



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 02:53 PM EDT

PDB ID : 9O0C / pdb_00009o0c
EMDB ID : EMD-49969
Title : The dimeric assembly of Listeria adhesion protein (LAP)
Deposited on : 2025-04-02
Resolution : 3.20 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

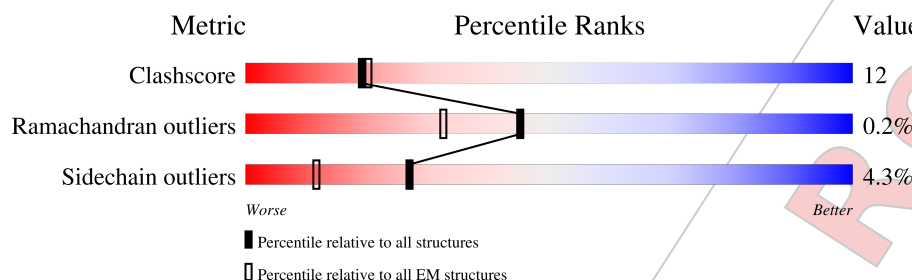
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	868	8% 69% 29% ..
1	B	868	8% 68% 30% ..
1	C	868	5% 34% 12% 53%
1	D	868	6% 34% 13% 53%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 19612 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 Aldehyde-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	860	Total	C	N	O	S	0	0
			6608	4215	1118	1245	30		
1	B	860	Total	C	N	O	S	0	0
			6608	4215	1118	1245	30		
1	C	408	Total	C	N	O	S	0	0
			3198	2058	531	596	13		
1	D	408	Total	C	N	O	S	0	0
			3198	2058	531	596	13		

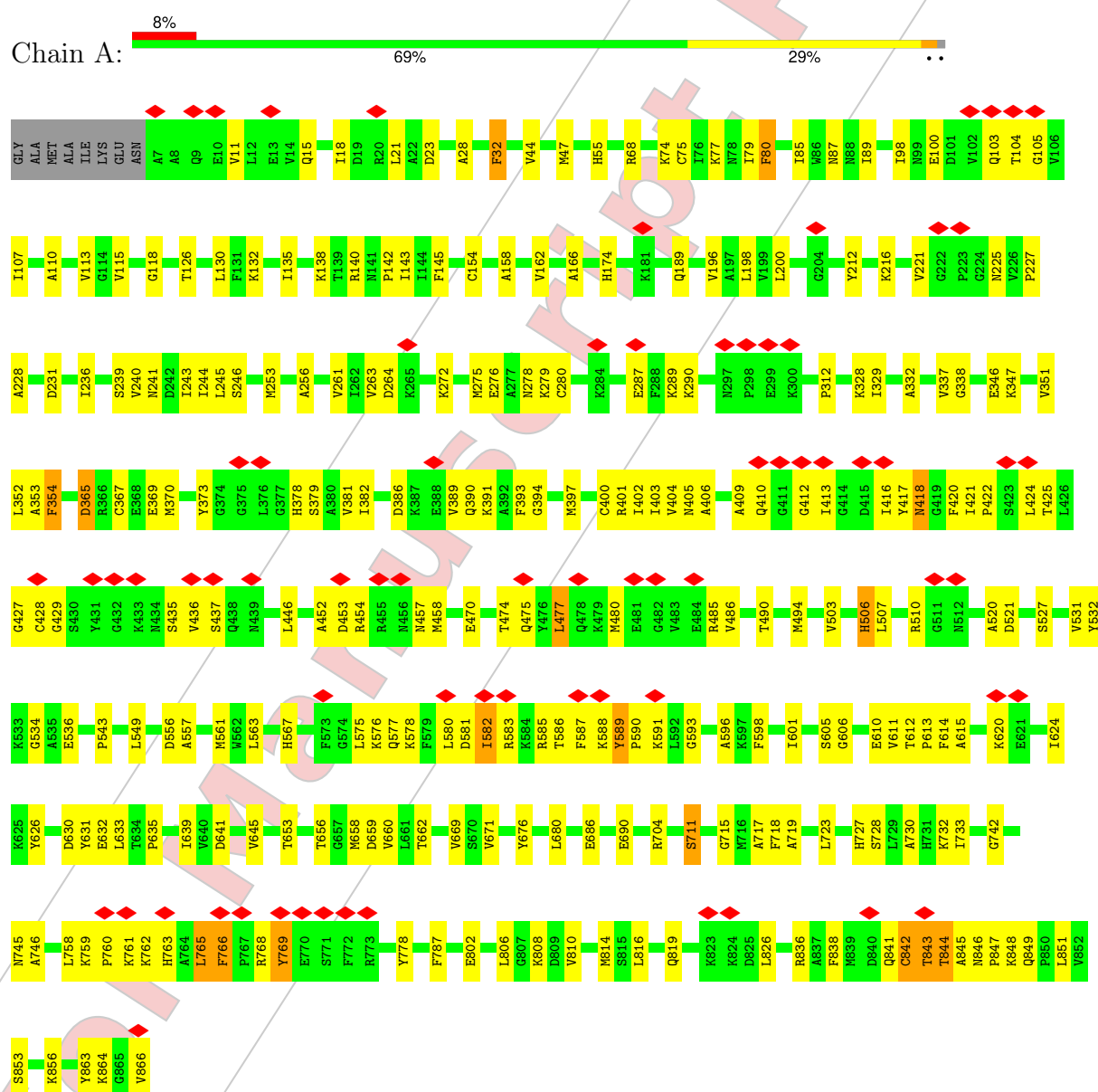
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6Q3I2
A	0	ALA	-	expression tag	UNP Q6Q3I2
B	-1	GLY	-	expression tag	UNP Q6Q3I2
B	0	ALA	-	expression tag	UNP Q6Q3I2
C	-1	GLY	-	expression tag	UNP Q6Q3I2
C	0	ALA	-	expression tag	UNP Q6Q3I2
D	-1	GLY	-	expression tag	UNP Q6Q3I2
D	0	ALA	-	expression tag	UNP Q6Q3I2

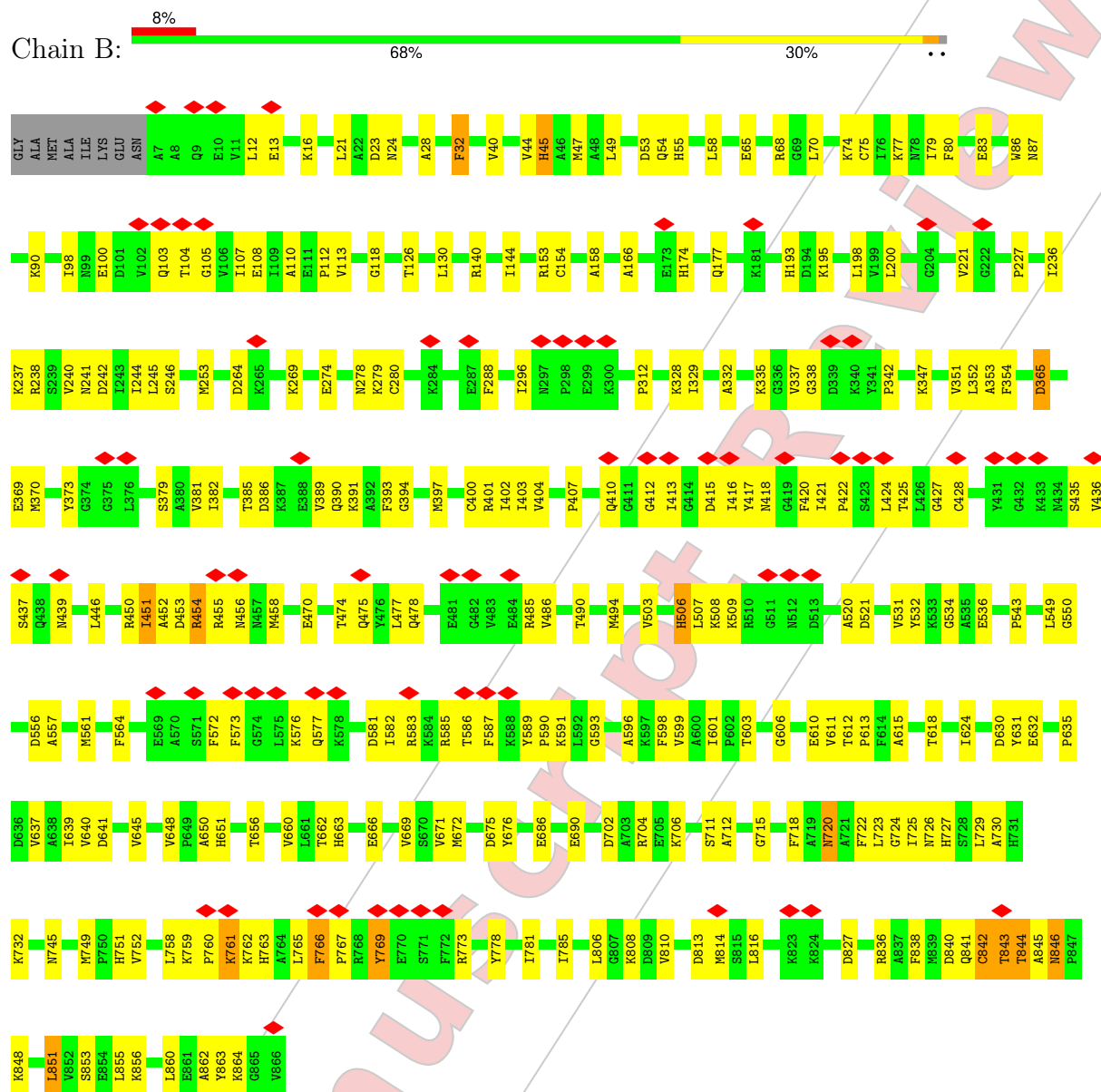
3 Residue-property plots

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.

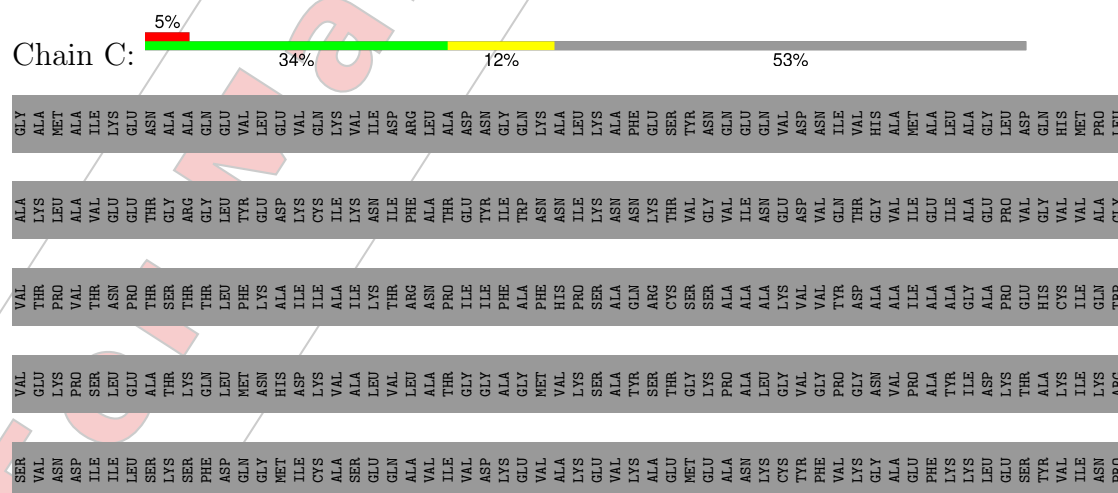
• Molecule 1: Aldehyde-alcohol dehydrogenase

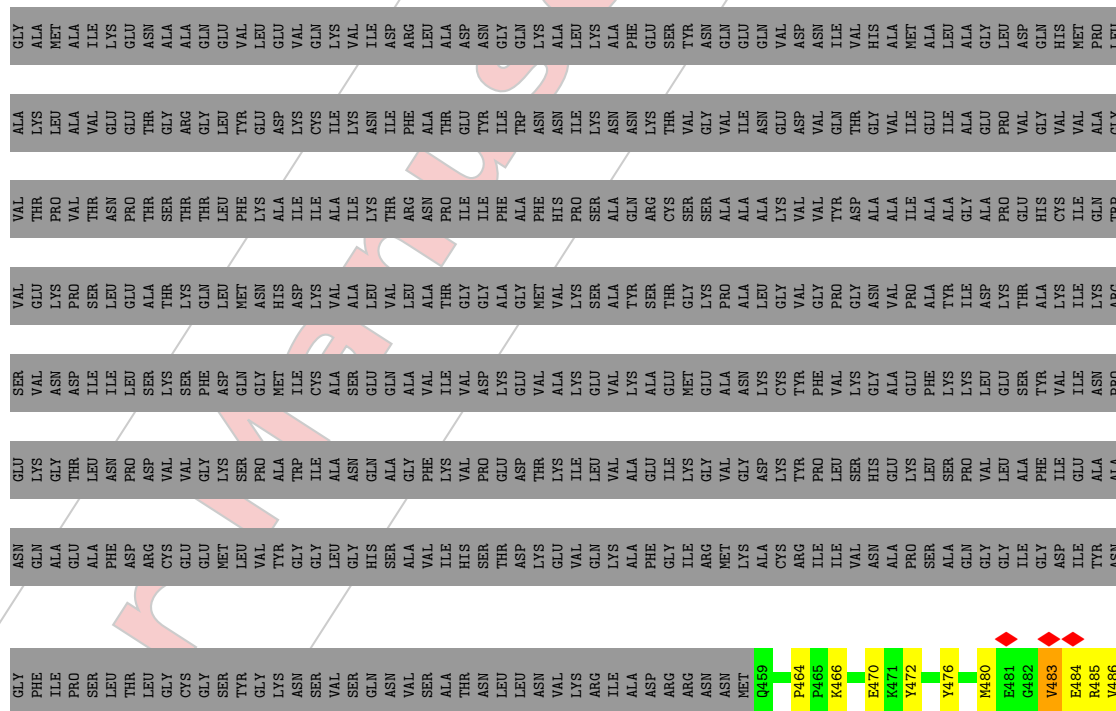


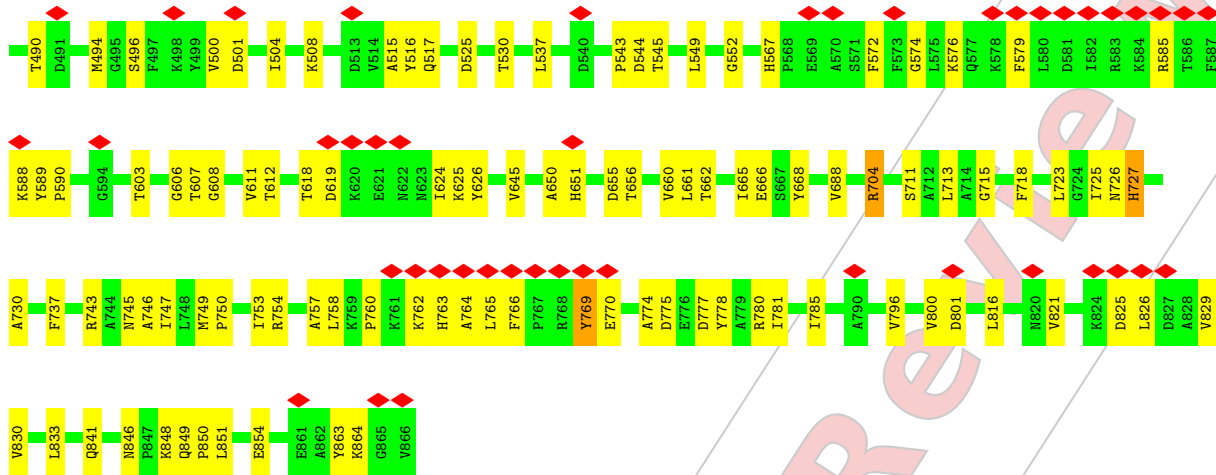
• Molecule 1: Aldehyde-alcohol dehydrogenase



- Molecule 1: Aldehyde-alcohol dehydrogenase







4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.230	Depositor
Minimum map value	-1.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	539.648, 539.648, 539.648	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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	0.27	0/6740	0.53	4/9124 (0.0%)
1	B	0.27	0/6740	0.53	3/9124 (0.0%)
1	C	0.26	0/3273	0.48	0/4430
1	D	0.26	0/3273	0.49	0/4430
All	All	0.27	0/20026	0.51	7/27108 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	LEU	CA-CB-CG	6.46	130.16	115.30
1	B	843	THR	N-CA-C	5.91	126.95	111.00
1	A	843	THR	N-CA-C	5.48	125.79	111.00
1	A	588	LYS	C-N-CA	5.45	135.33	121.70
1	A	842	CYS	C-N-CA	5.43	135.27	121.70
1	B	842	CYS	C-N-CA	5.41	135.24	121.70
1	B	365	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	ASN	Peptide
1	A	582	ILE	Peptide
1	A	759	LYS	Peptide
1	B	454	ARG	Sidechain
1	B	759	LYS	Peptide

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	6608	0	6661	211	0
1	B	6608	0	6658	209	0
1	C	3198	0	3201	65	0
1	D	3198	0	3201	71	0
All	All	19612	0	19721	490	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 12.

All (490) 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:C:606:GLY:HA3	1:C:656:THR:HB	1.55	0.88
1:D:606:GLY:HA2	1:D:660:VAL:HG23	1.57	0.87
1:D:606:GLY:HA3	1:D:656:THR:HB	1.58	0.85
1:C:606:GLY:HA2	1:C:660:VAL:HG23	1.62	0.82
1:B:606:GLY:HA3	1:B:656:THR:HB	1.61	0.80
1:A:768:ARG:HB2	1:B:238:ARG:HG2	1.64	0.80
1:A:578:LYS:HG3	1:B:49:LEU:HD21	1.64	0.79
1:A:382:ILE:HG23	1:A:404:VAL:HG12	1.66	0.77
1:A:606:GLY:HA3	1:A:656:THR:HB	1.67	0.77
1:B:582:ILE:HG22	1:B:583:ARG:H	1.50	0.76
1:A:413:ILE:HG13	1:B:671:VAL:HB	1.67	0.76
1:D:774:ALA:HA	1:D:777:ASP:HB2	1.68	0.76
1:A:261:VAL:HG23	1:A:352:LEU:HD21	1.67	0.75
1:A:580:LEU:HB3	1:A:841:GLN:HE21	1.52	0.75
1:B:337:VAL:HG11	1:B:370:MET:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:ALA:HA	1:C:777:ASP:HB2	1.69	0.73
1:A:279:LYS:HD2	1:B:760:PRO:HB3	1.70	0.72
1:B:424:LEU:HD12	1:B:425:THR:HG23	1.70	0.72
1:A:420:PHE:HD1	1:B:455:ARG:HG2	1.54	0.72
1:A:605:SER:HB2	1:A:645:VAL:HG21	1.71	0.72
1:B:421:ILE:HD12	1:B:439:ASN:HB3	1.72	0.72
1:A:221:VAL:HA	1:A:427:GLY:HA3	1.72	0.72
1:B:382:ILE:HG23	1:B:404:VAL:HG12	1.72	0.72
1:B:486:VAL:HG11	1:B:507:LEU:HD21	1.72	0.71
1:A:244:ILE:HD12	1:B:761:LYS:HE3	1.73	0.71
1:A:337:VAL:HG11	1:A:370:MET:HB2	1.72	0.70
1:A:394:GLY:HA2	1:A:402:ILE:HD13	1.73	0.69
1:D:816:LEU:HB2	1:D:863:TYR:HA	1.74	0.68
1:B:576:LYS:HG3	1:B:577:GLN:HG3	1.76	0.67
1:A:761:LYS:HD3	1:B:241:ASN:HA	1.76	0.67
1:A:557:ALA:O	1:A:561:MET:HG3	1.95	0.67
1:A:287:GLU:HA	1:A:290:LYS:HD3	1.76	0.67
1:B:240:VAL:HG21	1:B:274:GLU:HB2	1.78	0.66
1:C:508:LYS:HD3	1:D:508:LYS:HD3	1.76	0.66
1:A:400:CYS:HB2	1:A:436:VAL:HG13	1.77	0.66
1:A:241:ASN:HA	1:B:761:LYS:HD3	1.75	0.66
1:A:838:PHE:HA	1:A:842:CYS:SG	2.35	0.65
1:B:732:LYS:HE3	1:B:836:ARG:HG2	1.79	0.65
1:A:420:PHE:CD1	1:B:455:ARG:HG2	2.31	0.65
1:A:531:VAL:HA	1:A:561:MET:HG2	1.78	0.64
1:B:503:VAL:HG21	1:B:549:LEU:HD11	1.80	0.64
1:A:671:VAL:HG22	1:A:845:ALA:HB1	1.79	0.64
1:B:843:THR:HA	1:B:844:THR:O	1.98	0.63
1:B:401:ARG:HD3	1:B:421:ILE:HD11	1.79	0.63
1:A:503:VAL:HG21	1:A:549:LEU:HD11	1.80	0.63
1:A:676:TYR:HA	1:C:713:LEU:HD21	1.81	0.63
1:B:221:VAL:HA	1:B:427:GLY:HA3	1.80	0.63
1:C:645:VAL:HG12	1:C:704:ARG:HD3	1.79	0.63
1:B:726:ASN:HB2	1:B:752:VAL:HG11	1.78	0.63
1:B:842:CYS:HA	1:B:844:THR:HB	1.80	0.63
1:C:712:ALA:O	1:C:716:MET:HG3	1.99	0.63
1:D:645:VAL:HG12	1:D:704:ARG:HD3	1.79	0.62
1:B:557:ALA:O	1:B:561:MET:HG3	1.99	0.62
1:D:490:THR:HG21	1:D:500:VAL:HG22	1.82	0.62
1:A:765:LEU:HD22	1:B:412:GLY:HA2	1.81	0.62
1:A:100:GLU:HG3	1:A:107:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HD13	1:B:144:ILE:HG21	1.80	0.61
1:B:100:GLU:HB2	1:B:107:ILE:HG23	1.81	0.61
1:B:763:HIS:HD2	1:B:851:LEU:HD22	1.65	0.61
1:D:725:ILE:HG21	1:D:850:PRO:HG3	1.82	0.61
1:B:107:ILE:HD12	1:B:451:ILE:HD11	1.81	0.61
1:B:531:VAL:HA	1:B:561:MET:HG2	1.83	0.61
1:A:563:LEU:HD12	1:A:633:LEU:HD21	1.81	0.61
1:B:410:GLN:HG2	1:B:416:ILE:HD12	1.81	0.61
1:A:424:LEU:HD12	1:A:425:THR:HG23	1.82	0.61
1:B:724:GLY:HA2	1:B:844:THR:HG23	1.81	0.61
1:C:490:THR:HG21	1:C:500:VAL:HG22	1.83	0.60
1:C:816:LEU:HB2	1:C:863:TYR:HA	1.83	0.60
1:A:241:ASN:OD1	1:B:767:PRO:HD2	2.02	0.60
1:B:606:GLY:HA2	1:B:660:VAL:HG23	1.83	0.60
1:C:725:ILE:HG21	1:C:850:PRO:HG3	1.84	0.60
1:A:413:ILE:HG22	1:B:766:PHE:HD1	1.66	0.60
1:A:418:ASN:HD22	1:B:456:ASN:HB3	1.66	0.60
1:A:586:THR:HG23	1:A:587:PHE:CE1	2.36	0.60
1:B:534:GLY:HA3	1:B:561:MET:SD	2.42	0.60
1:A:239:SER:O	1:A:243:ILE:HG22	2.01	0.59
1:B:582:ILE:HG21	1:B:631:TYR:HE2	1.68	0.59
1:A:410:GLN:HG2	1:A:416:ILE:HD12	1.83	0.59
1:A:659:ASP:HB2	1:A:742:GLY:HA2	1.85	0.59
1:A:723:LEU:O	1:A:844:THR:HG23	2.03	0.59
1:B:666:GLU:OE2	1:B:726:ASN:HB3	2.03	0.59
1:B:672:MET:H	1:B:845:ALA:HB1	1.68	0.59
1:A:843:THR:HA	1:A:844:THR:O	2.03	0.59
1:B:28:ALA:O	1:B:32:PHE:HB2	2.03	0.59
1:A:236:ILE:O	1:A:240:VAL:HG23	2.03	0.58
1:A:107:ILE:HD13	1:B:391:LYS:HE2	1.85	0.58
1:B:763:HIS:CD2	1:B:851:LEU:HD22	2.38	0.58
1:D:725:ILE:HG23	1:D:846:ASN:ND2	2.18	0.58
1:B:676:TYR:HA	1:D:713:LEU:HD21	1.86	0.58
1:B:386:ASP:O	1:B:390:GLN:HG3	2.03	0.58
1:B:856:LYS:O	1:B:860:LEU:HG	2.04	0.58
1:A:587:PHE:HE1	1:B:87:ASN:HA	1.69	0.57
1:A:645:VAL:HG13	1:A:704:ARG:HG2	1.85	0.57
1:B:601:ILE:HD13	1:B:639:ILE:HB	1.86	0.57
1:A:428:CYS:SG	1:A:435:SER:HB2	2.44	0.57
1:A:864:LYS:HB3	1:A:866:VAL:HG23	1.85	0.57
1:B:532:TYR:O	1:B:536:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:HB2	1:B:454:ARG:NH1	2.20	0.57
1:A:580:LEU:HB3	1:A:841:GLN:NE2	2.18	0.57
1:A:113:VAL:HG11	1:A:198:LEU:HB2	1.85	0.57
1:A:105:GLY:HA3	1:A:453:ASP:HB2	1.87	0.56
1:A:587:PHE:CE1	1:B:87:ASN:HA	2.41	0.56
1:A:532:TYR:O	1:A:536:GLU:HG2	2.06	0.56
1:A:601:ILE:HD13	1:A:639:ILE:HB	1.88	0.56
1:A:457:ASN:HB3	1:B:415:ASP:OD1	2.05	0.56
1:A:534:GLY:HA3	1:A:561:MET:SD	2.46	0.56
1:A:420:PHE:HD2	1:A:421:ILE:HG12	1.70	0.56
1:A:227:PRO:HB3	1:A:370:MET:HG2	1.88	0.56
1:C:665:ILE:HG21	1:C:753:ILE:HD11	1.86	0.56
1:C:825:ASP:O	1:C:829:VAL:HG12	2.06	0.56
1:D:665:ILE:HG21	1:D:753:ILE:HD11	1.87	0.56
1:D:829:VAL:HG22	1:D:833:LEU:HG	1.87	0.56
1:A:766:PHE:H	1:B:245:LEU:HD13	1.71	0.55
1:A:843:THR:N	1:A:844:THR:HB	2.21	0.55
1:B:758:LEU:HB2	1:B:848:LYS:NZ	2.20	0.55
1:B:74:LYS:HG2	1:B:77:LYS:HE3	1.88	0.55
1:D:825:ASP:O	1:D:829:VAL:HG12	2.06	0.55
1:B:12:LEU:HD23	1:B:13:GLU:H	1.70	0.55
1:C:829:VAL:HG22	1:C:833:LEU:HG	1.87	0.55
1:B:842:CYS:HA	1:B:844:THR:CB	2.36	0.55
1:A:844:THR:HG22	1:A:846:ASN:H	1.72	0.55
1:A:347:LYS:HD2	1:A:351:VAL:HB	1.87	0.55
1:C:606:GLY:HA2	1:C:660:VAL:CG2	2.35	0.55
1:B:844:THR:HG22	1:B:846:ASN:H	1.71	0.55
1:B:613:PRO:HB3	1:B:631:TYR:HA	1.89	0.54
1:A:730:ALA:HB2	1:A:745:ASN:HB3	1.90	0.54
1:B:732:LYS:HE2	1:B:840:ASP:HB2	1.89	0.54
1:A:658:MET:O	1:A:662:THR:HG23	2.08	0.54
1:B:296:ILE:HD11	1:B:342:PRO:HB3	1.90	0.54
1:B:347:LYS:HD2	1:B:351:VAL:HB	1.88	0.54
1:B:842:CYS:C	1:B:844:THR:HB	2.27	0.54
1:C:851:LEU:HB2	1:C:854:GLU:HG3	1.90	0.54
1:A:280:CYS:SG	1:A:329:ILE:HB	2.48	0.54
1:A:758:LEU:HB2	1:A:848:LYS:NZ	2.23	0.54
1:B:589:TYR:CG	1:B:590:PRO:HD2	2.43	0.54
1:D:655:ASP:OD1	1:D:743:ARG:HG2	2.09	0.53
1:B:416:ILE:O	1:B:418:ASN:HA	2.09	0.53
1:A:846:ASN:OD1	1:A:847:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:O	1:A:390:GLN:HG3	2.08	0.53
1:A:452:ALA:HB1	1:A:454:ARG:HD2	1.91	0.53
1:B:686:GLU:O	1:B:690:GLU:HG2	2.09	0.53
1:D:486:VAL:HG22	1:D:545:THR:HB	1.91	0.53
1:D:851:LEU:HB2	1:D:854:GLU:HG3	1.89	0.53
1:A:761:LYS:HD2	1:B:244:ILE:HB	1.91	0.53
1:A:806:LEU:O	1:A:810:VAL:HG22	2.09	0.53
1:A:412:GLY:HA2	1:B:765:LEU:HD12	1.91	0.53
1:A:612:THR:HB	1:A:614:PHE:HD1	1.74	0.53
1:A:420:PHE:HB2	1:B:454:ARG:HA	1.91	0.53
1:D:501:ASP:HA	1:D:504:ILE:HG12	1.90	0.53
1:A:728:SER:O	1:A:732:LYS:HG2	2.09	0.52
1:D:766:PHE:HB3	1:D:769:TYR:HB2	1.91	0.52
1:A:390:GLN:HE21	1:A:404:VAL:HG11	1.74	0.52
1:B:662:THR:HB	1:B:749:MET:SD	2.49	0.52
1:A:245:LEU:HD22	1:B:766:PHE:H	1.74	0.52
1:A:454:ARG:CZ	1:B:418:ASN:HD21	2.22	0.52
1:C:501:ASP:HA	1:C:504:ILE:HG12	1.91	0.52
1:A:417:TYR:CZ	1:B:769:TYR:HD1	2.27	0.52
1:B:100:GLU:HG3	1:B:107:ILE:HG12	1.91	0.52
1:A:686:GLU:O	1:A:690:GLU:HG2	2.09	0.52
1:A:413:ILE:HG22	1:B:766:PHE:CD1	2.45	0.52
1:A:556:ASP:HB2	1:A:615:ALA:HA	1.92	0.52
1:D:781:ILE:O	1:D:785:ILE:HG12	2.10	0.52
1:A:581:ASP:HB3	1:A:841:GLN:NE2	2.25	0.52
1:C:486:VAL:HG22	1:C:545:THR:HB	1.91	0.52
1:A:844:THR:HG22	1:A:846:ASN:N	2.25	0.51
1:A:196:VAL:HG23	1:A:216:LYS:HE3	1.92	0.51
1:A:365:ASP:O	1:A:369:GLU:HG3	2.10	0.51
1:B:24:ASN:HB3	1:B:177:GLN:HE22	1.76	0.51
1:B:103:GLN:HB3	1:D:472:TYR:CE1	2.45	0.51
1:B:556:ASP:HB2	1:B:615:ALA:HA	1.91	0.51
1:C:662:THR:O	1:C:666:GLU:HG3	2.09	0.51
1:C:760:PRO:HA	1:C:848:LYS:HE3	1.92	0.51
1:D:606:GLY:HA2	1:D:660:VAL:CG2	2.35	0.51
1:A:761:LYS:HE3	1:B:244:ILE:HD12	1.91	0.51
1:B:113:VAL:HG11	1:B:198:LEU:HB2	1.91	0.51
1:B:365:ASP:O	1:B:369:GLU:HG3	2.10	0.51
1:B:723:LEU:HD13	1:B:727:HIS:CD2	2.46	0.51
1:A:763:HIS:HB3	1:A:849:GLN:O	2.11	0.51
1:B:236:ILE:O	1:B:240:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:CYS:SG	1:B:329:ILE:HB	2.50	0.51
1:A:379:SER:HA	1:A:401:ARG:O	2.10	0.50
1:A:240:VAL:HG12	1:A:244:ILE:HD12	1.93	0.50
1:B:110:ALA:HB1	1:B:446:LEU:HD21	1.93	0.50
1:A:610:GLU:HG2	1:A:611:VAL:HG13	1.92	0.50
1:C:781:ILE:O	1:C:785:ILE:HG12	2.10	0.50
1:A:74:LYS:HG2	1:A:77:LYS:HE3	1.94	0.50
1:A:338:GLY:HA2	1:A:373:TYR:CE2	2.47	0.50
1:A:763:HIS:CD2	1:A:851:LEU:HD22	2.47	0.50
1:A:87:ASN:HA	1:B:587:PHE:CZ	2.47	0.50
1:A:763:HIS:NE2	1:B:70:LEU:HD21	2.27	0.50
1:A:842:CYS:HA	1:A:844:THR:HB	1.94	0.50
1:B:610:GLU:HG2	1:B:611:VAL:HG13	1.93	0.50
1:A:68:ARG:HG3	1:A:253:MET:SD	2.52	0.49
1:B:45:HIS:CE1	1:B:86:TRP:HZ2	2.30	0.49
1:A:787:PHE:CE1	1:A:802:GLU:HG2	2.47	0.49
1:C:608:GLY:O	1:C:612:THR:HG23	2.12	0.49
1:A:417:TYR:HB2	1:B:766:PHE:CD1	2.48	0.49
1:B:816:LEU:HB2	1:B:863:TYR:HA	1.95	0.49
1:A:412:GLY:HA3	1:B:765:LEU:HB2	1.93	0.49
1:A:582:ILE:HG22	1:A:583:ARG:H	1.76	0.49
1:C:666:GLU:OE2	1:C:726:ASN:HB3	2.12	0.49
1:D:608:GLY:O	1:D:612:THR:HG23	2.12	0.49
1:A:110:ALA:HB1	1:A:446:LEU:HD21	1.94	0.49
1:D:579:PHE:H	1:D:841:GLN:NE2	2.11	0.49
1:B:725:ILE:HG12	1:B:846:ASN:OD1	2.12	0.49
1:D:567:HIS:CD2	1:D:590:PRO:HB2	2.47	0.49
1:D:760:PRO:HA	1:D:848:LYS:HE3	1.94	0.49
1:B:278:ASN:HD22	1:B:278:ASN:N	2.11	0.48
1:C:484:GLU:HB2	1:C:544:ASP:OD2	2.13	0.48
1:A:103:GLN:HB3	1:C:472:TYR:CE1	2.48	0.48
1:B:751:HIS:CD2	1:B:862:ALA:HA	2.49	0.48
1:C:579:PHE:H	1:C:841:GLN:NE2	2.10	0.48
1:C:757:ALA:HB2	1:C:778:TYR:HD2	1.78	0.48
1:A:44:VAL:HG21	1:A:138:LYS:HA	1.95	0.48
1:A:420:PHE:HB2	1:B:454:ARG:CA	2.44	0.48
1:A:453:ASP:HA	1:B:404:VAL:CG2	2.43	0.48
1:A:624:ILE:HG12	1:A:836:ARG:HD3	1.96	0.48
1:B:573:PHE:HA	1:B:576:LYS:HE3	1.95	0.48
1:C:724:GLY:HA3	1:C:846:ASN:HB3	1.95	0.48
1:C:762:LYS:HB2	1:C:762:LYS:HE3	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:HA	1:A:632:GLU:OE2	2.14	0.48
1:B:424:LEU:HD12	1:B:425:THR:CG2	2.42	0.48
1:C:737:PHE:HD1	1:C:821:VAL:HG22	1.78	0.48
1:A:582:ILE:HD11	1:A:630:ASP:HB2	1.96	0.48
1:B:729:LEU:HD21	1:B:855:LEU:HG	1.95	0.48
1:B:806:LEU:O	1:B:810:VAL:HG22	2.13	0.48
1:A:98:ILE:HD11	1:A:110:ALA:HB2	1.96	0.48
1:A:381:VAL:HA	1:A:403:ILE:O	2.14	0.48
1:A:428:CYS:HB2	1:A:437:SER:HB3	1.95	0.48
1:B:428:CYS:HB2	1:B:437:SER:HB3	1.95	0.48
1:B:843:THR:N	1:B:844:THR:HB	2.29	0.48
1:D:517:GLN:OE1	1:D:537:LEU:HD22	2.13	0.48
1:D:619:ASP:HB3	1:D:624:ILE:HG13	1.96	0.48
1:A:85:ILE:O	1:A:89:ILE:HG12	2.14	0.48
1:A:612:THR:HG21	1:A:718:PHE:CZ	2.49	0.48
1:A:768:ARG:NH1	1:B:238:ARG:HD3	2.29	0.48
1:B:422:PRO:HB2	1:B:424:LEU:O	2.14	0.48
1:B:624:ILE:HG12	1:B:836:ARG:HD3	1.95	0.48
1:A:126:THR:HB	1:A:154:CYS:SG	2.54	0.47
1:B:582:ILE:HD11	1:B:630:ASP:HA	1.95	0.47
1:D:737:PHE:HD2	1:D:821:VAL:HG22	1.79	0.47
1:B:55:HIS:CE1	1:B:79:ILE:HG12	2.49	0.47
1:B:581:ASP:HB3	1:B:841:GLN:OE1	2.14	0.47
1:C:567:HIS:HD2	1:C:590:PRO:HB2	1.79	0.47
1:D:485:ARG:HB3	1:D:515:ALA:HB3	1.96	0.47
1:A:842:CYS:HA	1:A:844:THR:CB	2.45	0.47
1:B:582:ILE:HG21	1:B:631:TYR:CE2	2.49	0.47
1:B:612:THR:HG21	1:B:718:PHE:CZ	2.49	0.47
1:C:567:HIS:CD2	1:C:590:PRO:HB2	2.49	0.47
1:D:484:GLU:HB2	1:D:544:ASP:OD2	2.14	0.47
1:B:582:ILE:HG22	1:B:583:ARG:N	2.26	0.47
1:B:838:PHE:HA	1:B:842:CYS:SG	2.55	0.47
1:D:612:THR:HG21	1:D:718:PHE:CZ	2.50	0.47
1:A:289:LYS:HA	1:A:289:LYS:HD3	1.64	0.47
1:A:723:LEU:HD13	1:A:727:HIS:CD2	2.49	0.47
1:B:126:THR:HB	1:B:154:CYS:SG	2.55	0.47
1:B:246:SER:HB2	1:B:407:PRO:CB	2.45	0.47
1:B:591:LYS:HA	1:B:632:GLU:OE2	2.14	0.47
1:A:272:LYS:O	1:A:275:MET:HB2	2.14	0.47
1:B:585:ARG:HH12	1:D:476:TYR:HD1	1.62	0.47
1:B:842:CYS:CA	1:B:844:THR:HB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:PHE:HB3	1:C:769:TYR:HB2	1.97	0.47
1:D:730:ALA:HB2	1:D:745:ASN:HB3	1.95	0.47
1:B:112:PRO:HG3	1:B:140:ARG:HB2	1.96	0.47
1:A:130:LEU:HD21	1:A:158:ALA:HB1	1.97	0.47
1:C:552:GLY:N	1:C:607:THR:HG21	2.29	0.47
1:A:18:ILE:HD13	1:A:189:GLN:HB3	1.96	0.47
1:A:577:GLN:OE1	1:B:53:ASP:HB2	2.15	0.47
1:C:612:THR:HG21	1:C:718:PHE:CZ	2.49	0.47
1:A:808:LYS:NZ	1:A:814:MET:HB3	2.30	0.46
1:A:55:HIS:CE1	1:A:79:ILE:HG12	2.50	0.46
1:C:464:PRO:HG2	1:C:611:VAL:HG12	1.97	0.46
1:A:585:ARG:O	1:A:587:PHE:HA	2.15	0.46
1:B:118:GLY:HA2	1:B:200:LEU:O	2.16	0.46
1:A:28:ALA:O	1:A:32:PHE:HB2	2.15	0.46
1:A:225:ASN:HB3	1:A:346:GLU:HB3	1.96	0.46
1:A:606:GLY:HA2	1:A:660:VAL:HG23	1.98	0.46
1:B:586:THR:HA	1:B:587:PHE:HA	1.62	0.46
1:B:808:LYS:NZ	1:B:814:MET:HB3	2.30	0.46
1:A:244:ILE:HD11	1:A:275:MET:SD	2.55	0.46
1:A:244:ILE:HB	1:B:761:LYS:HD2	1.98	0.46
1:A:645:VAL:O	1:A:704:ARG:HD3	2.15	0.46
1:B:105:GLY:HA3	1:B:453:ASP:HB2	1.97	0.46
1:B:582:ILE:HB	1:B:722:PHE:CZ	2.51	0.46
1:C:537:LEU:HD21	1:D:537:LEU:HD21	1.96	0.46
1:D:552:GLY:N	1:D:607:THR:HG21	2.31	0.46
1:A:231:ASP:HA	1:A:264:ASP:HB2	1.98	0.46
1:A:842:CYS:C	1:A:844:THR:HB	2.36	0.46
1:A:680:LEU:HB2	1:A:717:ALA:HB2	1.98	0.46
1:B:296:ILE:CD1	1:B:342:PRO:HB3	2.46	0.46
1:C:725:ILE:HG12	1:C:846:ASN:HD22	1.79	0.46
1:C:730:ALA:HB2	1:C:745:ASN:HB3	1.97	0.46
1:A:424:LEU:HD12	1:A:425:THR:CG2	2.46	0.46
1:A:613:PRO:HB3	1:A:631:TYR:HA	1.98	0.46
1:B:762:LYS:HG3	1:B:763:HIS:N	2.31	0.46
1:C:826:LEU:O	1:C:830:VAL:HB	2.15	0.46
1:D:662:THR:O	1:D:666:GLU:HG3	2.16	0.46
1:A:352:LEU:HD23	1:A:353:ALA:N	2.31	0.46
1:A:769:TYR:HD1	1:B:417:TYR:CZ	2.34	0.46
1:B:108:GLU:HG3	1:B:450:ARG:HG2	1.98	0.45
1:B:474:THR:HG22	1:B:641:ASP:OD2	2.16	0.45
1:B:715:GLY:HA2	1:B:718:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:GLY:HA2	1:B:718:PHE:CE2	2.50	0.45
1:D:567:HIS:HD2	1:D:590:PRO:HB2	1.80	0.45
1:D:494:MET:HE3	1:D:494:MET:HB3	1.86	0.45
1:D:668:TYR:OH	1:D:780:ARG:HD2	2.17	0.45
1:A:417:TYR:CD2	1:B:769:TYR:HB3	2.52	0.45
1:A:758:LEU:HB2	1:A:848:LYS:HZ3	1.79	0.45
1:A:760:PRO:HB2	1:A:762:LYS:HG2	1.97	0.45
1:A:761:LYS:N	1:B:328:LYS:HZ2	2.15	0.45
1:B:564:PHE:HZ	1:B:572:PHE:CD1	2.34	0.45
1:A:581:ASP:HB3	1:A:841:GLN:CD	2.37	0.45
1:B:68:ARG:HG3	1:B:253:MET:SD	2.55	0.45
1:A:416:ILE:O	1:A:418:ASN:HA	2.17	0.45
1:A:763:HIS:O	1:A:849:GLN:HB3	2.17	0.45
1:B:386:ASP:HB3	1:B:389:VAL:HG12	1.97	0.45
1:B:416:ILE:C	1:B:418:ASN:HA	2.36	0.45
1:D:464:PRO:HG2	1:D:611:VAL:HG12	1.99	0.45
1:C:668:TYR:OH	1:C:780:ARG:HD2	2.17	0.45
1:D:494:MET:HE1	1:D:603:THR:HG21	1.98	0.45
1:A:575:LEU:HD11	1:A:589:TYR:OH	2.16	0.45
1:B:312:PRO:HG3	1:B:328:LYS:HA	1.98	0.45
1:A:118:GLY:HA2	1:A:200:LEU:O	2.17	0.45
1:A:458:MET:HE1	1:C:476:TYR:HB2	1.98	0.45
1:A:413:ILE:HG21	1:B:767:PRO:HA	1.99	0.44
1:A:669:VAL:HG11	1:A:778:TYR:CE1	2.51	0.44
1:A:527:SER:OG	1:A:620:LYS:HB2	2.17	0.44
1:A:332:ALA:O	1:A:353:ALA:HA	2.17	0.44
1:B:338:GLY:HA2	1:B:373:TYR:CE2	2.52	0.44
1:B:730:ALA:HB2	1:B:745:ASN:HB3	1.99	0.44
1:A:768:ARG:HH11	1:B:238:ARG:HD3	1.83	0.44
1:A:80:PHE:CZ	1:A:422:PRO:HG3	2.52	0.44
1:C:743:ARG:HA	1:C:746:ALA:HB3	1.98	0.44
1:A:454:ARG:HG3	1:B:420:PHE:HE1	1.83	0.44
1:B:130:LEU:HD21	1:B:158:ALA:HB1	1.99	0.44
1:B:400:CYS:HB2	1:B:436:VAL:HG13	1.99	0.44
1:C:740:PRO:HD2	1:C:743:ARG:HE	1.82	0.44
1:D:770:GLU:H	1:D:770:GLU:HG3	1.65	0.44
1:A:256:ALA:HB2	1:A:378:HIS:CD2	2.52	0.44
1:A:452:ALA:O	1:B:404:VAL:HG22	2.18	0.44
1:B:485:ARG:HB2	1:B:543:PRO:HA	2.00	0.44
1:A:760:PRO:HB3	1:B:279:LYS:HD2	2.00	0.44
1:D:725:ILE:HG23	1:D:846:ASN:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:757:ALA:HB2	1:D:778:TYR:HD2	1.83	0.44
1:B:381:VAL:HA	1:B:403:ILE:O	2.18	0.43
1:B:645:VAL:O	1:B:648:VAL:HG22	2.17	0.43
1:D:762:LYS:HE3	1:D:762:LYS:HB2	1.69	0.43
1:A:474:THR:HG22	1:A:641:ASP:OD2	2.18	0.43
1:A:485:ARG:HB2	1:A:543:PRO:HA	2.00	0.43
1:A:653:THR:HG21	1:A:704:ARG:NH2	2.33	0.43
1:B:550:GLY:HA2	1:B:603:THR:HB	2.00	0.43
1:B:598:PHE:HB3	1:B:635:PRO:HA	2.00	0.43
1:C:490:THR:HG23	1:C:549:LEU:HD22	2.00	0.43
1:C:763:HIS:O	1:C:765:LEU:HD23	2.17	0.43
1:A:104:THR:HG22	1:C:472:TYR:CD2	2.53	0.43
1:B:98:ILE:HD11	1:B:110:ALA:HB2	1.99	0.43
1:D:661:LEU:HB2	1:D:688:VAL:HG11	1.99	0.43
1:B:193:HIS:CE1	1:B:195:LYS:HG2	2.52	0.43
1:B:606:GLY:HA2	1:B:660:VAL:CG2	2.46	0.43
1:A:458:MET:HB2	1:A:458:MET:HE2	1.79	0.43
1:A:853:SER:O	1:A:856:LYS:HG2	2.19	0.43
1:D:826:LEU:O	1:D:830:VAL:HB	2.19	0.43
1:A:246:SER:HA	1:A:409:ALA:HB2	2.00	0.43
1:B:477:LEU:HB3	1:B:506:HIS:NE2	2.34	0.43
1:B:671:VAL:HG22	1:B:845:ALA:HB1	2.00	0.43
1:D:487:PHE:HB2	1:D:543:PRO:HG3	1.99	0.43
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.84	0.43
1:B:663:HIS:CE1	1:B:727:HIS:HE2	2.37	0.43
1:A:490:THR:O	1:A:520:ALA:HA	2.19	0.43
1:A:723:LEU:HD22	1:A:727:HIS:CD2	2.54	0.43
1:B:65:GLU:HG3	1:B:153:ARG:HB2	2.01	0.43
1:B:669:VAL:HG11	1:B:778:TYR:CE1	2.53	0.43
1:C:484:GLU:HB2	1:C:544:ASP:CG	2.39	0.43
1:C:726:ASN:HB2	1:C:752:VAL:HG11	2.00	0.43
1:D:650:ALA:HB1	1:D:651:HIS:ND1	2.34	0.43
1:A:386:ASP:HB3	1:A:389:VAL:HG12	1.99	0.43
1:A:671:VAL:HG21	1:B:413:ILE:HA	2.00	0.43
1:A:416:ILE:HG13	1:B:766:PHE:CZ	2.54	0.43
1:A:768:ARG:HH21	1:B:417:TYR:HB3	1.84	0.43
1:B:246:SER:HB2	1:B:407:PRO:HB2	2.00	0.43
1:B:458:MET:HB2	1:D:470:GLU:HB2	2.00	0.43
1:D:588:LYS:HA	1:D:588:LYS:HD3	1.65	0.43
1:D:723:LEU:HD22	1:D:727:HIS:CG	2.54	0.43
1:A:228:ALA:O	1:A:261:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:HB2	1:B:269:LYS:HE2	1.79	0.42
1:C:492:PRO:HB3	1:C:520:ALA:O	2.19	0.42
1:D:484:GLU:HB2	1:D:544:ASP:CG	2.40	0.42
1:A:11:VAL:O	1:A:15:GLN:HB2	2.19	0.42
1:A:47:MET:SD	1:A:166:ALA:HB2	2.59	0.42
1:B:572:PHE:O	1:B:576:LYS:HB3	2.19	0.42
1:A:612:THR:HG22	1:A:719:ALA:HB2	2.00	0.42
1:B:394:GLY:HA2	1:B:402:ILE:HD13	2.02	0.42
1:B:576:LYS:CG	1:B:577:GLN:HG3	2.48	0.42
1:B:631:TYR:OH	1:B:720:ASN:HA	2.19	0.42
1:C:486:VAL:O	1:C:516:TYR:HA	2.19	0.42
1:A:816:LEU:HB2	1:A:863:TYR:HA	2.01	0.42
1:A:842:CYS:HA	1:A:844:THR:OG1	2.19	0.42
1:B:47:MET:SD	1:B:166:ALA:HB2	2.59	0.42
1:B:352:LEU:HD23	1:B:353:ALA:N	2.34	0.42
1:C:487:PHE:HB2	1:C:543:PRO:HG3	2.01	0.42
1:D:743:ARG:O	1:D:747:ILE:HG12	2.19	0.42
1:A:576:LYS:HD2	1:A:626:TYR:CZ	2.54	0.42
1:B:593:GLY:HA2	1:B:596:ALA:O	2.19	0.42
1:C:737:PHE:HE1	1:C:821:VAL:HG13	1.84	0.42
1:D:764:ALA:HB2	1:D:849:GLN:N	2.35	0.42
1:A:212:TYR:CE2	1:A:429:GLY:HA2	2.54	0.42
1:A:393:PHE:CE2	1:A:397:MET:HG3	2.55	0.42
1:A:486:VAL:HG11	1:A:507:LEU:HD21	2.01	0.42
1:A:624:ILE:HG23	1:A:732:LYS:NZ	2.35	0.42
1:A:715:GLY:HA2	1:A:718:PHE:CD2	2.55	0.42
1:B:475:GLN:HA	1:B:506:HIS:CG	2.54	0.42
1:B:599:VAL:HG13	1:B:637:VAL:HG13	1.99	0.42
1:C:674:SER:O	1:C:678:ARG:HG3	2.20	0.42
1:A:420:PHE:CD2	1:A:421:ILE:HG12	2.53	0.42
1:C:483:VAL:O	1:C:484:GLU:HG2	2.20	0.42
1:B:379:SER:HA	1:B:401:ARG:O	2.20	0.42
1:C:754:ARG:HG3	1:C:800:VAL:HG21	2.02	0.42
1:D:743:ARG:HA	1:D:746:ALA:HB3	2.00	0.42
1:A:115:VAL:HG22	1:A:142:PRO:HG2	2.02	0.42
1:A:766:PHE:HD1	1:B:413:ILE:HG22	1.85	0.42
1:B:40:VAL:O	1:B:44:VAL:HG23	2.19	0.42
1:B:702:ASP:OD1	1:B:706:LYS:HD3	2.19	0.42
1:D:737:PHE:HE2	1:D:821:VAL:HG13	1.84	0.42
1:D:816:LEU:HD23	1:D:816:LEU:HA	1.89	0.42
1:B:650:ALA:HA	1:B:651:HIS:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:ALA:HB2	1:C:849:GLN:N	2.34	0.41
1:D:494:MET:CE	1:D:603:THR:HG21	2.50	0.41
1:D:749:MET:HB3	1:D:750:PRO:HD3	2.02	0.41
1:A:312:PRO:HG3	1:A:328:LYS:HA	2.01	0.41
1:A:417:TYR:CE2	1:B:769:TYR:HB3	2.55	0.41
1:A:475:GLN:HA	1:A:506:HIS:CG	2.54	0.41
1:A:733:ILE:HG12	1:A:816:LEU:HD21	2.03	0.41
1:C:650:ALA:HB1	1:C:651:HIS:ND1	2.35	0.41
1:C:661:LEU:HB2	1:C:688:VAL:HG11	2.01	0.41
1:D:618:THR:HG23	1:D:625:LYS:HD2	2.02	0.41
1:D:754:ARG:HG3	1:D:800:VAL:HG21	2.01	0.41
1:D:778:TYR:HB2	1:D:796:VAL:HG22	2.02	0.41
1:B:842:CYS:SG	1:B:842:CYS:O	2.79	0.41
1:A:420:PHE:HB2	1:B:454:ARG:N	2.36	0.41
1:A:593:GLY:HA2	1:A:596:ALA:O	2.20	0.41
1:A:598:PHE:HB3	1:A:635:PRO:HA	2.02	0.41
1:B:490:THR:O	1:B:520:ALA:HA	2.19	0.41
1:D:483:VAL:O	1:D:484:GLU:HG2	2.20	0.41
1:A:263:VAL:HG21	1:A:354:PHE:CZ	2.56	0.41
1:A:278:ASN:N	1:A:278:ASN:HD22	2.17	0.41
1:A:404:VAL:HG22	1:B:452:ALA:O	2.20	0.41
1:A:506:HIS:CE1	1:A:510:ARG:HE	2.39	0.41
1:A:658:MET:HB3	1:A:746:ALA:HB2	2.02	0.41
1:B:227:PRO:HB3	1:B:370:MET:HG2	2.02	0.41
1:A:567:HIS:ND1	1:A:590:PRO:HB2	2.35	0.41
1:B:400:CYS:HB3	1:B:437:SER:O	2.20	0.41
1:D:758:LEU:HD23	1:D:758:LEU:HA	1.92	0.41
1:A:413:ILE:HD13	1:A:417:TYR:CE2	2.56	0.41
1:B:288:PHE:HE1	1:B:332:ALA:HB1	1.85	0.41
1:B:853:SER:O	1:B:856:LYS:HG2	2.21	0.41
1:B:104:THR:HG22	1:D:472:TYR:CD2	2.56	0.41
1:B:332:ALA:O	1:B:353:ALA:HA	2.21	0.41
1:C:564:PHE:HE1	1:C:570:ALA:HB3	1.86	0.41
1:C:572:PHE:C	1:C:574:GLY:H	2.23	0.41
1:C:778:TYR:HB2	1:C:796:VAL:HG22	2.03	0.41
1:C:864:LYS:HD2	1:C:864:LYS:C	2.40	0.41
1:D:490:THR:HG23	1:D:549:LEU:HG	2.02	0.41
1:D:715:GLY:HA2	1:D:718:PHE:CE1	2.55	0.41
1:D:763:HIS:O	1:D:765:LEU:HD23	2.20	0.41
1:A:723:LEU:HD13	1:A:727:HIS:CG	2.55	0.41
1:B:781:ILE:O	1:B:785:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:O	1:A:162:VAL:HG22	2.21	0.40
1:A:842:CYS:SG	1:A:842:CYS:O	2.79	0.40
1:B:55:HIS:NE2	1:B:79:ILE:HG12	2.36	0.40
1:A:143:ILE:HG12	1:A:145:PHE:CZ	2.57	0.40
1:A:391:LYS:HE2	1:B:107:ILE:HD13	2.04	0.40
1:A:477:LEU:HG	1:A:480:MET:HG3	2.03	0.40
1:A:586:THR:HG21	1:B:83:GLU:HG3	2.02	0.40
1:B:393:PHE:CE2	1:B:397:MET:HG3	2.56	0.40
1:B:864:LYS:HB3	1:B:864:LYS:HE3	1.84	0.40
1:A:613:PRO:HB2	1:A:630:ASP:O	2.21	0.40
1:A:660:VAL:HG21	1:A:711:SER:HA	2.02	0.40
1:C:485:ARG:HG3	1:C:543:PRO:HA	2.02	0.40
1:C:758:LEU:HD12	1:C:758:LEU:HA	1.87	0.40
1:A:404:VAL:CG2	1:B:453:ASP:HA	2.52	0.40
1:B:54:GLN:HB3	1:B:58:LEU:HD13	2.04	0.40
1:B:338:GLY:HA2	1:B:373:TYR:CZ	2.57	0.40
1:B:428:CYS:SG	1:B:435:SER:HB2	2.61	0.40
1:C:733:ILE:HD12	1:C:859:TYR:CE1	2.57	0.40
1:D:486:VAL:O	1:D:516:TYR:HA	2.21	0.40
1:D:572:PHE:C	1:D:574:GLY:H	2.23	0.40
1:A:132:LYS:HA	1:A:135:ILE:HG12	2.03	0.40
1:A:587:PHE:CG	1:B:90:LYS:HD3	2.56	0.40
1:B:509:LYS:HB2	1:B:509:LYS:HE3	1.89	0.40
1:B:640:VAL:HG11	1:B:712:ALA:HB2	2.04	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	856/868 (99%)	794 (93%)	60 (7%)	2 (0%)	44 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	856/868 (99%)	797 (93%)	57 (7%)	2 (0%)	44	75
1	C	406/868 (47%)	379 (93%)	27 (7%)	0	100	100
1	D	406/868 (47%)	378 (93%)	28 (7%)	0	100	100
All	All	2524/3472 (73%)	2348 (93%)	172 (7%)	4 (0%)	45	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	GLU
1	B	470	GLU
1	B	844	THR
1	A	844	THR

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	703/708 (99%)	681 (97%)	22 (3%)	35	66
1	B	703/708 (99%)	671 (95%)	32 (5%)	23	56
1	C	340/708 (48%)	323 (95%)	17 (5%)	20	54
1	D	340/708 (48%)	322 (95%)	18 (5%)	19	52
All	All	2086/2832 (74%)	1997 (96%)	89 (4%)	27	57

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	23	ASP
1	A	32	PHE
1	A	75	CYS
1	A	80	PHE
1	A	140	ARG
1	A	174	HIS

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Mol	Chain	Res	Type
1	A	276	GLU
1	A	354	PHE
1	A	365	ASP
1	A	367	CYS
1	A	405	ASN
1	A	494	MET
1	A	506	HIS
1	A	521	ASP
1	A	589	TYR
1	A	711	SER
1	A	765	LEU
1	A	766	PHE
1	A	769	TYR
1	A	819	GLN
1	A	826	LEU
1	B	16	LYS
1	B	23	ASP
1	B	32	PHE
1	B	45	HIS
1	B	75	CYS
1	B	80	PHE
1	B	174	HIS
1	B	237	LYS
1	B	242	ASP
1	B	264	ASP
1	B	335	LYS
1	B	354	PHE
1	B	385	THR
1	B	451	ILE
1	B	478	GLN
1	B	494	MET
1	B	506	HIS
1	B	508	LYS
1	B	521	ASP
1	B	618	THR
1	B	675	ASP
1	B	704	ARG
1	B	711	SER
1	B	720	ASN
1	B	761	LYS
1	B	766	PHE
1	B	769	TYR

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Mol	Chain	Res	Type
1	B	773	ARG
1	B	813	ASP
1	B	827	ASP
1	B	846	ASN
1	B	851	LEU
1	C	466	LYS
1	C	480	MET
1	C	483	VAL
1	C	496	SER
1	C	525	ASP
1	C	576	LYS
1	C	585	ARG
1	C	589	TYR
1	C	626	TYR
1	C	704	ARG
1	C	711	SER
1	C	726	ASN
1	C	727	HIS
1	C	775	ASP
1	C	801	ASP
1	C	831	ASP
1	C	864	LYS
1	D	466	LYS
1	D	480	MET
1	D	483	VAL
1	D	496	SER
1	D	525	ASP
1	D	530	THR
1	D	576	LYS
1	D	585	ARG
1	D	589	TYR
1	D	626	TYR
1	D	704	ARG
1	D	711	SER
1	D	726	ASN
1	D	727	HIS
1	D	769	TYR
1	D	775	ASP
1	D	801	ASP
1	D	864	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	189	GLN
1	A	390	GLN
1	A	841	GLN
1	B	54	GLN
1	B	278	ASN
1	B	390	GLN
1	B	756	ASN
1	B	763	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	453:ASP	C	454:ARG	N	8.06
1	B	453:ASP	C	454:ARG	N	7.01

For Manuscript Review

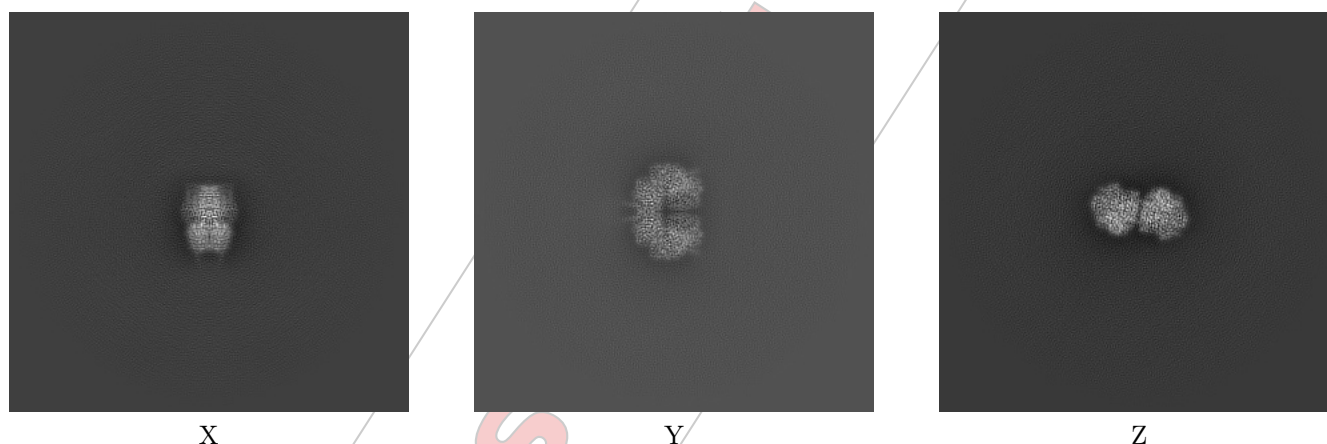
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49969. These allow visual inspection of the internal detail of the map and identification of artifacts.

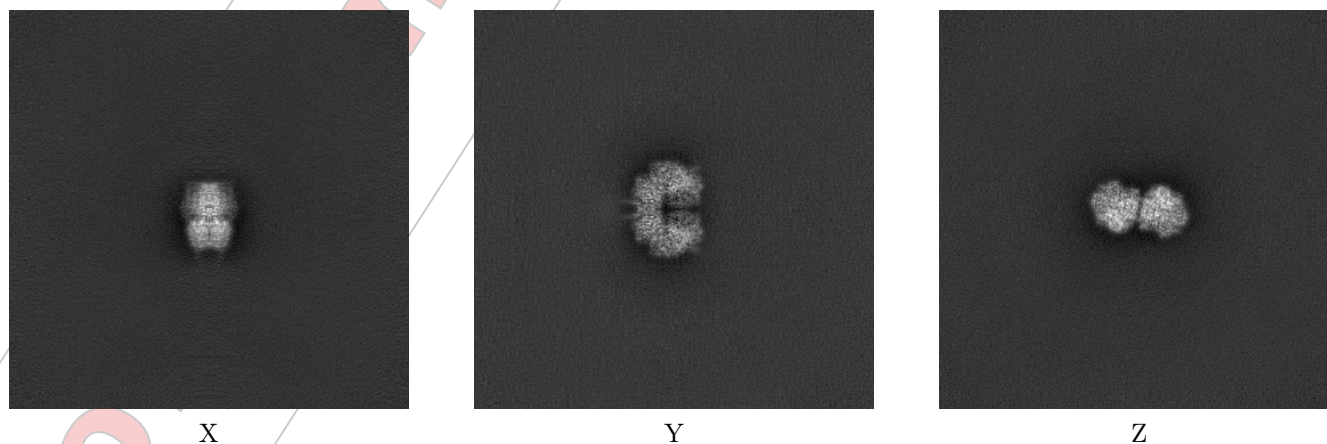
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



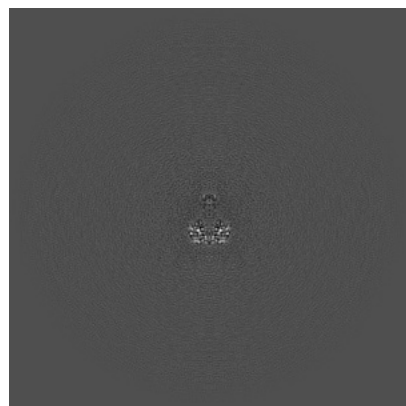
6.1.2 Raw map



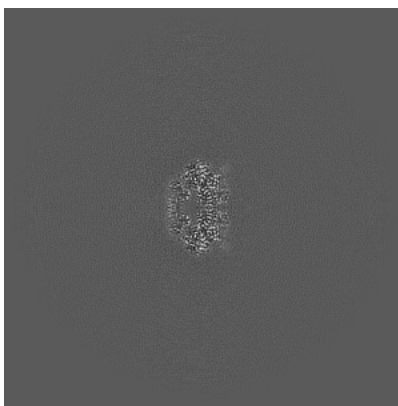
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

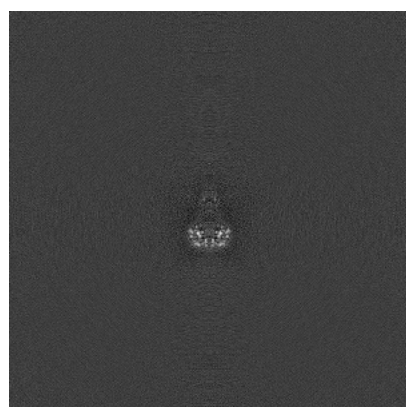


Y Index: 256

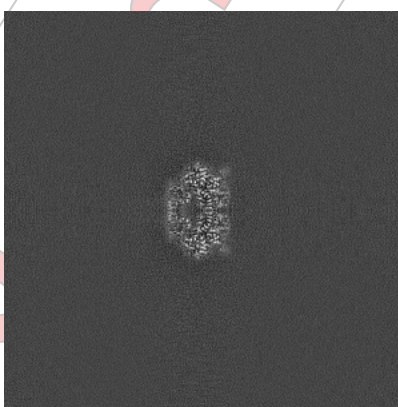


Z Index: 256

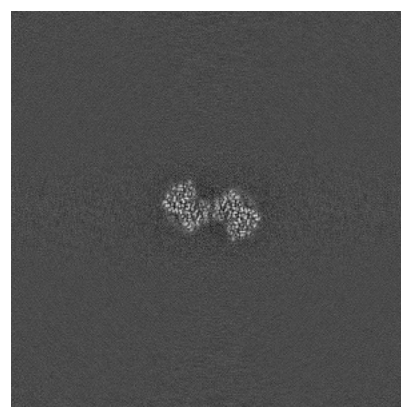
6.2.2 Raw map



X Index: 256



Y Index: 256

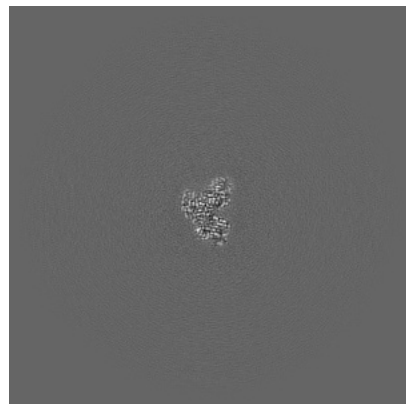


Z Index: 256

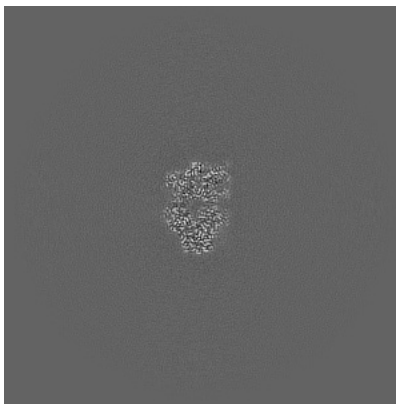
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

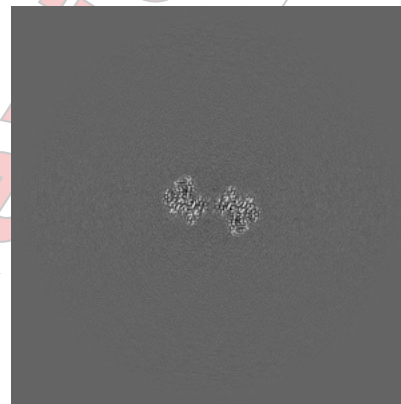
6.3.1 Primary map



X Index: 287

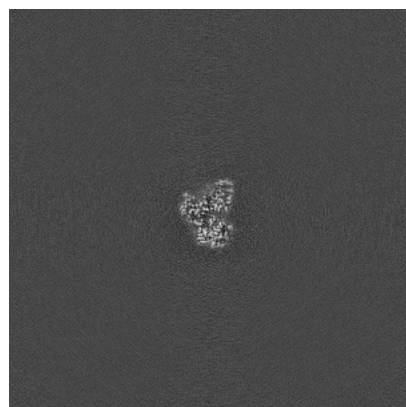


Y Index: 263

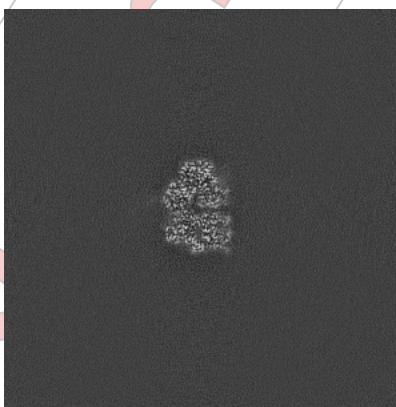


Z Index: 254

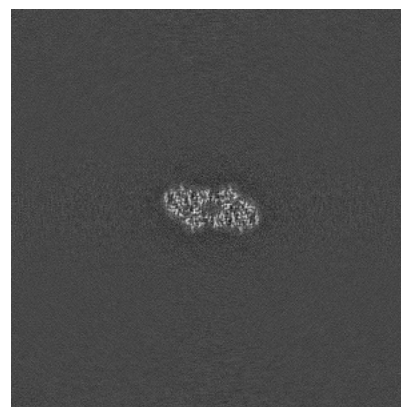
6.3.2 Raw map



X Index: 285



Y Index: 248

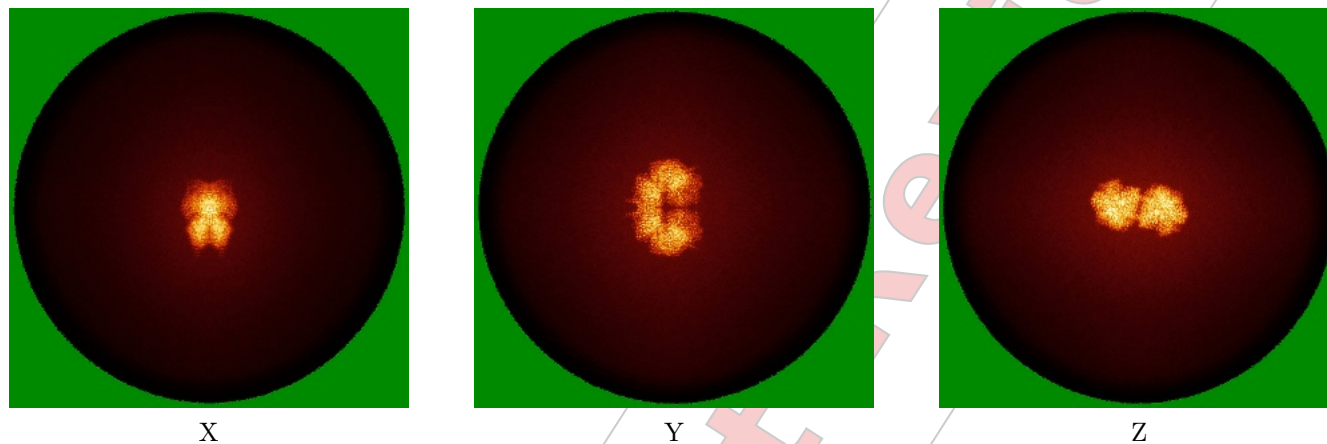


Z Index: 237

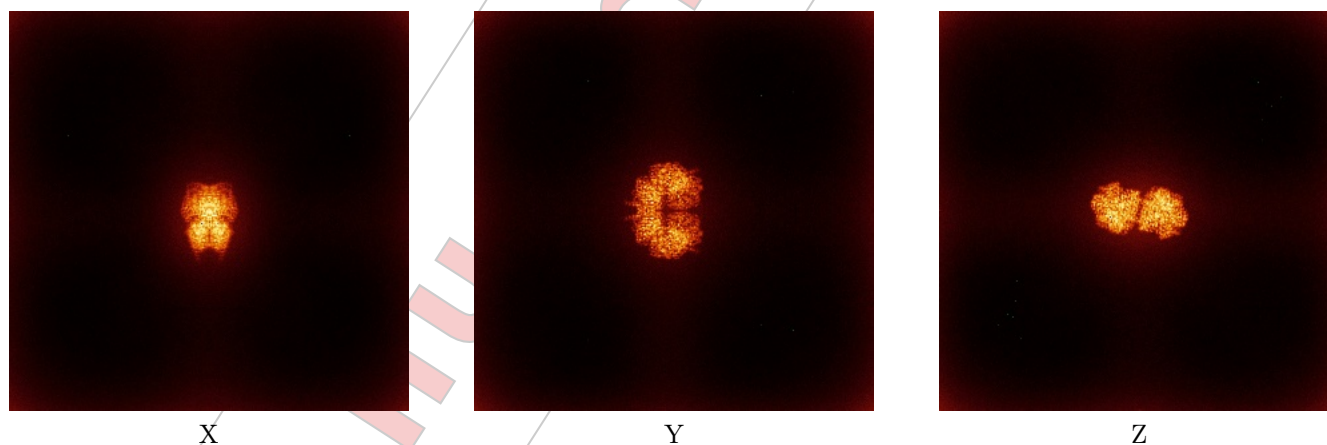
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

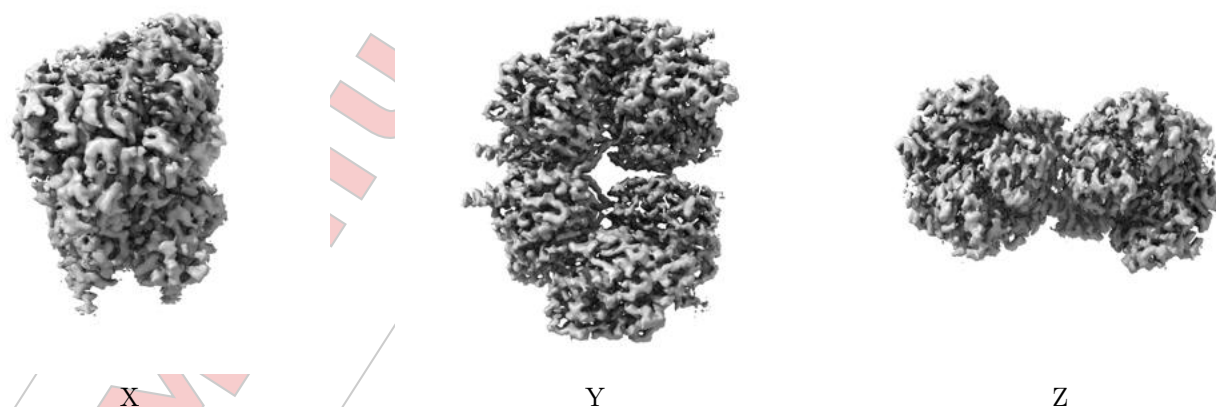
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



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

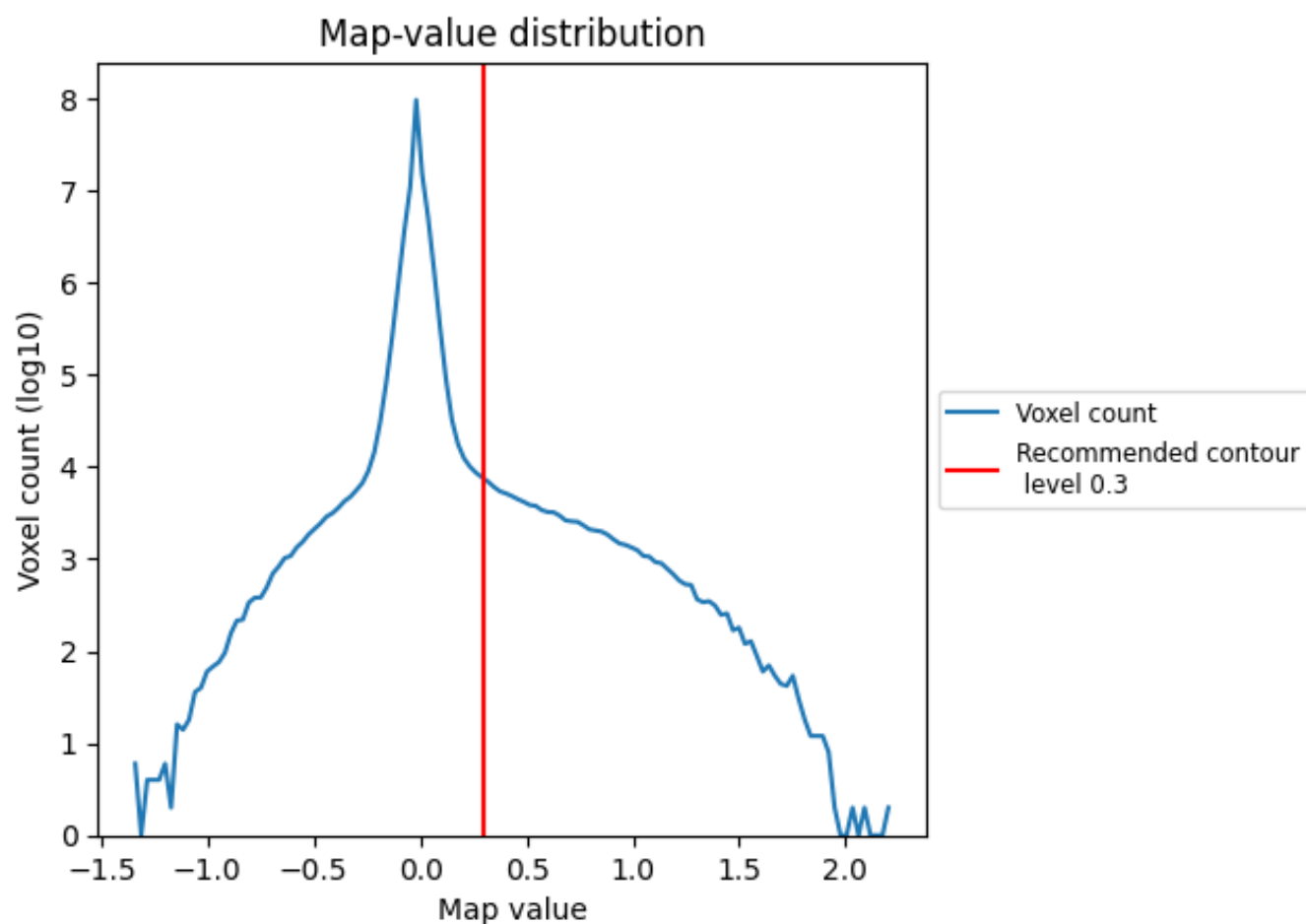
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

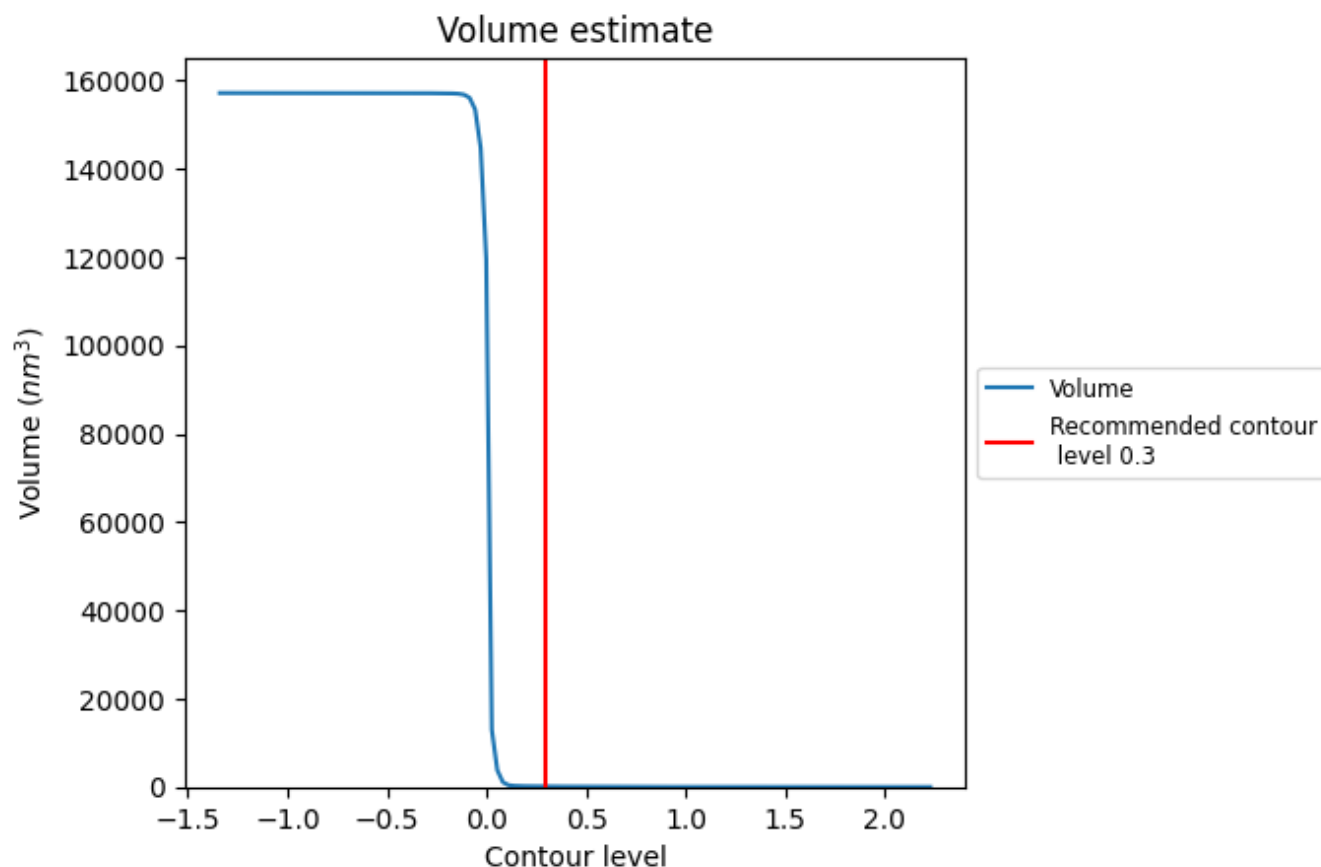
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

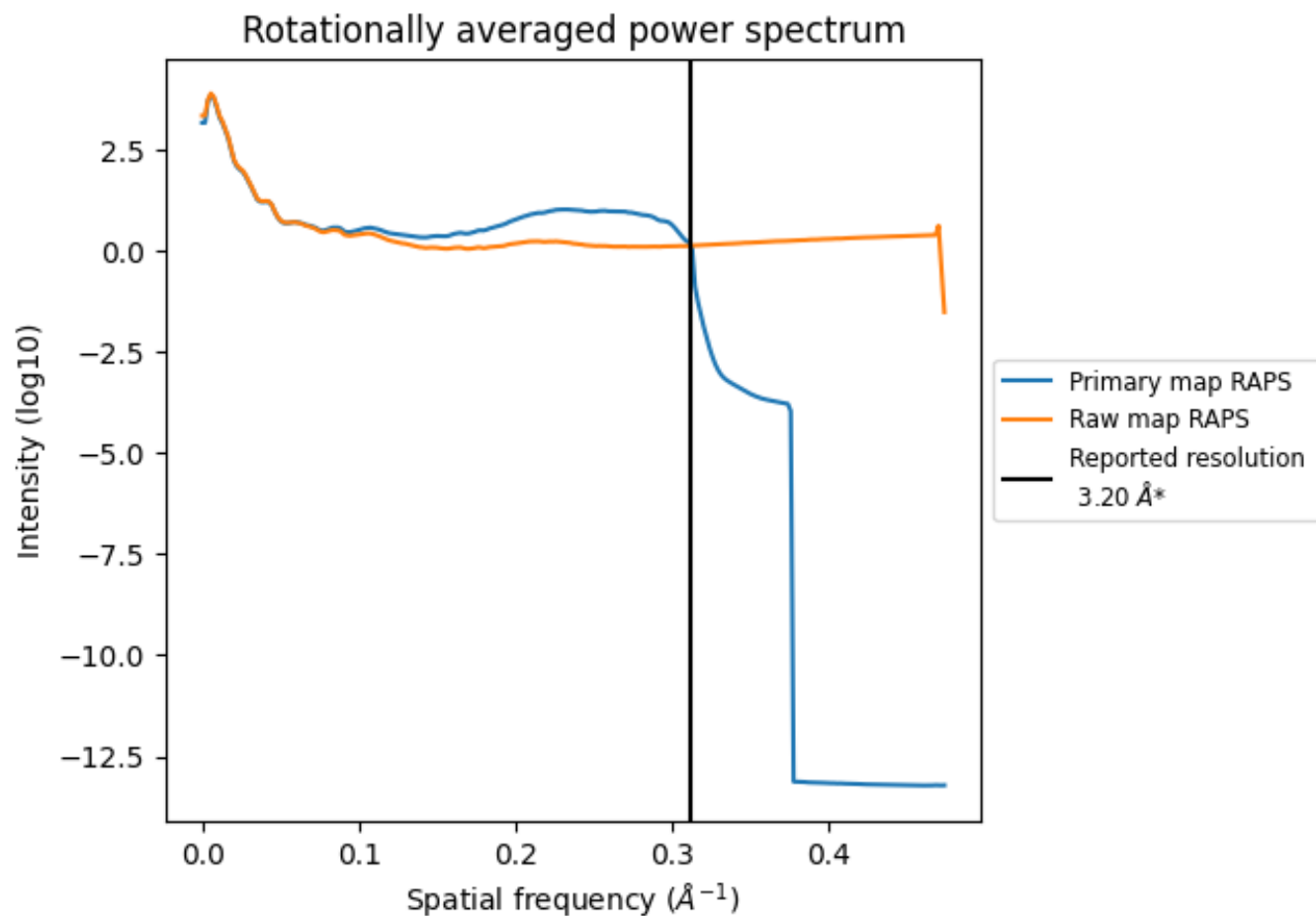
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm^3 ; this corresponds to an approximate mass of 103 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 ⓘ

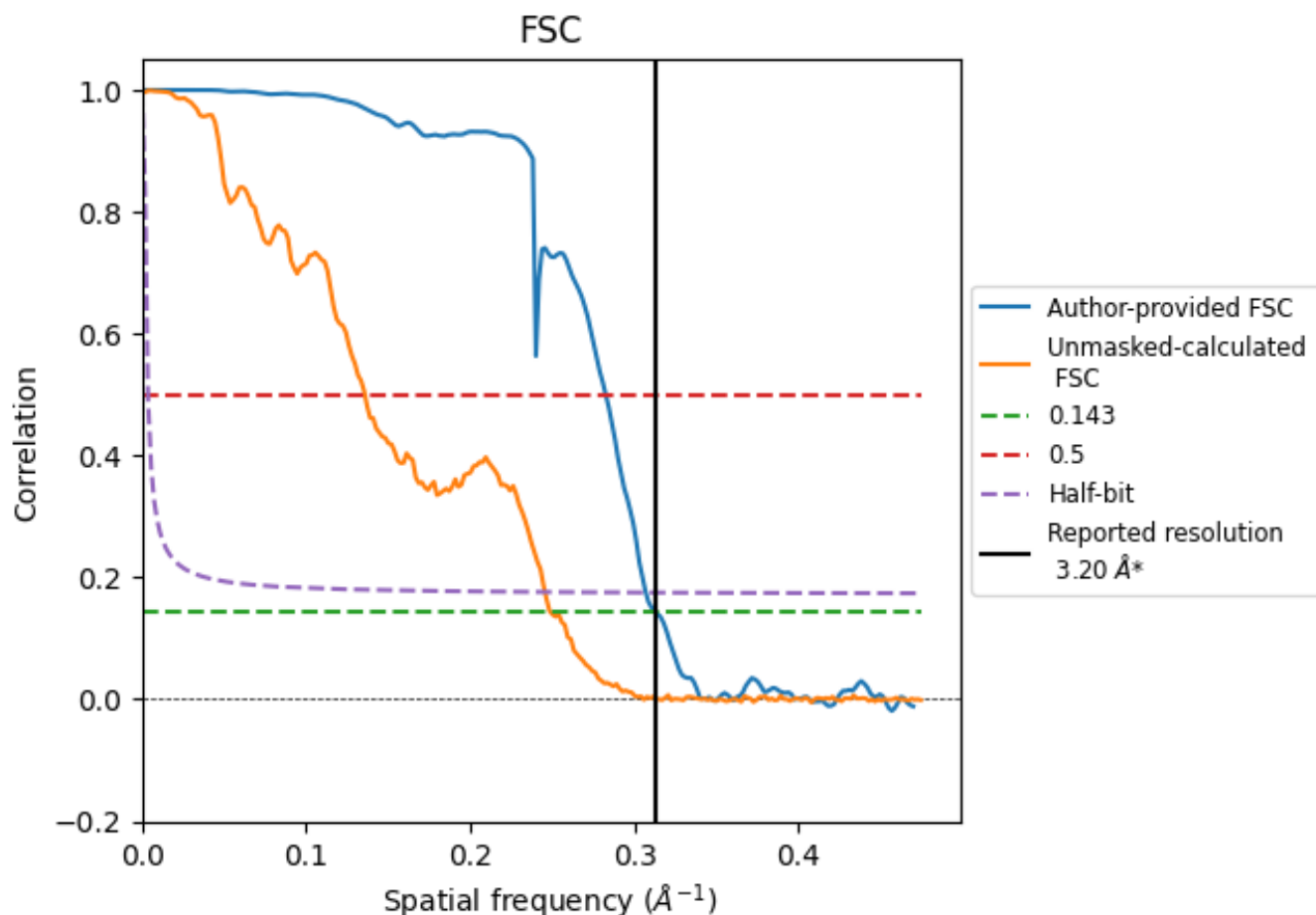


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

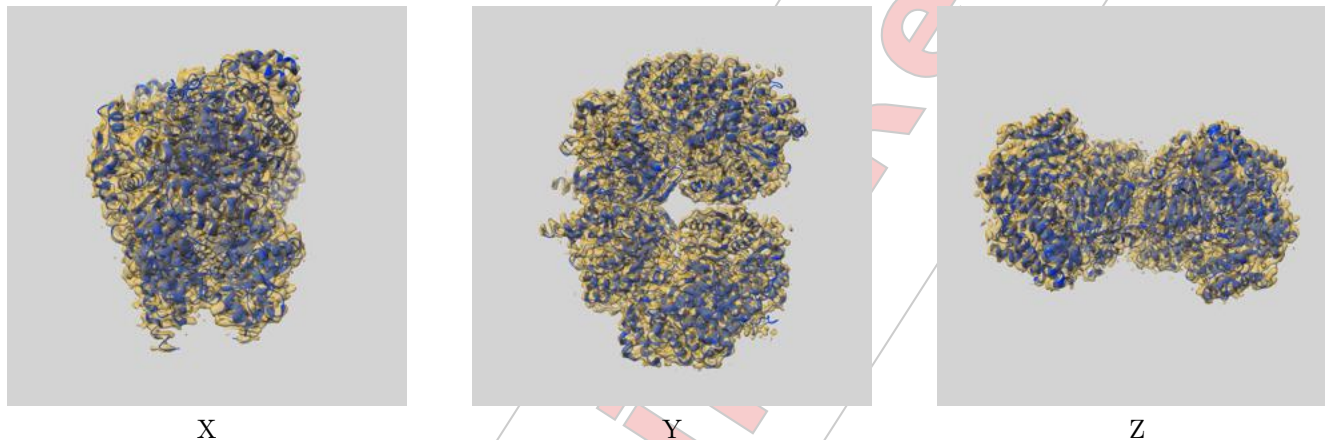
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.54	3.26
Unmasked-calculated*	4.02	7.37	4.07

*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 4.02 differs from the reported value 3.2 by more than 10 %

9 Map-model fit ⓘ

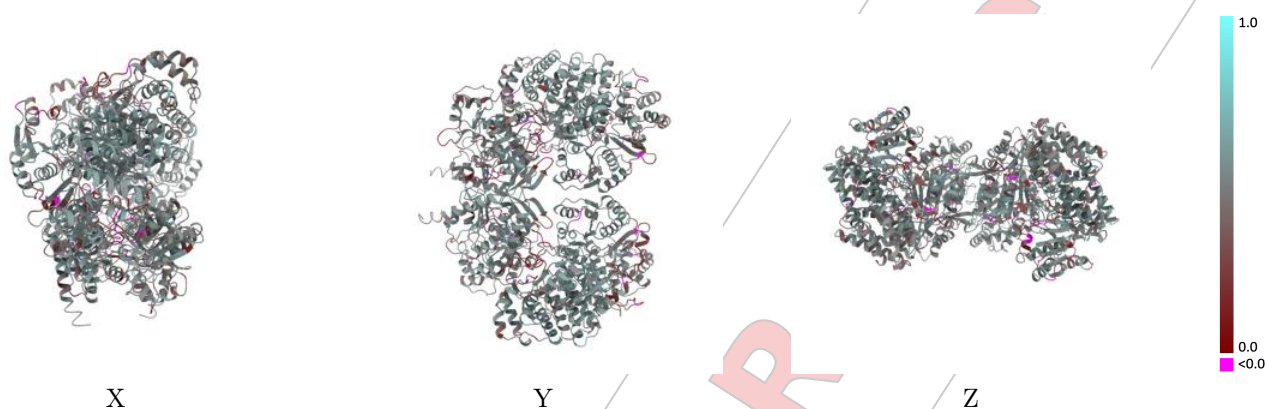
This section contains information regarding the fit between EMDB map EMD-49969 and PDB model 9O0C. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ



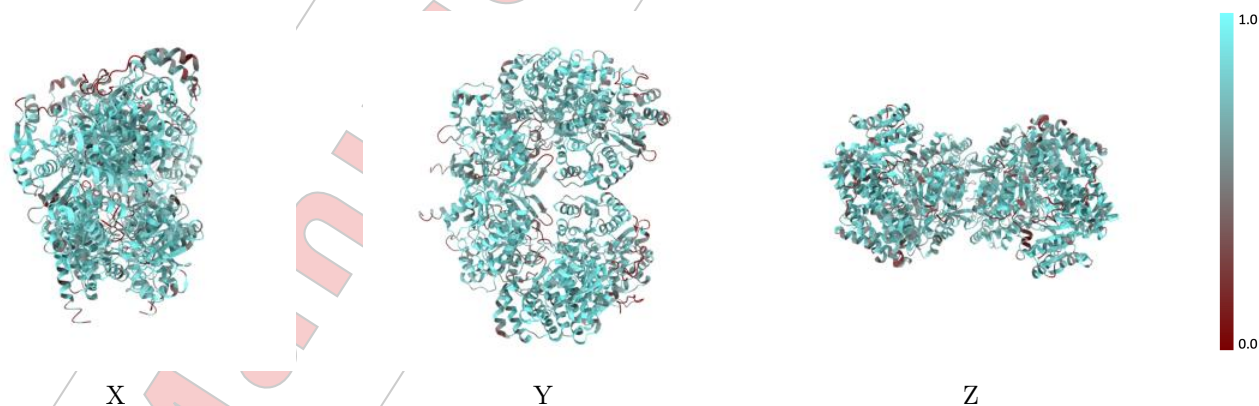
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



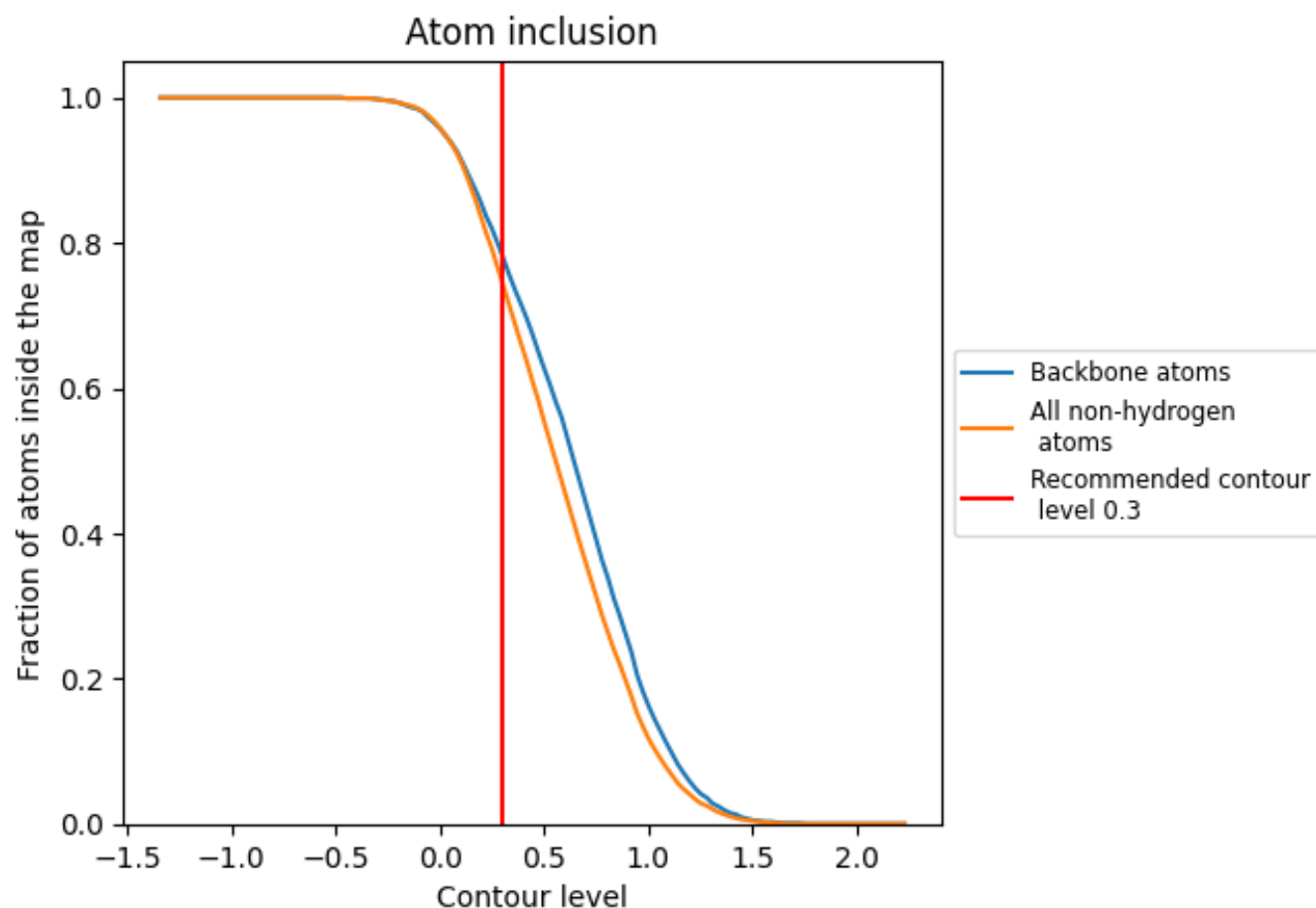
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.4730
A	 0.7580	 0.4710
B	 0.7590	 0.4660
C	 0.7170	 0.4810
D	 0.7160	 0.4810

