26599 (0.0%)
2	C	0.09	0/8232	0.25	0/11104
All	All	0.17	0/27881	0.45	3/37703 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2182	ILE	CG1-CB-CG2	-5.73	93.52	110.70
1	A	3992	LEU	CA-C-N	5.49	129.55	120.94
1	A	3992	LEU	C-N-CA	5.49	129.55	120.94

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	19304	0	19682	223	0
2	C	8044	0	7839	89	0
All	All	27348	0	27521	310	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 (310) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:987:GLU:HA	2:C:1011:ILE:O	1.68	0.94
2:C:1039:LYS:HB2	2:C:1080:ASP:HB3	1.65	0.77
1:A:956:THR:HG21	1:A:960:LEU:HG	1.67	0.76
1:A:1913:ASN:HB2	1:A:2690:ARG:HH22	1.49	0.76
1:A:3598:LEU:HD22	1:A:3741:ARG:HD3	1.71	0.73
1:A:631:PHE:HB3	1:A:684:LEU:HD11	1.71	0.72
2:C:815:ASN:HB3	2:C:862:ARG:HB2	1.72	0.72
1:A:1495:LEU:HD12	1:A:1526:LEU:HD12	1.75	0.69
1:A:3994:PHE:HB2	1:A:4246:GLU:HG2	1.75	0.69
1:A:3293:ALA:HB3	1:A:3296:CYS:HB3	1.74	0.69
2:C:797:ILE:HG12	2:C:810:VAL:HG22	1.75	0.68
1:A:1503:THR:HA	2:C:957:GLU:HA	1.75	0.68
1:A:263:LEU:HD21	1:A:3294:LEU:HD21	1.76	0.68
1:A:3867:LEU:HD13	1:A:3876:VAL:HA	1.74	0.67
1:A:3880:GLN:HG3	1:A:3969:ILE:HD12	1.77	0.67
1:A:3434:LEU:HA	1:A:3437:MET:HG3	1.80	0.64
2:C:1013:GLN:HG3	2:C:1060:LEU:HD21	1.79	0.64
2:C:452:ALA:HB3	2:C:517:VAL:HB	1.80	0.63
2:C:992:VAL:HG22	2:C:1077:LEU:HB3	1.79	0.63
1:A:3302:GLN:HE21	1:A:3325:HIS:HB2	1.63	0.62
2:C:1018:ARG:HA	2:C:1021:MET:HE3	1.81	0.62
1:A:464:VAL:HG21	1:A:539:SER:HB2	1.81	0.62
2:C:620:ILE:HG22	2:C:664:THR:HG22	1.81	0.62
1:A:1508:LYS:HG3	1:A:1512:GLU:HB2	1.81	0.61
1:A:2229:PRO:HB3	1:A:3192:LEU:HD21	1.83	0.60
1:A:550:TYR:HB3	1:A:554:LEU:HD23	1.83	0.60
1:A:1854:THR:HG21	1:A:1872:ARG:HH12	1.66	0.60
2:C:467:VAL:HG13	2:C:480:PHE:HB2	1.83	0.60
1:A:1809:GLN:HA	1:A:2065:LEU:HD13	1.83	0.60
1:A:3989:ILE:HD13	1:A:4241:ILE:HA	1.83	0.60
2:C:865:LEU:HB3	2:C:874:LYS:HD3	1.84	0.59
2:C:865:LEU:HD22	2:C:874:LYS:HB3	1.83	0.59
1:A:3581:LEU:O	1:A:3585:VAL:HG23	2.02	0.59
1:A:1897:LEU:HD11	1:A:2685:GLU:HG3	1.83	0.59
1:A:1805:LEU:HD13	1:A:1952:ALA:HB2	1.84	0.59
1:A:3438:LEU:HD22	1:A:3585:VAL:HG21	1.85	0.59
1:A:3976:HIS:HB3	1:A:3979:ASP:OD2	2.03	0.59
1:A:573:LEU:HD23	1:A:614:ASN:HB2	1.85	0.58
1:A:123:LEU:HD23	1:A:162:ARG:HB3	1.86	0.58
2:C:838:GLN:HB2	2:C:881:LEU:HD11	1.86	0.58
1:A:526:ASP:HB3	1:A:4123:LEU:HD12	1.85	0.57
1:A:918:ARG:HH22	1:A:1076:GLY:HA2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:892:ARG:HH12	2:C:894:PHE:HB2	1.69	0.57
1:A:425:GLN:O	1:A:429:VAL:HG23	2.04	0.57
1:A:4115:ALA:HB1	1:A:4234:ILE:HG12	1.85	0.57
1:A:1756:THR:HG22	1:A:1794:MET:HE1	1.87	0.56
1:A:1682:LEU:HD11	1:A:2668:SER:HB3	1.87	0.56
1:A:236:PRO:HG3	1:A:265:HIS:CG	2.40	0.56
2:C:620:ILE:HB	2:C:662:LEU:HD11	1.86	0.56
1:A:3876:VAL:HG11	1:A:3965:VAL:HG13	1.88	0.56
2:C:119:LEU:HD13	2:C:193:VAL:HG11	1.88	0.56
2:C:637:MET:HE3	2:C:681:LYS:HB3	1.88	0.56
1:A:873:GLU:OE2	1:A:890:THR:HA	2.06	0.56
2:C:470:ASN:HD21	2:C:475:GLY:H	1.54	0.56
1:A:1770:VAL:HG23	1:A:1771:ASP:H	1.72	0.56
2:C:690:LYS:HB2	2:C:767:VAL:HG22	1.88	0.56
1:A:2663:MET:O	1:A:2667:VAL:HG23	2.06	0.55
1:A:236:PRO:HG3	1:A:265:HIS:CD2	2.42	0.55
1:A:4093:ILE:HD12	1:A:4219:ILE:HD12	1.87	0.55
2:C:780:LEU:HD13	2:C:786:TYR:HA	1.89	0.55
2:C:855:HIS:HB3	2:C:885:ILE:HD13	1.89	0.55
1:A:3867:LEU:HB3	1:A:3876:VAL:HG22	1.88	0.54
1:A:926:GLY:HA3	1:A:1097:ALA:HB1	1.89	0.54
1:A:1545:ALA:HB2	1:A:1596:THR:HG21	1.89	0.54
1:A:4157:LEU:HD22	1:A:4207:VAL:HG13	1.89	0.54
2:C:140:ILE:HD12	2:C:171:MET:HE3	1.89	0.54
1:A:157:THR:OG1	1:A:158:PRO:HD3	2.08	0.54
2:C:184:ILE:HD11	2:C:187:ASP:HA	1.88	0.54
1:A:1939:PRO:HD2	1:A:1942:ILE:HD12	1.90	0.54
2:C:99:ILE:HG23	2:C:117:PHE:HE1	1.73	0.54
2:C:454:LEU:HB2	2:C:515:MET:HB3	1.90	0.54
1:A:3965:VAL:O	1:A:3969:ILE:HG12	2.08	0.54
2:C:602:LEU:HB3	2:C:644:GLY:HA2	1.90	0.54
1:A:1882:PRO:O	1:A:1886:THR:HG23	2.08	0.53
1:A:4087:ASP:HB2	1:A:4090:THR:HG22	1.88	0.53
1:A:4160:LEU:HD21	1:A:4203:LYS:HD2	1.91	0.53
1:A:544:ILE:HG23	1:A:555:PHE:HE1	1.74	0.53
1:A:1679:MET:HE1	1:A:1868:ASN:ND2	2.24	0.53
1:A:1775:LEU:HA	1:A:1778:THR:HG22	1.90	0.53
2:C:833:ASP:HB3	2:C:836:LEU:HG	1.91	0.53
2:C:983:ASP:HB3	2:C:986:ASN:HB2	1.90	0.53
1:A:2117:LEU:HG	1:A:2178:ALA:HB1	1.90	0.53
1:A:3579:ASN:O	1:A:3583:LEU:HD13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MET:HE2	1:A:257:LEU:HD23	1.91	0.53
1:A:1615:ASN:HB3	1:A:1680:LEU:HD21	1.91	0.52
1:A:1469:ILE:HD13	1:A:1540:LEU:HD11	1.91	0.52
1:A:370:MET:HE3	1:A:419:LEU:HD11	1.92	0.52
1:A:874:LEU:HD22	1:A:1052:LEU:HD11	1.91	0.52
1:A:1253:ILE:HG21	1:A:1277:LEU:HD21	1.91	0.52
1:A:117:GLU:HG3	1:A:155:LYS:HD3	1.91	0.52
1:A:4339:HIS:HB2	1:A:4344:GLN:HB3	1.91	0.52
1:A:1630:TYR:HB2	1:A:1635:ASN:OD1	2.10	0.52
1:A:637:PRO:HA	1:A:640:LEU:HG	1.92	0.51
2:C:381:ALA:HB3	2:C:384:HIS:HB2	1.92	0.51
2:C:222:THR:HB	2:C:225:MET:HE2	1.93	0.51
1:A:1063:LEU:HG	1:A:1067:PHE:CE2	2.45	0.51
1:A:4133:TYR:HE1	1:A:4251:ILE:HD12	1.76	0.51
2:C:964:PRO:HA	2:C:970:PHE:HE2	1.75	0.51
1:A:3606:LEU:O	1:A:3610:ARG:HG3	2.11	0.51
1:A:4199:THR:HG23	1:A:4202:ASN:HD22	1.76	0.51
2:C:1017:PHE:O	2:C:1020:VAL:HG12	2.11	0.51
1:A:1165:ALA:O	1:A:1169:THR:HG23	2.12	0.50
1:A:1499:ALA:HB2	1:A:1517:MET:SD	2.51	0.50
1:A:4317:MET:HE3	1:A:4341:CYS:HB2	1.93	0.50
1:A:3211:ASN:HA	1:A:3214:TYR:CD2	2.47	0.50
1:A:240:MET:HG3	1:A:258:PHE:HD1	1.77	0.50
1:A:611:LEU:O	1:A:617:GLY:HA3	2.11	0.50
1:A:696:LYS:HE2	1:A:697:TYR:CZ	2.47	0.50
1:A:693:ARG:HH21	1:A:804:THR:HG21	1.77	0.50
2:C:941:LEU:HD11	2:C:970:PHE:HB3	1.94	0.50
1:A:2176:LEU:O	1:A:2180:MET:HG2	2.12	0.50
1:A:1510:VAL:O	1:A:1514:ILE:HG23	2.12	0.49
1:A:1132:ILE:HG12	1:A:1198:PHE:HA	1.94	0.49
1:A:1779:LEU:HB3	1:A:1819:LEU:HD22	1.95	0.49
1:A:4149:GLU:HG3	1:A:4215:MET:SD	2.52	0.49
2:C:200:PRO:HG2	2:C:203:VAL:HG21	1.94	0.49
1:A:778:GLU:HB2	1:A:827:VAL:HG22	1.95	0.49
1:A:3190:LEU:O	1:A:3194:PHE:HD1	1.96	0.49
1:A:4199:THR:O	1:A:4203:LYS:HG3	2.12	0.49
1:A:582:THR:HA	1:A:585:MET:HE3	1.94	0.49
1:A:3444:ARG:HH21	1:A:3588:LEU:HD12	1.78	0.49
1:A:3863:CYS:SG	1:A:3879:LEU:HD11	2.52	0.49
1:A:1444:LEU:HD11	1:A:1480:ILE:HG12	1.95	0.48
1:A:240:MET:HE1	1:A:254:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:986:ASN:HB3	2:C:1013:GLN:OE1	2.13	0.48
2:C:1065:PRO:HD3	2:C:1074:ARG:HB3	1.95	0.48
1:A:423:GLN:NE2	1:A:501:ILE:HD11	2.29	0.48
1:A:938:SER:HB3	1:A:1108:LEU:HD13	1.96	0.48
1:A:3982:PHE:O	1:A:3985:LEU:HG	2.14	0.48
2:C:995:PHE:O	2:C:1080:ASP:HA	2.13	0.48
1:A:4130:ARG:HH21	1:A:4298:GLN:HB3	1.77	0.48
1:A:1498:ALA:O	1:A:1517:MET:HE1	2.13	0.48
1:A:4015:GLU:H	1:A:4044:ASN:ND2	2.12	0.48
1:A:529:ARG:HH12	1:A:4067:MET:HG3	1.79	0.48
1:A:600:VAL:O	1:A:604:LEU:HG	2.14	0.48
1:A:918:ARG:HH21	1:A:1073:LEU:HA	1.79	0.48
1:A:1159:CYS:HB2	1:A:1421:CYS:HB2	1.96	0.48
1:A:3875:ALA:O	1:A:3878:VAL:HG22	2.13	0.48
2:C:1063:PHE:CD1	2:C:1063:PHE:N	2.82	0.48
1:A:1817:THR:OG1	1:A:1818:PRO:HD3	2.14	0.47
1:A:4141:VAL:HG21	1:A:4215:MET:HG3	1.96	0.47
1:A:4355:LYS:HD2	1:A:4359:MET:HE2	1.95	0.47
2:C:326:GLY:HA3	2:C:399:PRO:HD3	1.95	0.47
1:A:423:GLN:HE21	1:A:501:ILE:HD11	1.78	0.47
1:A:663:VAL:O	1:A:667:MET:HG3	2.13	0.47
1:A:3189:LEU:HD23	1:A:3192:LEU:HD12	1.97	0.47
1:A:3454:LEU:HD21	1:A:3585:VAL:HG11	1.95	0.47
2:C:990:VAL:HG21	2:C:1063:PHE:CZ	2.50	0.47
1:A:558:ALA:O	1:A:562:VAL:HG23	2.15	0.47
1:A:2069:SER:HB2	1:A:2131:LEU:HD12	1.96	0.47
2:C:799:CYS:SG	2:C:875:LYS:HE3	2.54	0.47
1:A:229:LEU:HD13	1:A:232:ILE:HD12	1.95	0.47
1:A:1911:PHE:HA	1:A:1914:LEU:HB2	1.95	0.47
2:C:942:LEU:HD12	2:C:952:VAL:HG22	1.97	0.47
1:A:1591:ASP:OD1	1:A:1591:ASP:C	2.57	0.47
1:A:3437:MET:HA	1:A:3440:HIS:ND1	2.29	0.47
2:C:100:MET:HB3	2:C:118:PHE:HB2	1.97	0.47
2:C:1015:GLU:HB3	2:C:1058:VAL:HG11	1.96	0.47
2:C:1063:PHE:N	2:C:1063:PHE:HD1	2.12	0.47
1:A:951:LEU:HD22	1:A:1049:ILE:HG23	1.97	0.47
1:A:3602:ALA:O	1:A:3606:LEU:HG	2.14	0.47
1:A:820:ALA:O	1:A:824:VAL:HG23	2.15	0.46
1:A:3292:ALA:HB1	1:A:3327:GLN:HB3	1.96	0.46
1:A:1523:ALA:HB1	1:A:1582:TRP:HD1	1.80	0.46
1:A:765:PRO:HG2	1:A:769:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:CYS:HB2	2:C:465:TYR:HB2	1.97	0.46
2:C:455:VAL:HA	2:C:513:ALA:HA	1.97	0.46
1:A:667:MET:SD	1:A:674:LYS:HA	2.56	0.46
1:A:3195:VAL:HG22	1:A:3288:VAL:HG11	1.97	0.46
2:C:242:VAL:HG13	2:C:245:MET:HE2	1.97	0.46
1:A:544:ILE:HA	1:A:555:PHE:CD1	2.51	0.46
1:A:359:LEU:HB3	1:A:360:PRO:HD3	1.98	0.45
1:A:1504:THR:HG22	2:C:956:ASP:HB3	1.97	0.45
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.84	0.45
1:A:2212:ILE:HG13	1:A:2213:ILE:N	2.31	0.45
1:A:1630:TYR:HB3	1:A:1634:ASN:HB2	1.99	0.45
1:A:2126:LYS:HG3	1:A:2127:ASP:OD1	2.16	0.45
1:A:4151:TYR:HB2	1:A:4317:MET:HE1	1.98	0.45
2:C:159:PHE:CE2	2:C:161:LYS:HB2	2.52	0.45
1:A:1568:LEU:HB3	1:A:1768:VAL:HG21	1.99	0.45
1:A:2226:ALA:CB	1:A:3185:ALA:HB1	2.47	0.45
2:C:329:VAL:HG22	2:C:344:ARG:HG2	1.98	0.45
2:C:944:ILE:HG12	2:C:949:ILE:HA	1.99	0.45
1:A:1290:ARG:HA	1:A:1293:LYS:HB2	1.98	0.45
1:A:104:ILE:HG12	1:A:141:PHE:CZ	2.52	0.45
1:A:3636:LYS:O	1:A:3640:THR:HG23	2.16	0.45
1:A:4189:LEU:HD22	1:A:4209:LEU:HB3	1.99	0.45
1:A:2655:CYS:SG	1:A:2663:MET:HG3	2.57	0.45
1:A:3219:ARG:HG2	1:A:3223:ILE:HD12	1.98	0.45
1:A:774:MET:HG3	1:A:824:VAL:HG22	1.99	0.45
1:A:938:SER:CB	1:A:1108:LEU:HD13	2.47	0.45
2:C:68:GLU:HA	2:C:195:VAL:O	2.17	0.45
2:C:997:LYS:HZ2	2:C:997:LYS:HB2	1.82	0.45
1:A:188:MET:HE3	1:A:191:TYR:HD2	1.81	0.44
1:A:1679:MET:HE1	1:A:1868:ASN:HD22	1.81	0.44
2:C:128:THR:HA	2:C:160:HIS:HB3	1.99	0.44
1:A:468:ARG:HD3	1:A:542:HIS:CD2	2.52	0.44
1:A:633:VAL:HG13	1:A:639:TYR:CG	2.53	0.44
1:A:3607:GLN:OE1	1:A:3610:ARG:HD2	2.17	0.44
1:A:3726:MET:O	1:A:3730:THR:HG23	2.17	0.44
2:C:216:LEU:HD23	2:C:274:VAL:HB	1.98	0.44
1:A:1123:THR:HG22	1:A:1125:ARG:H	1.82	0.44
2:C:160:HIS:CD2	2:C:161:LYS:HG3	2.53	0.44
2:C:285:TRP:HB3	2:C:289:ASP:HB2	1.99	0.44
1:A:2671:LYS:O	1:A:2675:VAL:HG22	2.16	0.44
1:A:1267:GLY:HA2	1:A:1454:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2225:LEU:HA	1:A:2228:VAL:HG23	1.99	0.44
2:C:297:GLN:HE22	2:C:351:GLN:HE21	1.64	0.44
2:C:757:LEU:HD21	2:C:766:ILE:HD11	1.99	0.44
2:C:931:LEU:HD13	2:C:937:GLY:HA2	1.98	0.44
1:A:1495:LEU:HA	1:A:1498:ALA:HB3	1.99	0.44
1:A:3726:MET:SD	1:A:3878:VAL:HG11	2.57	0.44
1:A:61:PHE:O	1:A:65:LEU:HG	2.17	0.44
1:A:1049:ILE:HA	1:A:1052:LEU:HD13	1.99	0.44
1:A:3296:CYS:SG	1:A:3298:THR:HG23	2.58	0.44
1:A:3860:LEU:HD12	1:A:3879:LEU:HD13	2.00	0.44
1:A:403:LEU:HD22	1:A:408:MET:HG3	2.00	0.43
1:A:544:ILE:HA	1:A:555:PHE:HD1	1.83	0.43
1:A:1170:PHE:CE2	1:A:1252:CYS:HB3	2.53	0.43
1:A:1099:ARG:O	1:A:1156:LYS:HE3	2.18	0.43
1:A:4315:GLU:HA	1:A:4320:ILE:HA	2.00	0.43
2:C:982:ILE:HB	2:C:987:GLU:HB2	2.00	0.43
1:A:823:ALA:O	1:A:827:VAL:HG23	2.19	0.43
2:C:689:LEU:HB3	2:C:768:PHE:HE2	1.83	0.43
2:C:997:LYS:HG3	2:C:1082:PHE:HE1	1.83	0.43
2:C:1042:ILE:HG13	2:C:1051:ILE:HD11	2.00	0.43
1:A:135:LEU:HB3	1:A:282:HIS:HB3	1.99	0.43
1:A:1619:TRP:CE2	1:A:1628:CYS:HB2	2.52	0.43
1:A:1044:ALA:O	1:A:1048:GLN:HG2	2.19	0.43
1:A:1216:LEU:HD13	1:A:1290:ARG:NH1	2.34	0.43
1:A:3290:MET:HE3	1:A:3290:MET:HB2	1.82	0.43
1:A:3864:LEU:HD22	1:A:3965:VAL:HG11	2.00	0.43
2:C:735:TYR:HB3	2:C:743:THR:HG22	2.01	0.43
1:A:1620:PHE:HB2	1:A:1627:TRP:CZ3	2.54	0.43
1:A:1824:LEU:O	1:A:1828:ILE:HG12	2.19	0.43
1:A:3338:ASP:O	1:A:3342:GLN:HG2	2.18	0.43
1:A:4208:HIS:O	1:A:4212:GLN:HG2	2.19	0.43
2:C:912:PRO:HG3	2:C:921:LEU:HD13	2.01	0.43
1:A:968:GLN:O	1:A:972:GLN:HG2	2.18	0.43
1:A:1195:THR:O	1:A:1199:LEU:HG	2.18	0.43
1:A:163:LEU:HB2	1:A:287:LEU:HD21	2.00	0.42
1:A:3193:LEU:HD12	1:A:3193:LEU:HA	1.86	0.42
1:A:529:ARG:NH1	1:A:4067:MET:HG3	2.34	0.42
2:C:949:ILE:HG13	2:C:1006:PRO:HB2	2.00	0.42
1:A:576:LEU:HA	1:A:579:ASN:ND2	2.35	0.42
1:A:4065:TRP:O	1:A:4068:ILE:HG22	2.19	0.42
2:C:297:GLN:NE2	2:C:351:GLN:HE21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1546:TRP:HB2	1:A:1745:ILE:HG23	2.02	0.42
2:C:892:ARG:HD2	2:C:914:LYS:HA	2.01	0.42
1:A:376:ASP:HA	1:A:377:PRO:HD3	1.79	0.42
1:A:1824:LEU:HD13	1:A:2074:LEU:HD21	2.01	0.42
1:A:799:LEU:HD22	1:A:840:VAL:HG13	2.01	0.42
1:A:3988:TYR:O	1:A:3991:VAL:HG22	2.20	0.42
2:C:320:ILE:HB	2:C:321:PRO:HD3	2.01	0.42
1:A:1152:LEU:HD11	1:A:1156:LYS:HE2	2.02	0.42
2:C:1070:MET:HG3	2:C:1071:SER:H	1.84	0.42
1:A:1128:LEU:O	1:A:1132:ILE:HG13	2.19	0.42
1:A:1451:LEU:HD11	1:A:1532:LEU:HD22	2.02	0.42
1:A:1611:GLN:HB3	1:A:1683:LEU:HD11	2.02	0.42
2:C:87:SER:HB3	2:C:99:ILE:HB	2.02	0.42
1:A:4245:GLN:O	1:A:4249:LEU:HG	2.19	0.42
2:C:945:VAL:HB	2:C:950:ILE:HG21	2.01	0.42
1:A:1052:LEU:N	1:A:1052:LEU:HD12	2.35	0.41
1:A:543:ILE:HA	1:A:550:TYR:CD2	2.55	0.41
1:A:1620:PHE:HB2	1:A:1627:TRP:CH2	2.55	0.41
1:A:1770:VAL:HG23	1:A:1771:ASP:N	2.34	0.41
1:A:3225:SER:O	1:A:3229:ILE:HG13	2.20	0.41
2:C:652:SER:HB3	2:C:658:TRP:CE3	2.54	0.41
2:C:976:PRO:O	2:C:980:VAL:HG23	2.20	0.41
2:C:71:PHE:HE2	2:C:99:ILE:HG13	1.85	0.41
1:A:2230:HIS:CD2	1:A:3395:LEU:HD22	2.56	0.41
2:C:172:ALA:HB3	2:C:175:GLU:HG3	2.02	0.41
2:C:234:PHE:CD2	2:C:469:LEU:HD13	2.55	0.41
2:C:1041:ALA:O	2:C:1077:LEU:HD12	2.20	0.41
1:A:3739:PHE:CZ	1:A:3743:LEU:HD11	2.56	0.41
1:A:4107:PHE:HA	1:A:4110:VAL:HG12	2.01	0.41
1:A:403:LEU:HA	1:A:406:CYS:SG	2.61	0.41
1:A:1940:ASP:O	1:A:1944:GLU:HG3	2.21	0.41
1:A:4207:VAL:HA	1:A:4210:VAL:HG12	2.03	0.41
1:A:1661:GLN:O	1:A:1665:MET:N	2.54	0.41
1:A:525:SER:HB2	1:A:4063:ARG:NH1	2.35	0.41
1:A:1500:LEU:HD23	1:A:1500:LEU:HA	1.82	0.41
2:C:1016:HIS:HA	2:C:1056:TYR:HB3	2.03	0.41
1:A:143:LYS:HA	1:A:289:TYR:CD1	2.56	0.41
1:A:419:LEU:HA	1:A:419:LEU:HD23	1.84	0.41
1:A:779:SER:O	1:A:783:ASN:HB2	2.21	0.41
1:A:4050:PHE:HE2	1:A:4061:LEU:HD22	1.86	0.41
1:A:918:ARG:NH2	1:A:1076:GLY:HA2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:ALA:HB1	1:A:1582:TRP:CD1	2.55	0.41
1:A:3857:TRP:CZ2	1:A:3889:VAL:HG11	2.56	0.41
2:C:373:LEU:O	2:C:388:GLU:HA	2.21	0.41
2:C:549:ARG:O	2:C:553:GLN:HG2	2.20	0.41
1:A:2239:MET:HG3	1:A:2240:ALA:N	2.36	0.40
1:A:3434:LEU:O	1:A:3437:MET:HB2	2.21	0.40
1:A:4050:PHE:CE2	1:A:4061:LEU:HD22	2.56	0.40
2:C:318:GLY:C	2:C:321:PRO:HD2	2.46	0.40
2:C:925:CYS:O	2:C:929:VAL:HG22	2.21	0.40
1:A:903:ILE:HD13	1:A:1063:LEU:HD13	2.01	0.40
1:A:3187:SER:OG	1:A:3395:LEU:HD11	2.21	0.40
1:A:4200:GLU:HA	1:A:4203:LYS:HE2	2.02	0.40
1:A:284:ILE:O	1:A:288:VAL:HG23	2.21	0.40
1:A:874:LEU:HD12	1:A:874:LEU:HA	1.95	0.40
1:A:4178:VAL:HG21	1:A:4213:MET:HG3	2.03	0.40
2:C:814:SER:HB3	2:C:817:MET:HG3	2.03	0.40
1:A:680:ALA:O	1:A:684:LEU:HG	2.21	0.40
1:A:1572:LYS:HD3	1:A:1768:VAL:HG12	2.04	0.40
1:A:2668:SER:O	1:A:2672:VAL:HG23	2.21	0.40
1:A:3444:ARG:NH2	1:A:3588:LEU:HD12	2.37	0.40
2:C:211:THR:HG22	2:C:487:ARG:HG3	2.03	0.40
2:C:455:VAL:HG13	2:C:512:ASN:C	2.46	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	2383/4374 (54%)	2323 (98%)	60 (2%)	0	100	100
2	C	963/1102 (87%)	940 (98%)	22 (2%)	1 (0%)	48	74
All	All	3346/5476 (61%)	3263 (98%)	82 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	461	HIS

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	2166/3808 (57%)	2116 (98%)	50 (2%)	44	74
2	C	896/1004 (89%)	880 (98%)	16 (2%)	51	78
All	All	3062/4812 (64%)	2996 (98%)	66 (2%)	45	75

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	SER
1	A	864	SER
1	A	1052	LEU
1	A	1139	SER
1	A	1210	VAL
1	A	1442	THR
1	A	1502	LEU
1	A	1510	VAL
1	A	1511	SER
1	A	1539	GLU
1	A	1558	ILE
1	A	1591	ASP
1	A	1596	THR
1	A	1613	ASN
1	A	1622	ASP
1	A	1870	ILE
1	A	1894	ARG
1	A	1930	LEU
1	A	2083	VAL
1	A	2108	VAL
1	A	2113	LEU
1	A	2127	ASP

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Mol	Chain	Res	Type
1	A	2144	SER
1	A	2146	THR
1	A	2169	SER
1	A	2182	ILE
1	A	2185	THR
1	A	2239	MET
1	A	2250	LEU
1	A	2521	VAL
1	A	2662	SER
1	A	2685	GLU
1	A	2692	LYS
1	A	3284	SER
1	A	3303	ILE
1	A	3583	LEU
1	A	3598	LEU
1	A	3615	THR
1	A	3621	LYS
1	A	3870	SER
1	A	3888	LEU
1	A	3974	THR
1	A	4002	ARG
1	A	4130	ARG
1	A	4162	GLU
1	A	4183	VAL
1	A	4186	VAL
1	A	4209	LEU
1	A	4301	THR
1	A	4330	ARG
2	C	223	CYS
2	C	460	ASN
2	C	501	HIS
2	C	512	ASN
2	C	554	LYS
2	C	707	THR
2	C	743	THR
2	C	892	ARG
2	C	991	THR
2	C	1013	GLN
2	C	1020	VAL
2	C	1057	GLU
2	C	1058	VAL
2	C	1063	PHE

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Mol	Chain	Res	Type
2	C	1066	GLN
2	C	1074	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	175	ASN
1	A	265	HIS
1	A	278	GLN
1	A	568	GLN
1	A	859	HIS
1	A	923	ASN
1	A	924	GLN
1	A	1155	GLN
1	A	1255	ASN
1	A	1574	GLN
1	A	1809	GLN
1	A	1868	ASN
1	A	1913	ASN
1	A	2119	HIS
1	A	2223	ASN
1	A	2664	HIS
1	A	3302	GLN
1	A	3436	ASN
1	A	3582	GLN
1	A	3748	GLN
1	A	4044	ASN
1	A	4202	ASN
1	A	4212	GLN
2	C	156	HIS
2	C	351	GLN
2	C	414	GLN
2	C	417	GLN
2	C	438	GLN
2	C	470	ASN
2	C	553	GLN
2	C	581	ASN
2	C	792	HIS
2	C	986	ASN
2	C	996	HIS

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](#)

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.

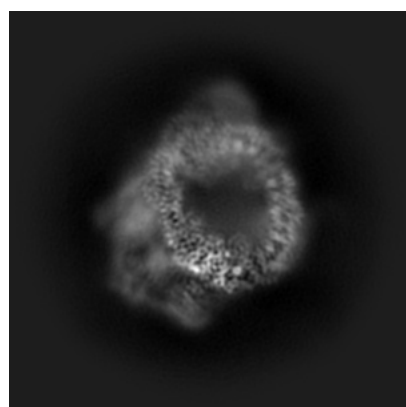
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71721. These allow visual inspection of the internal detail of the map and identification of artifacts.

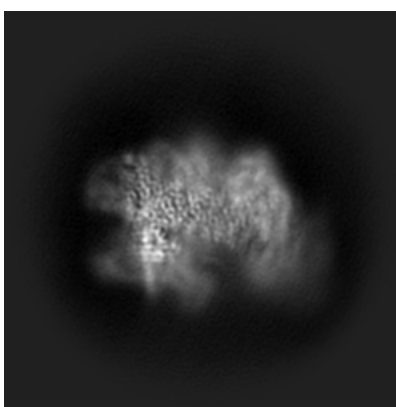
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

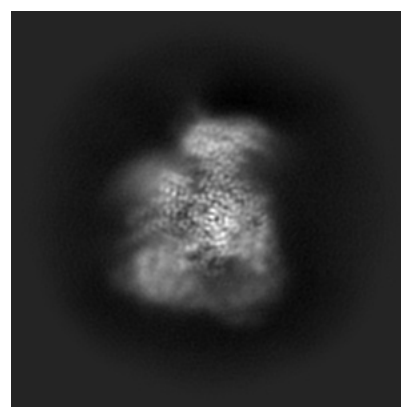
6.1.1 Primary map



X



Y

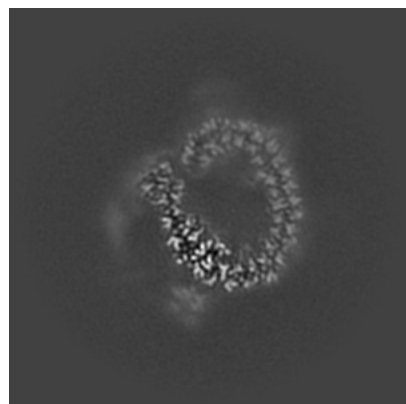


Z

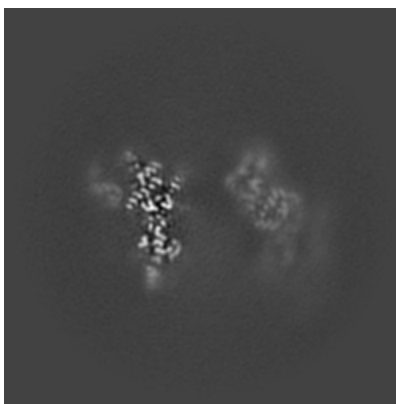
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

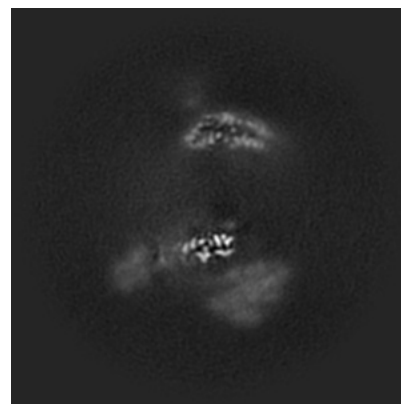
6.2.1 Primary map



X Index: 190



Y Index: 190

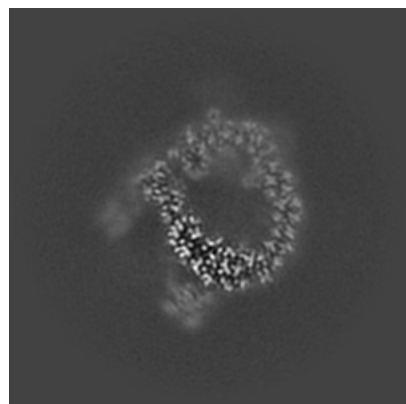


Z Index: 190

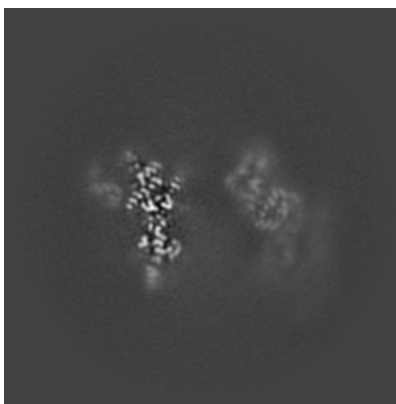
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

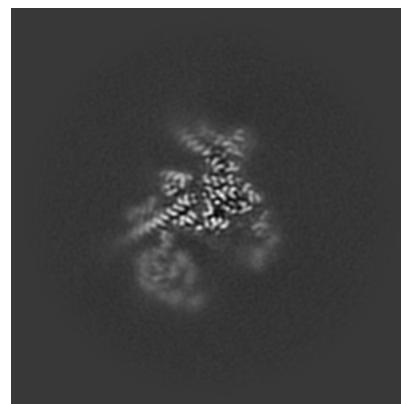
6.3.1 Primary map



X Index: 197



Y Index: 190

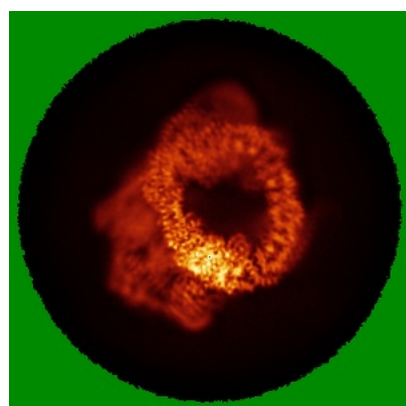


Z Index: 135

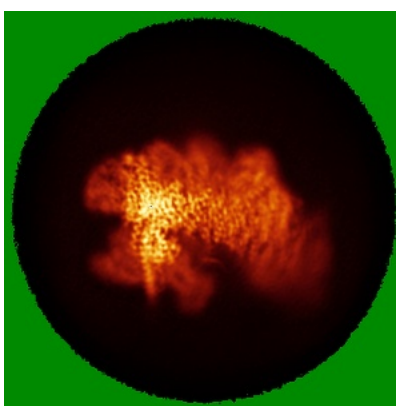
The images above show the largest variance slices of the map in three orthogonal directions.

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

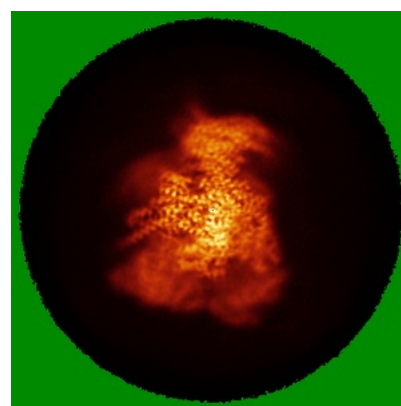
6.4.1 Primary map



X



Y

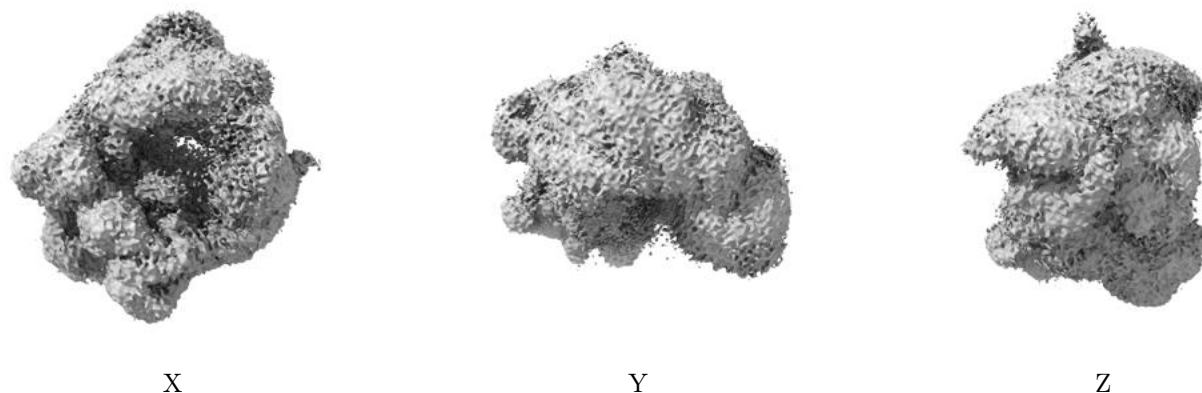


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

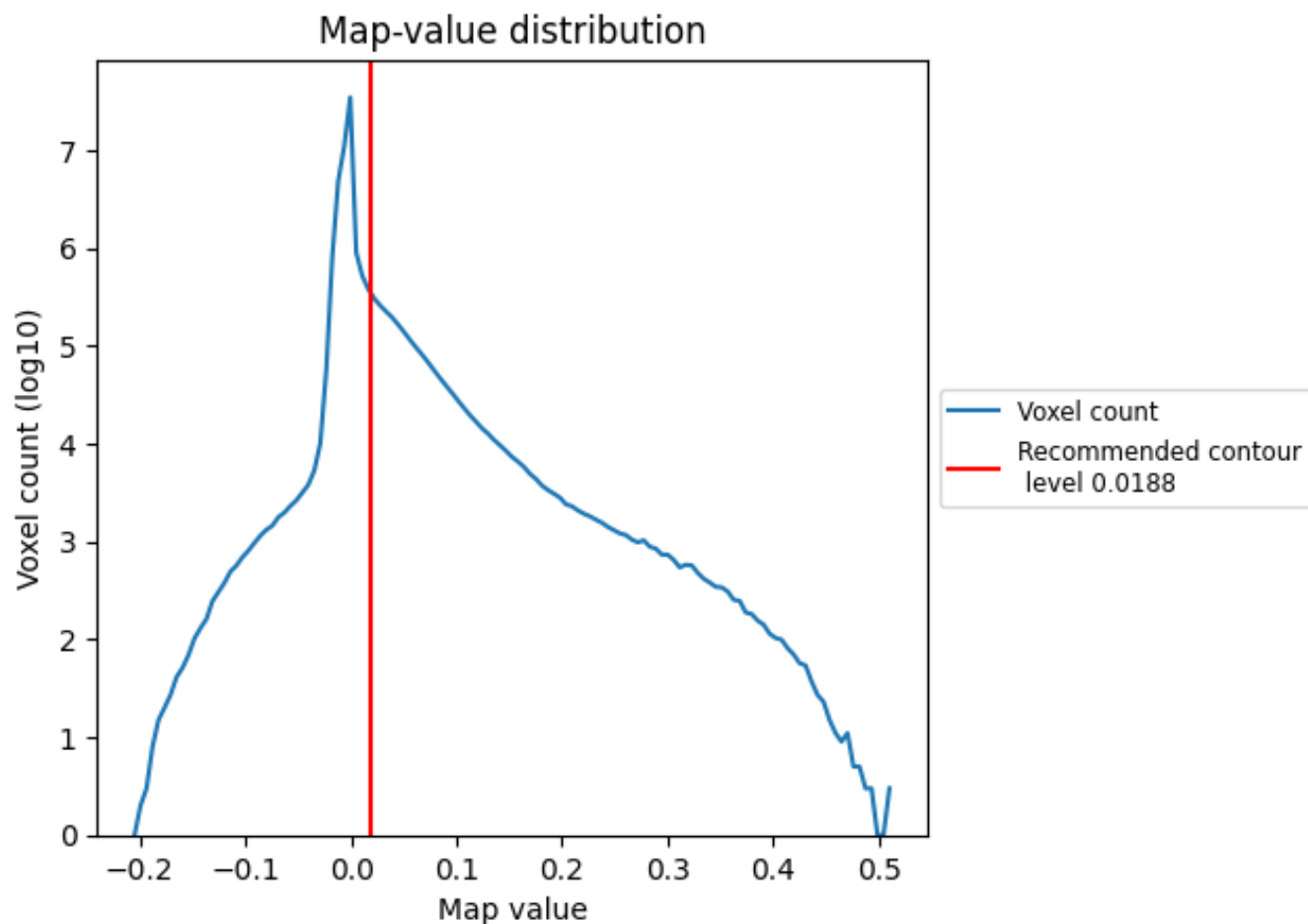
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

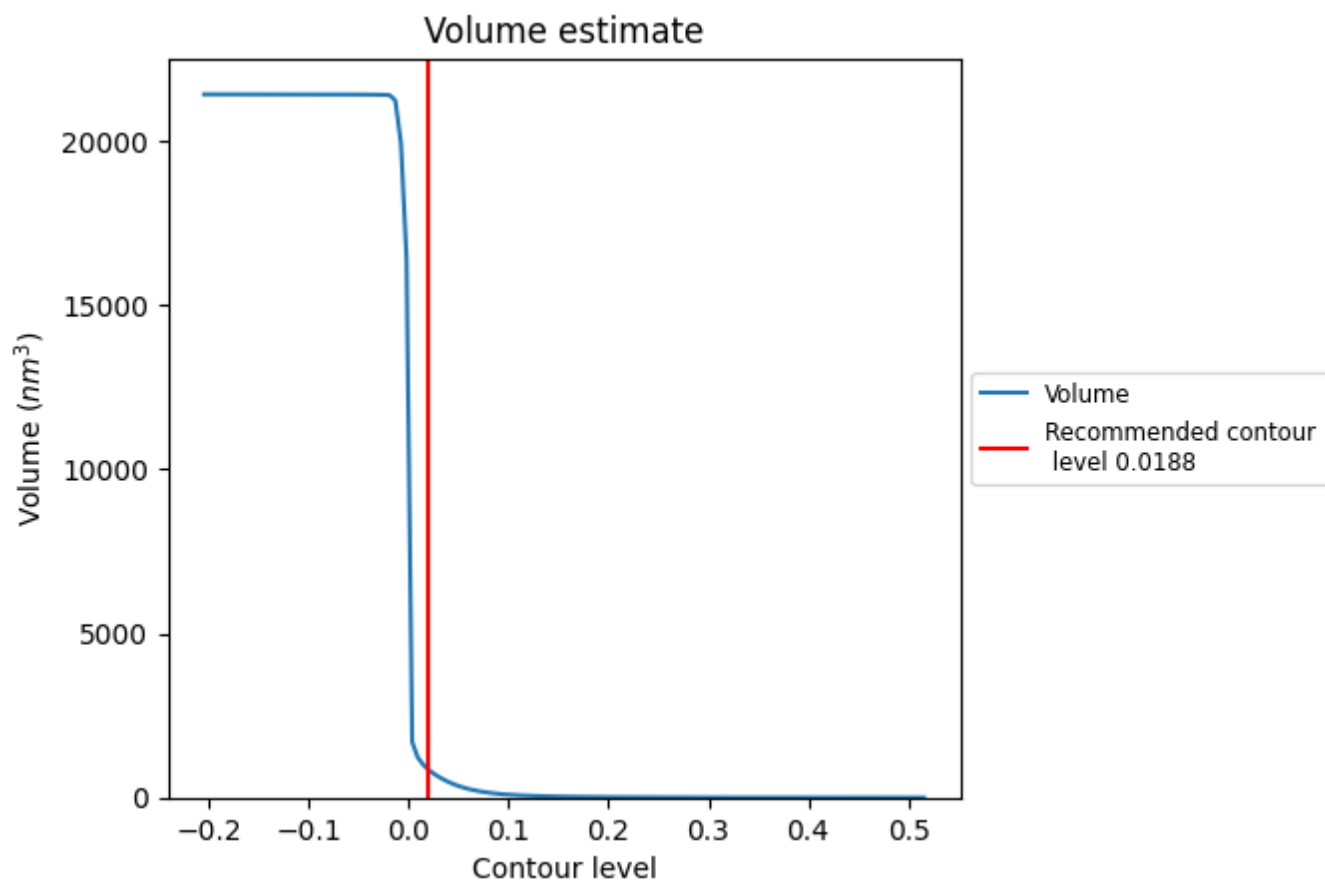
This section contains the results of statistical analysis of the map.

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.

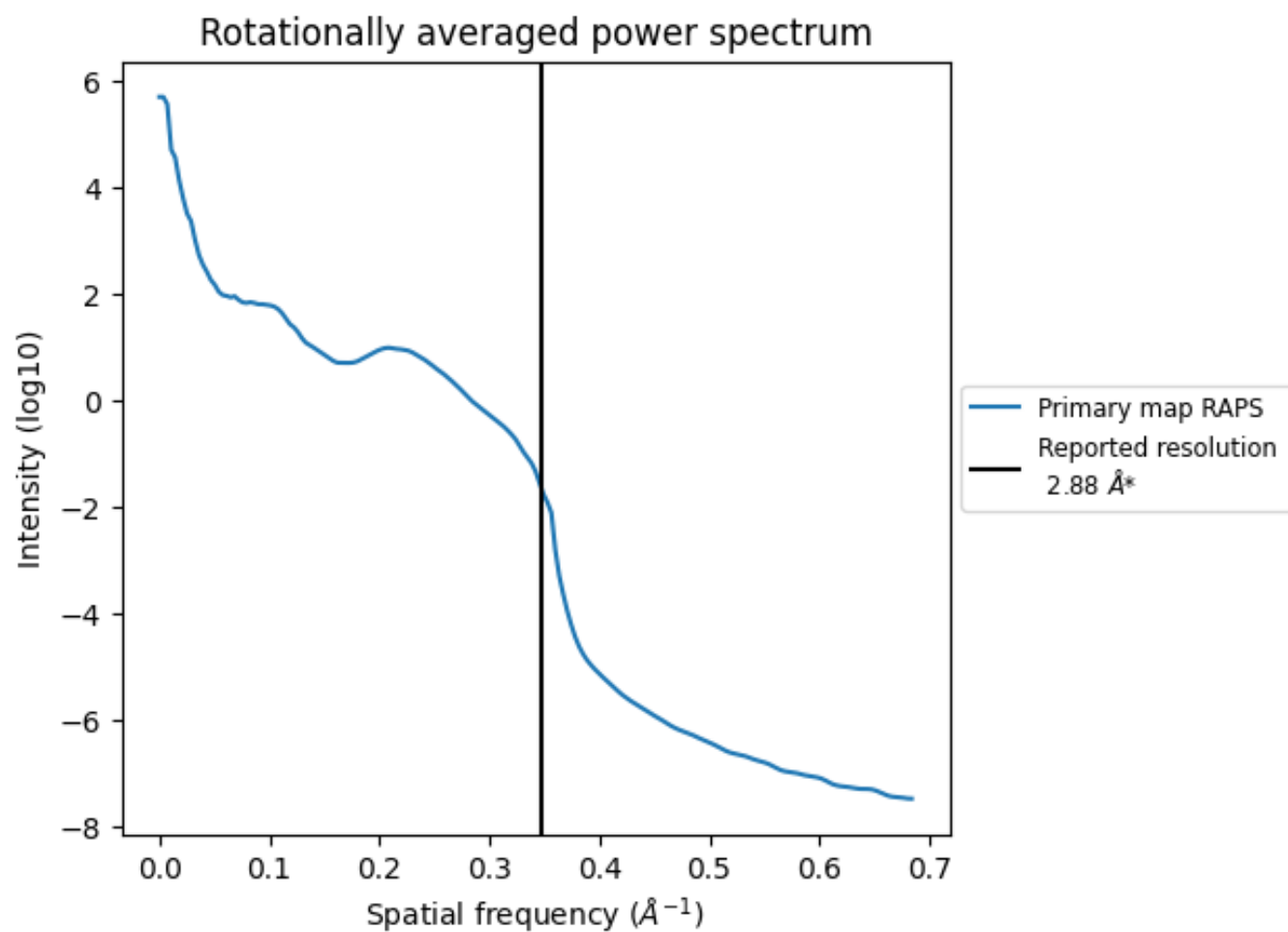
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 874 nm³; this corresponds to an approximate mass of 790 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 0.347 Å⁻¹

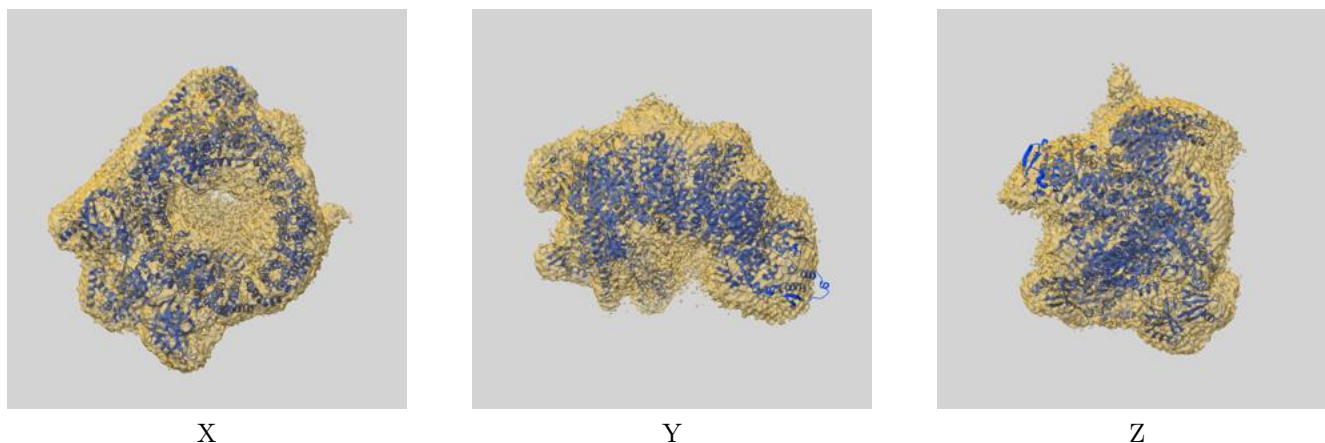
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

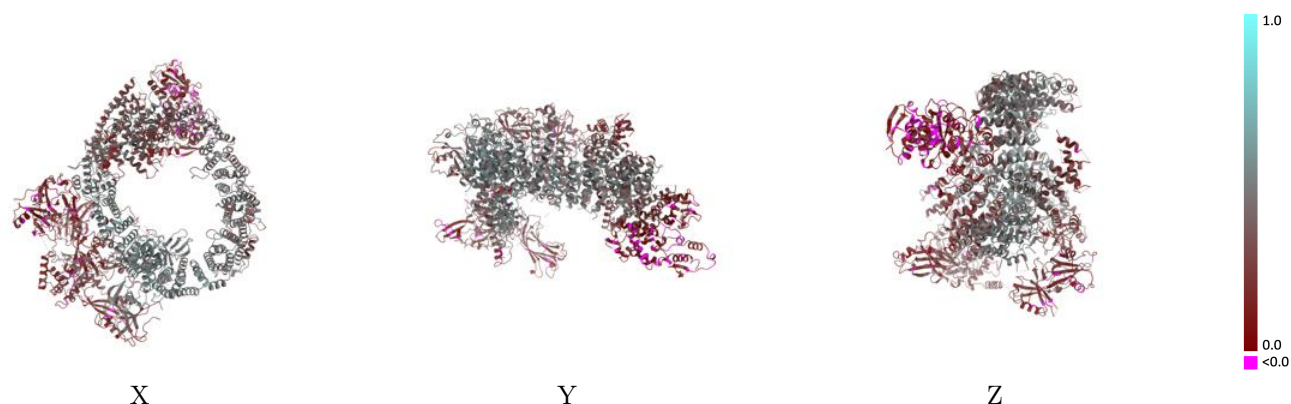
This section contains information regarding the fit between EMDB map EMD-71721 and PDB model 9PLR. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



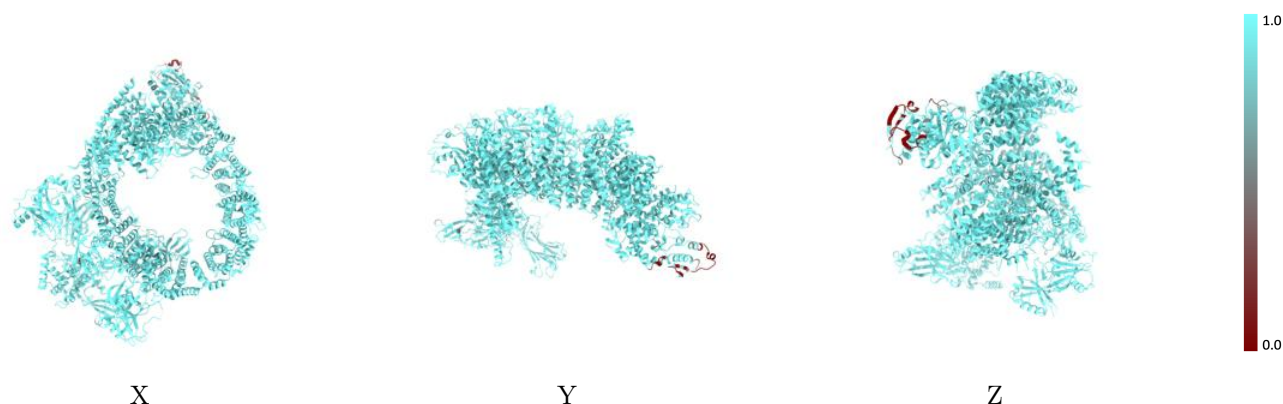
The images above show the 3D surface view of the map at the recommended contour level 0.0188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



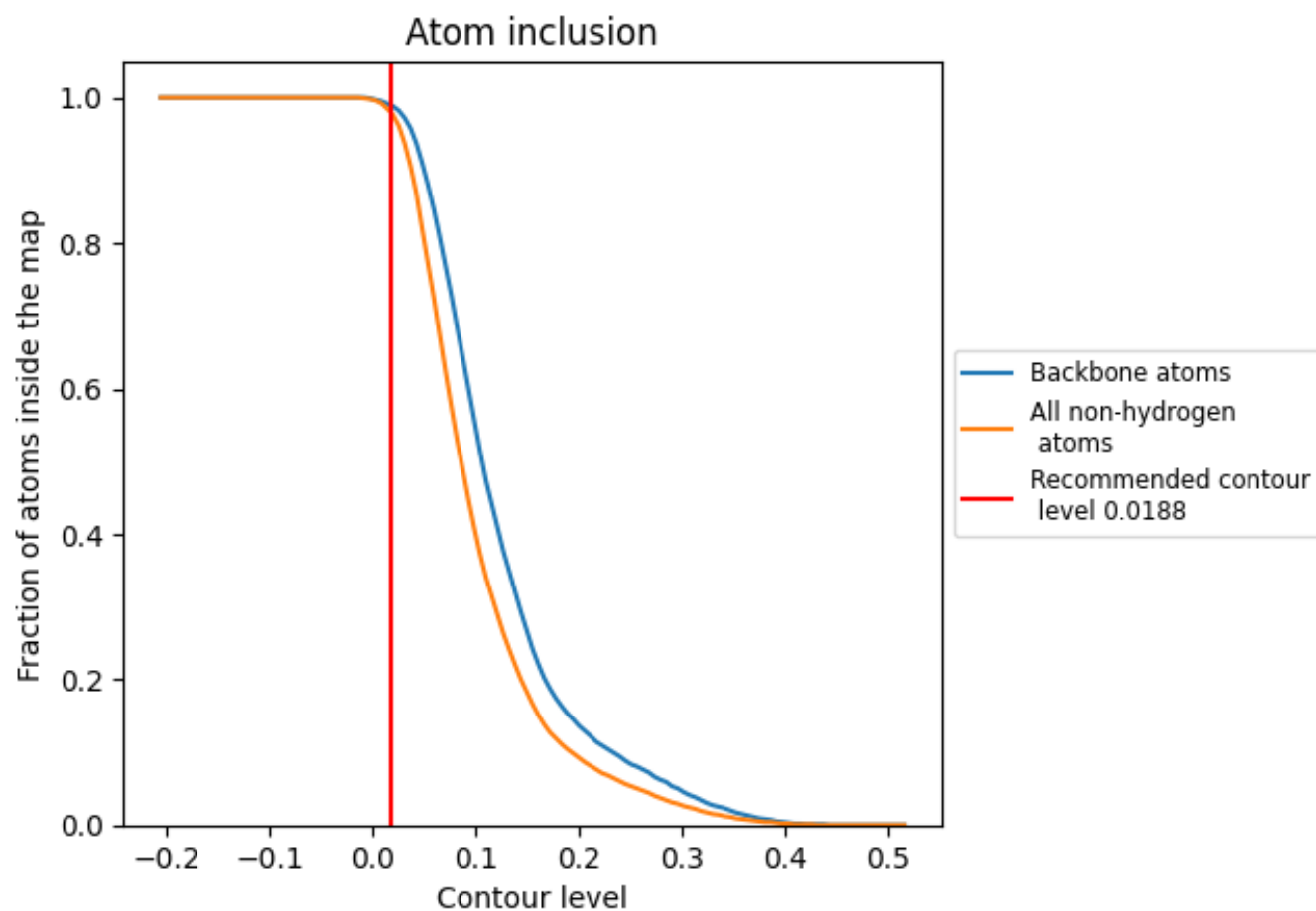
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0188).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9790	0.3410
A	0.9770	0.3860
C	0.9840	0.2340

