



Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 12:50 PM EDT

PDB ID : 11XU / pdb_000011xu
EMDB ID : EMD-76173
Title : In situ subtomogram average of the transition zone linker in human airway cilia (composite map)
Authors : Zhou, H.; Brown, A.
Deposited on : 2026-03-17
Resolution : 9.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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

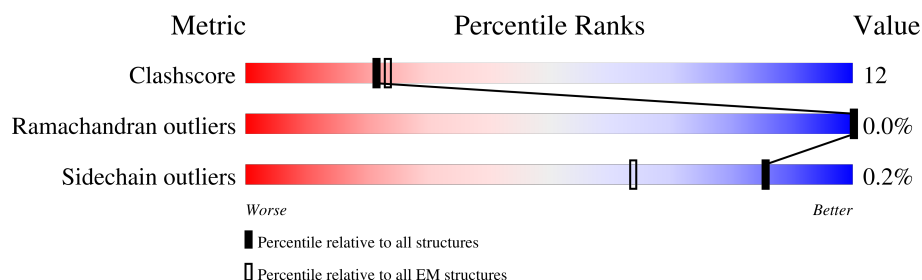
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.60 Å.

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



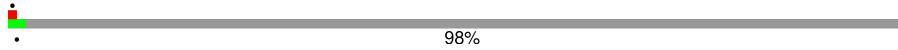
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A1	904	
1	B1	904	
2	C1	163	
2	D1	163	
3	E1	89	
3	F1	89	
4	G1	752	
4	H1	752	

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Mol	Chain	Length	Quality of chain
4	I1	752	 98%
4	J1	752	 9% 90%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17865 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 Epithelial cell-transforming sequence 2 oncogene-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	747	Total	C	N	O	S	0	0
			6108	3945	1029	1105	29		
1	B1	696	Total	C	N	O	S	0	0
			5697	3688	962	1024	23		

- Molecule 2 is a protein called S-phase kinase-associated protein 1.

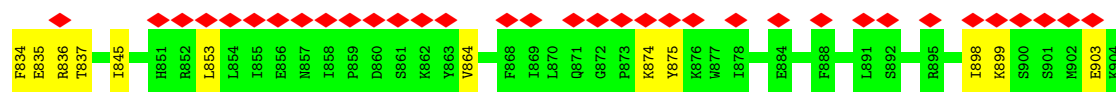
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	163	Total	C	N	O	S	0	0
			1308	820	211	270	7		
2	D1	163	Total	C	N	O	S	0	0
			1308	820	211	270	7		

- Molecule 3 is a protein called Dynein light chain 1, cytoplasmic.

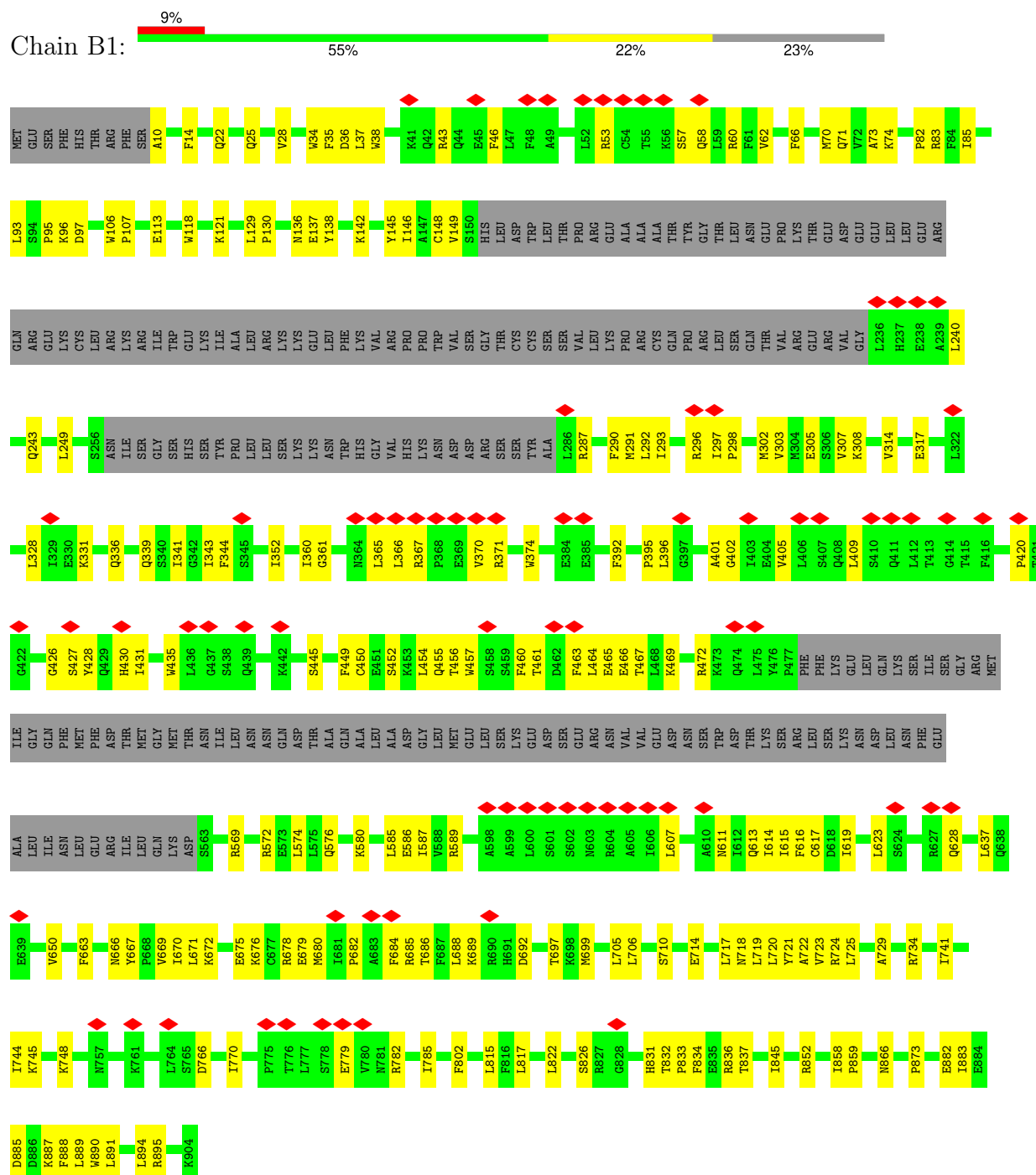
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E1	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
3	F1	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

- Molecule 4 is a protein called Double zinc ribbon and ankyrin repeat-containing protein 1.

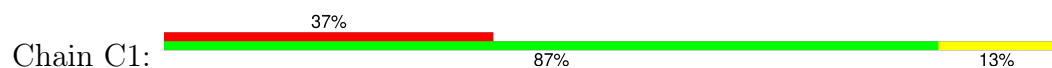
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G1	104	Total	C	N	O	S	0	0
			832	516	159	153	4		
4	H1	66	Total	C	N	O	S	0	0
			526	327	101	95	3		
4	I1	13	Total	C	N	O		0	0
			92	55	18	19			
4	J1	74	Total	C	N	O	S	0	0
			538	330	96	102	10		

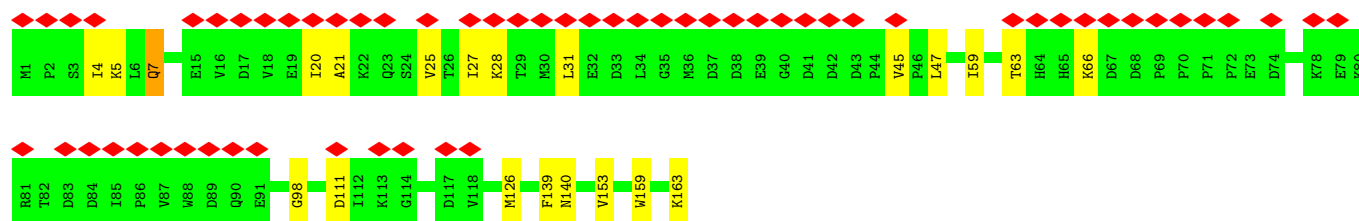


- Molecule 1: Epithelial cell-transforming sequence 2 oncogene-like

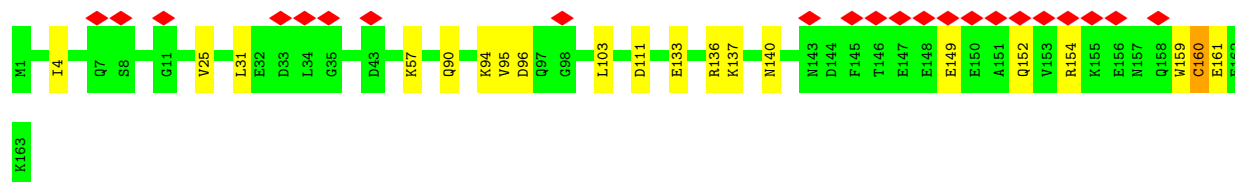
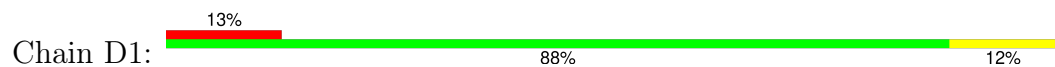


- Molecule 2: S-phase kinase-associated protein 1

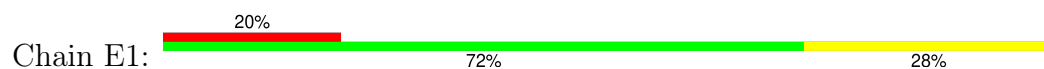




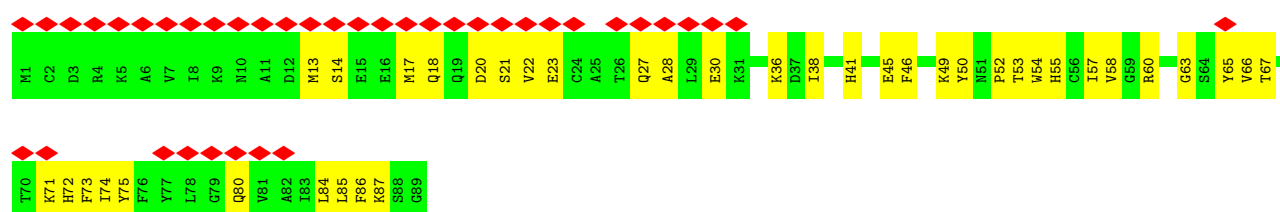
• Molecule 2: S-phase kinase-associated protein 1



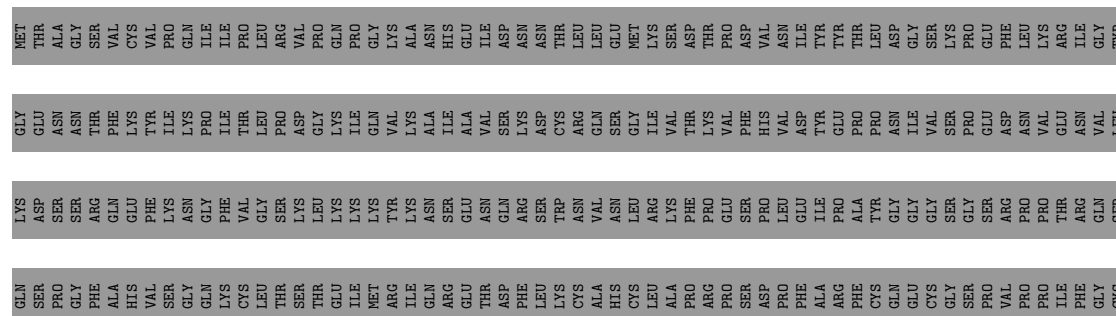
• Molecule 3: Dynein light chain 1, cytoplasmic



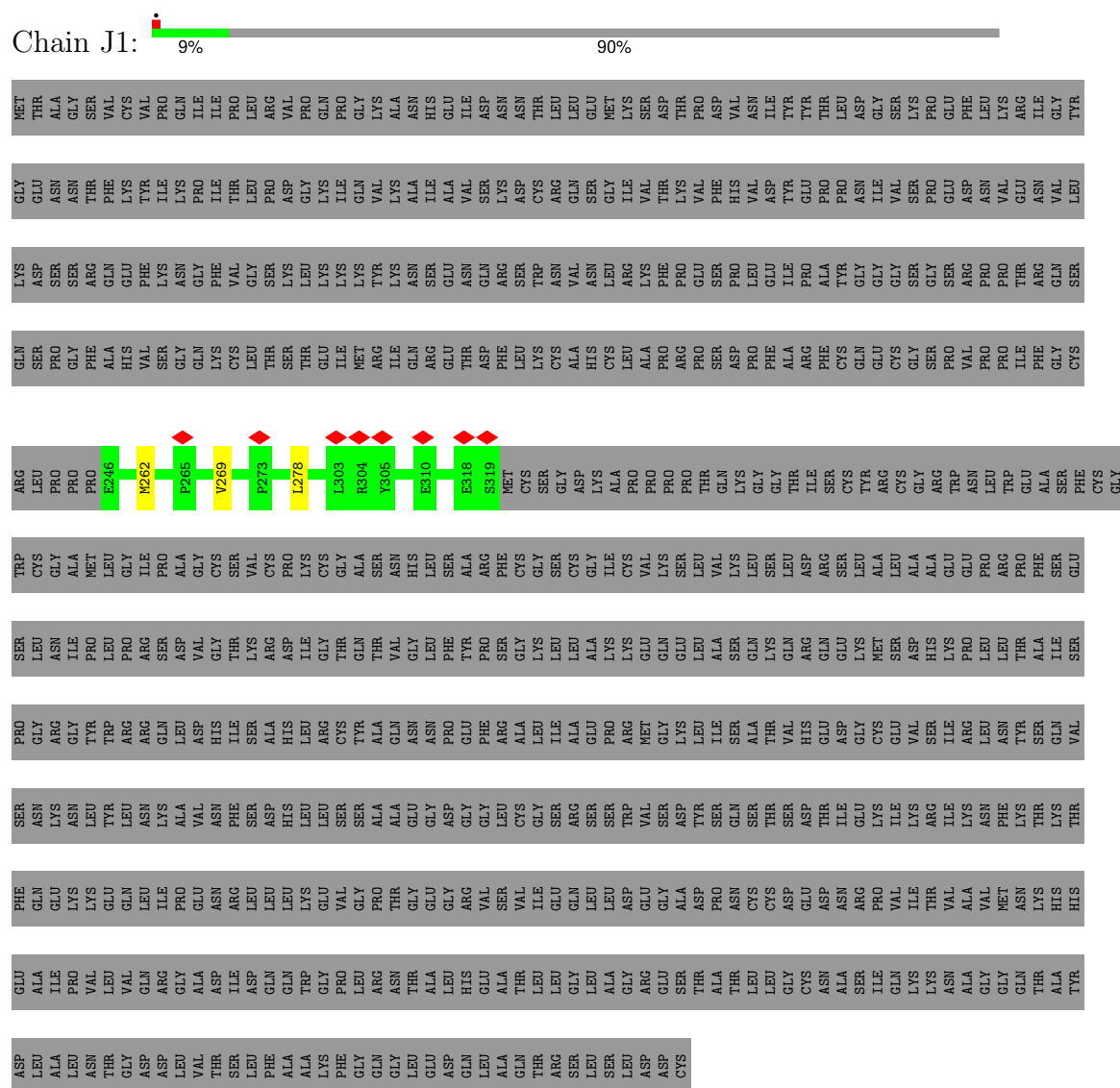
• Molecule 3: Dynein light chain 1, cytoplasmic



• Molecule 4: Double zinc ribbon and ankyrin repeat-containing protein 1



Chain J1: 9% 90%



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	12237	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 ($e^-/\text{\AA}^2$)	154.44	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0005	Depositor
Map size (Å)	450.216, 506.012, 359.788	wwPDB
Map dimensions	234, 263, 187	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.924, 1.924, 1.924	Depositor

5 Model quality

5.1 Standard geometry

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	A1	0.16	0/6254	0.41	5/8459 (0.1%)
1	B1	0.16	0/5836	0.38	0/7904
2	C1	0.10	0/1331	0.30	0/1801
2	D1	0.27	0/1331	0.47	2/1801 (0.1%)
3	E1	0.47	0/744	0.74	0/997
3	F1	0.17	0/744	0.46	0/997
4	G1	0.16	0/846	0.43	0/1133
4	H1	0.14	0/537	0.34	0/726
4	I1	0.17	0/91	0.39	0/121
4	J1	0.19	0/546	0.50	0/741
All	All	0.19	0/18260	0.42	7/24680 (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	A1	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D1	160	CYS	N-CA-C	6.17	117.84	110.44
1	A1	291	MET	CB-CG-SD	-5.95	94.86	112.70
1	A1	136	ASN	CA-CB-CG	5.92	118.52	112.60
1	A1	350	ARG	CB-CG-CD	5.75	124.53	111.30
2	D1	161	GLU	CA-CB-CG	-5.59	102.91	114.10
1	A1	136	ASN	CB-CA-C	-5.50	99.48	110.42
1	A1	136	ASN	N-CA-CB	5.43	119.66	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	136	ASN	Peptide
1	A1	349	SER	Peptide

5.2 Too-close contacts

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	A1	6108	0	6106	183	0
1	B1	5697	0	5713	194	0
2	C1	1308	0	1280	17	0
2	D1	1308	0	1280	14	0
3	E1	728	0	714	23	0
3	F1	728	0	714	30	0
4	G1	832	0	831	36	0
4	H1	526	0	518	24	0
4	I1	92	0	96	1	0
4	J1	538	0	542	3	0
All	All	17865	0	17794	417	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 (417) 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:A1:707:LEU:HD22	1:B1:836:ARG:HB2	1.47	0.97
2:D1:136:ARG:HH22	2:D1:154:ARG:HH22	1.21	0.88
1:A1:478:PHE:HB3	1:B1:467:THR:HG23	1.56	0.87
4:G1:529:LEU:HD11	4:H1:491:LEU:HD13	1.57	0.87
1:B1:678:ARG:HD3	1:B1:688:LEU:HD12	1.56	0.85
3:F1:80:GLN:HG3	4:G1:443:GLY:HA3	1.59	0.84
1:A1:471:VAL:O	1:A1:475:LEU:HB3	1.79	0.81
1:A1:794:HIS:HB2	1:A1:810:ILE:HD11	1.64	0.80
1:B1:298:PRO:HB2	1:B1:464:LEU:HD13	1.62	0.79
1:A1:350:ARG:HG3	1:B1:721:TYR:CD1	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:427:SER:HB3	1:B1:466:GLU:HG3	1.65	0.78
1:A1:808:GLU:HG2	1:B1:682:PRO:HG2	1.66	0.77
4:G1:533:GLN:HE22	4:H1:525:VAL:HB	1.52	0.74
1:A1:365:LEU:HD11	1:A1:409:LEU:HD21	1.71	0.73
1:A1:698:LYS:O	1:A1:699:MET:HG2	1.88	0.73
1:B1:589:ARG:HH11	1:B1:623:LEU:HD21	1.55	0.72
2:C1:20:ILE:HD13	2:C1:63:THR:HG22	1.72	0.72
3:E1:21:SER:HA	3:E1:46:PHE:HZ	1.53	0.72
1:A1:137:GLU:HB2	1:B1:136:ASN:HB3	1.72	0.71
1:A1:59:LEU:HB3	1:B1:70:MET:HE2	1.71	0.71
1:A1:352:ILE:HD11	1:A1:396:LEU:HD11	1.72	0.71
1:A1:764:LEU:HD23	1:A1:768:GLN:HE22	1.56	0.70
1:B1:360:ILE:HD13	1:B1:374:TRP:HH2	1.57	0.70
1:B1:352:ILE:HD11	1:B1:396:LEU:HD21	1.72	0.70
1:B1:365:LEU:HD11	1:B1:405:VAL:HG13	1.73	0.70
1:A1:326:LEU:HD11	1:A1:373:PHE:HA	1.74	0.69
1:B1:574:LEU:HD22	1:B1:719:LEU:HD22	1.73	0.69
1:A1:318:HIS:HB3	1:A1:356:GLN:HG3	1.74	0.69
1:B1:428:TYR:CD2	1:B1:461:THR:HB	2.27	0.69
1:A1:130:PRO:HA	1:A1:690:ARG:HE	1.57	0.68
1:B1:66:PHE:CD1	1:B1:70:MET:HE3	2.28	0.68
1:B1:586:GLU:HG2	1:B1:589:ARG:HH12	1.59	0.68
4:G1:487:ILE:HG12	4:H1:531:TYR:HE2	1.58	0.68
1:B1:882:GLU:HG2	1:B1:883:ILE:HG13	1.77	0.67
3:F1:45:GLU:O	3:F1:49:LYS:HG2	1.95	0.67
1:A1:713:PHE:HA	1:A1:716:TYR:HD2	1.59	0.66
1:A1:302:MET:HE2	1:A1:457:TRP:CG	2.31	0.66
1:A1:471:VAL:O	1:A1:475:LEU:CB	2.45	0.65
1:A1:712:ARG:HG3	1:A1:716:TYR:CE2	2.32	0.65
1:B1:95:PRO:HG3	1:B1:121:LYS:HD3	1.79	0.65
1:B1:93:LEU:HB3	1:B1:97:ASP:HB2	1.78	0.65
1:B1:569:ARG:HE	1:B1:572:ARG:HH21	1.44	0.65
2:C1:4:ILE:HD12	2:C1:31:LEU:HD21	1.79	0.64
1:A1:676:LYS:HD3	1:A1:680:MET:HE1	1.79	0.64
1:A1:807:TYR:HB2	1:A1:864:VAL:HG21	1.80	0.64
1:B1:572:ARG:HG2	1:B1:637:LEU:HD21	1.79	0.64
1:B1:717:LEU:HD11	1:B1:745:LYS:HA	1.80	0.63
3:E1:36:LYS:HE3	4:I1:434:GLN:HB2	1.79	0.63
3:F1:36:LYS:HB2	4:G1:434:GLN:HB2	1.80	0.63
4:J1:262:MET:HB2	4:J1:278:LEU:HD21	1.79	0.63
1:A1:577:SER:HB2	1:A1:712:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:302:MET:HE1	1:B1:457:TRP:HA	1.80	0.63
1:A1:794:HIS:HB3	1:A1:808:GLU:HB3	1.81	0.62
1:B1:82:PRO:HD2	1:B1:85:ILE:HD12	1.81	0.62
1:A1:27:ARG:O	1:A1:31:ILE:HG13	1.99	0.62
1:B1:287:ARG:HE	1:B1:339:GLN:HA	1.63	0.62
1:A1:618:ASP:HB3	1:A1:663:PHE:HB2	1.82	0.62
1:B1:146:ILE:HG12	2:D1:159:TRP:NE1	2.14	0.62
1:A1:699:MET:HE1	1:B1:456:THR:O	1.99	0.62
1:A1:82:PRO:HD2	1:A1:85:ILE:HD12	1.82	0.61
1:A1:423:ILE:HD13	1:B1:719:LEU:HD23	1.81	0.61
3:E1:66:VAL:HG12	3:F1:55:HIS:HB3	1.81	0.61
1:A1:462:ASP:HB3	1:A1:836:ARG:HH22	1.64	0.61
3:E1:55:HIS:HB3	3:F1:66:VAL:HG12	1.83	0.61
3:F1:73:PHE:HD1	3:F1:86:PHE:HB3	1.66	0.61
1:A1:136:ASN:CG	1:B1:137:GLU:C	2.68	0.61
1:A1:136:ASN:OD1	1:B1:138:TYR:HA	1.99	0.61
1:A1:7:ARG:HA	1:A1:23:LEU:HD11	1.83	0.60
1:A1:136:ASN:HB2	1:B1:136:ASN:C	2.26	0.60
1:A1:113:GLU:HA	1:A1:118:TRP:HE1	1.66	0.60
1:B1:883:ILE:HG22	1:B1:885:ASP:H	1.66	0.60
2:C1:25:VAL:HB	2:C1:111:ASP:HB3	1.84	0.59
1:B1:249:LEU:HD22	1:B1:895:ARG:HG2	1.84	0.59
1:B1:607:LEU:HD22	1:B1:611:ASN:HD22	1.67	0.59
1:A1:136:ASN:C	1:B1:138:TYR:HB2	2.25	0.59
1:A1:758:ILE:HD11	1:B1:834:PHE:HD2	1.67	0.59
1:B1:308:LYS:HE3	1:B1:450:CYS:HA	1.84	0.59
1:B1:366:LEU:HD13	1:B1:371:ARG:HH12	1.68	0.59
1:B1:303:VAL:HG22	1:B1:457:TRP:CD1	2.38	0.59
1:B1:96:LYS:HG3	2:D1:160:CYS:HB3	1.84	0.59
1:B1:779:GLU:HB2	1:B1:782:ARG:HB2	1.85	0.59
1:A1:462:ASP:HA	1:A1:836:ARG:HH12	1.68	0.59
4:G1:491:LEU:HD13	4:H1:484:LEU:HD22	1.85	0.59
1:A1:512:GLN:HB3	1:B1:699:MET:HG2	1.85	0.58
1:B1:717:LEU:HD12	1:B1:748:LYS:HD3	1.84	0.58
1:A1:424:ALA:HB3	1:B1:718:ASN:HD22	1.67	0.58
4:H1:486:HIS:O	4:H1:490:HIS:HD2	1.86	0.58
1:A1:10:ALA:HA	1:B1:34:TRP:HE1	1.68	0.58
1:A1:320:VAL:HG13	1:A1:324:SER:HB2	1.86	0.58
1:A1:325:LEU:O	1:A1:329:ILE:HG12	2.04	0.58
1:A1:136:ASN:HB2	1:B1:137:GLU:N	2.19	0.58
1:A1:699:MET:SD	1:B1:456:THR:HG23	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:426:GLY:O	1:B1:465:GLU:HB3	2.04	0.57
1:B1:460:PHE:O	1:B1:464:LEU:HG	2.04	0.57
1:A1:853:LEU:HD23	1:A1:898:ILE:HD11	1.85	0.57
1:B1:142:LYS:HE2	1:B1:146:ILE:HD11	1.85	0.57
1:B1:574:LEU:HD13	1:B1:719:LEU:HD13	1.86	0.57
1:B1:129:LEU:HD12	1:B1:130:PRO:HD2	1.87	0.57
1:B1:650:VAL:HG11	1:B1:720:LEU:HD11	1.86	0.57
1:A1:496:PHE:HA	1:A1:499:MET:HG2	1.87	0.57
1:A1:593:VAL:HG11	1:A1:620:LEU:HD11	1.86	0.57
1:A1:810:ILE:HG22	1:A1:811:HIS:ND1	2.20	0.57
2:D1:4:ILE:HD12	2:D1:31:LEU:HD21	1.86	0.57
1:B1:74:LYS:HG3	2:D1:140:ASN:HB2	1.86	0.56
1:B1:291:MET:SD	1:B1:293:ILE:HG13	2.45	0.56
4:G1:459:ARG:HA	4:G1:462:LYS:HD2	1.88	0.56
1:A1:34:TRP:HE1	1:B1:10:ALA:HA	1.71	0.56
1:A1:469:LYS:HE3	1:A1:837:THR:HG21	1.88	0.56
4:G1:450:GLU:HA	4:G1:453:LEU:HD12	1.88	0.56
1:A1:350:ARG:HG3	1:B1:721:TYR:CG	2.41	0.55
1:A1:571:VAL:HG12	1:A1:637:LEU:HD11	1.88	0.55
1:A1:290:PHE:HD2	1:A1:341:ILE:HG23	1.71	0.55
1:A1:493:GLN:NE2	1:B1:296:ARG:HA	2.22	0.55
1:B1:852:ARG:HG3	1:B1:873:PRO:HD3	1.88	0.55
4:G1:494:TYR:CG	4:H1:513:LEU:HD23	2.42	0.55
1:A1:899:LYS:O	1:A1:903:GLU:HG3	2.07	0.55
1:B1:885:ASP:O	1:B1:889:LEU:HG	2.06	0.55
1:B1:36:ASP:HA	1:B1:43:ARG:HH21	1.71	0.54
2:D1:25:VAL:HB	2:D1:111:ASP:HB3	1.89	0.54
1:A1:324:SER:HB3	1:B1:889:LEU:HD13	1.90	0.54
1:A1:478:PHE:HB3	1:B1:467:THR:CG2	2.34	0.54
3:E1:21:SER:HA	3:E1:46:PHE:CZ	2.40	0.54
3:E1:26:THR:O	3:E1:29:LEU:HG	2.08	0.54
1:A1:482:LEU:HD11	1:B1:464:LEU:HD21	1.90	0.54
1:A1:292:LEU:HD21	1:A1:325:LEU:HD11	1.90	0.54
2:C1:27:ILE:HD11	2:C1:47:LEU:HD21	1.90	0.54
1:A1:498:THR:O	1:A1:501:MET:HG2	2.08	0.54
1:A1:615:ILE:HD11	1:A1:673:THR:HB	1.89	0.54
1:A1:751:ILE:HA	1:A1:754:MET:HG2	1.90	0.54
1:A1:409:LEU:HB3	1:A1:417:PHE:HE2	1.72	0.53
2:C1:4:ILE:HD11	2:C1:45:VAL:HG21	1.90	0.53
3:F1:46:PHE:HE2	3:F1:85:LEU:HD13	1.72	0.53
1:A1:493:GLN:HE22	1:B1:296:ARG:HA	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:667:TYR:CE2	1:A1:671:LEU:HD11	2.44	0.53
3:F1:13:MET:HG2	3:F1:74:ILE:HD11	1.91	0.53
1:A1:763:HIS:O	1:A1:767:ILE:HG12	2.09	0.53
1:B1:614:ILE:HG13	4:G1:528:ARG:NH1	2.22	0.53
3:F1:13:MET:SD	3:F1:17:MET:HE3	2.48	0.53
1:A1:106:TRP:CE2	1:B1:83:ARG:HD3	2.43	0.53
1:A1:395:PRO:HA	1:A1:420:PRO:HD2	1.90	0.53
3:F1:14:SER:HB3	3:F1:71:LYS:HE2	1.91	0.53
1:A1:664:PHE:HB3	1:B1:834:PHE:HE1	1.74	0.52
1:A1:309:ALA:HB2	1:B1:317:GLU:HG3	1.89	0.52
2:C1:5:LYS:HZ3	2:C1:7:GLN:HB3	1.74	0.52
1:B1:614:ILE:HG13	4:G1:528:ARG:HH11	1.74	0.52
1:B1:721:TYR:O	1:B1:724:ARG:HG2	2.10	0.52
4:G1:447:ALA:O	4:G1:450:GLU:HG3	2.09	0.52
1:A1:800:ILE:HB	1:A1:805:ARG:NH1	2.24	0.52
1:B1:667:TYR:HE1	1:B1:706:LEU:HG	1.74	0.52
1:B1:25:GLN:HA	1:B1:28:VAL:HG12	1.90	0.52
1:A1:129:LEU:HD12	1:A1:130:PRO:HD2	1.92	0.51
1:A1:398:ALA:HA	1:B1:725:LEU:HD22	1.92	0.51
1:A1:585:LEU:HB2	1:A1:623:LEU:HD13	1.92	0.51
1:B1:679:GLU:HA	1:B1:685:ARG:NH2	2.25	0.51
1:B1:826:SER:HB3	1:B1:845:ILE:HD11	1.92	0.51
4:H1:513:LEU:HD13	4:H1:531:TYR:CE1	2.45	0.51
2:D1:133:GLU:HB3	2:D1:137:LYS:NZ	2.25	0.51
4:G1:533:GLN:NE2	4:H1:525:VAL:HB	2.22	0.51
1:A1:753:GLN:O	1:A1:756:GLN:HG3	2.10	0.51
1:A1:764:LEU:HD13	1:A1:783:TYR:HA	1.93	0.51
1:A1:834:PHE:CE1	1:B1:710:SER:HB2	2.45	0.51
1:B1:669:VAL:HA	1:B1:672:LYS:HE3	1.93	0.51
2:C1:163:LYS:HB3	4:J1:269:VAL:HG21	1.92	0.51
4:G1:483:GLN:HG3	4:H1:506:ALA:HA	1.93	0.51
1:A1:146:ILE:HG12	2:C1:159:TRP:CE2	2.45	0.51
1:A1:324:SER:HA	1:B1:889:LEU:HD22	1.92	0.51
1:A1:698:LYS:O	1:A1:700:LEU:HG	2.10	0.51
1:A1:475:LEU:HD23	1:A1:491:ILE:HG12	1.92	0.51
1:B1:461:THR:HG22	1:B1:464:LEU:HD12	1.92	0.51
1:B1:307:VAL:HG22	1:B1:449:PHE:HE1	1.77	0.50
1:A1:748:LYS:O	1:A1:751:ILE:HG22	2.11	0.50
1:B1:576:GLN:HG3	1:B1:580:LYS:HE3	1.93	0.50
1:B1:669:VAL:HA	1:B1:672:LYS:HG2	1.92	0.50
1:B1:719:LEU:O	1:B1:723:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F1:21:SER:HA	3:F1:46:PHE:HZ	1.77	0.50
1:A1:698:LYS:C	1:A1:699:MET:HG2	2.36	0.50
1:B1:817:LEU:HD22	1:B1:894:LEU:HD23	1.93	0.50
1:B1:290:PHE:HB3	1:B1:341:ILE:HG12	1.94	0.50
1:A1:32:SER:HB3	1:B1:53:ARG:NE	2.27	0.50
1:A1:289:HIS:HB2	1:A1:311:VAL:HG22	1.93	0.50
1:A1:103:GLN:HG2	2:C1:153:VAL:HG12	1.93	0.50
1:A1:575:LEU:HD22	1:A1:637:LEU:HD22	1.94	0.49
1:A1:134:THR:HG23	1:B1:136:ASN:O	2.13	0.49
1:B1:569:ARG:HE	1:B1:572:ARG:NH2	2.09	0.49
1:A1:347:GLY:HA2	1:A1:353:ASN:ND2	2.28	0.49
1:A1:826:SER:HB2	1:A1:845:ILE:HD11	1.94	0.49
1:A1:793:LEU:HB3	1:A1:807:TYR:HB3	1.94	0.49
1:A1:611:ASN:O	1:A1:615:ILE:HG12	2.12	0.49
1:A1:715:GLU:O	1:A1:719:LEU:HG	2.12	0.49
1:A1:390:VAL:HB	1:A1:417:PHE:CD1	2.48	0.49
1:B1:73:ALA:HB2	2:D1:96:ASP:HB2	1.94	0.49
1:B1:613:GLN:O	1:B1:617:CYS:HB2	2.12	0.49
1:B1:614:ILE:N	4:G1:528:ARG:HH12	2.11	0.49
1:B1:669:VAL:HG11	4:H1:501:PHE:HZ	1.78	0.49
3:E1:41:HIS:HA	3:E1:44:LYS:HE2	1.93	0.48
1:A1:650:VAL:HG11	1:A1:720:LEU:HD11	1.95	0.48
1:A1:805:ARG:CZ	1:A1:805:ARG:HA	2.42	0.48
1:B1:457:TRP:NE1	1:B1:461:THR:HG21	2.28	0.48
1:B1:666:ASN:O	1:B1:670:ILE:HD12	2.13	0.48
4:G1:453:LEU:HA	4:G1:456:GLN:OE1	2.14	0.48
1:A1:74:LYS:HB2	2:C1:140:ASN:HB2	1.94	0.48
1:A1:302:MET:HE2	1:A1:457:TRP:CD2	2.49	0.48
1:A1:679:GLU:HA	1:A1:685:ARG:NH2	2.29	0.48
1:B1:370:VAL:HG13	1:B1:374:TRP:CZ3	2.49	0.48
1:A1:613:GLN:NE2	1:A1:614:ILE:HG13	2.29	0.48
1:B1:586:GLU:HG2	1:B1:589:ARG:NH1	2.26	0.48
1:A1:615:ILE:HD12	1:A1:674:ILE:HG23	1.95	0.48
1:A1:832:THR:HB	1:A1:835:GLU:HB2	1.95	0.48
2:C1:21:ALA:HB1	2:C1:27:ILE:HG21	1.95	0.48
3:E1:43:LYS:HB3	3:F1:65:TYR:HD2	1.79	0.48
1:B1:396:LEU:HD12	1:B1:402:GLY:HA2	1.96	0.47
1:B1:431:ILE:HD12	1:B1:457:TRP:HH2	1.79	0.47
3:F1:50:TYR:HB2	3:F1:54:TRP:HZ2	1.78	0.47
1:B1:589:ARG:NH1	1:B1:623:LEU:HD21	2.28	0.47
3:E1:38:ILE:O	3:E1:42:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:671:LEU:HA	1:A1:674:ILE:HG12	1.96	0.47
4:H1:484:LEU:HA	4:H1:487:ILE:HG12	1.97	0.47
1:A1:314:VAL:HG21	1:A1:332:ALA:HB2	1.96	0.47
1:B1:430:HIS:CD2	1:B1:431:ILE:HG13	2.50	0.47
1:A1:106:TRP:CZ2	1:B1:83:ARG:HD3	2.50	0.47
1:A1:349:SER:O	1:A1:396:LEU:HA	2.14	0.47
4:G1:527:ILE:HD13	4:H1:505:ILE:HD13	1.97	0.47
1:B1:766:ASP:O	1:B1:770:ILE:HG12	2.15	0.47
3:F1:57:ILE:HB	3:F1:84:LEU:HB3	1.96	0.47
1:B1:697:THR:HB	1:B1:705:LEU:HD11	1.98	0.46
4:G1:506:ALA:HB1	4:H1:478:GLY:HA2	1.97	0.46
1:B1:113:GLU:HB2	1:B1:138:TYR:OH	2.15	0.46
3:F1:53:THR:N	3:F1:87:LYS:HZ2	2.12	0.46
1:B1:96:LYS:HA	2:D1:160:CYS:SG	2.55	0.46
1:A1:137:GLU:HB2	1:B1:136:ASN:CB	2.44	0.46
1:A1:292:LEU:HD11	1:A1:325:LEU:HD11	1.98	0.46
1:A1:663:PHE:CE1	1:A1:706:LEU:HD12	2.50	0.46
1:B1:287:ARG:HG3	1:B1:336:GLN:HE22	1.81	0.46
1:B1:374:TRP:CD1	1:B1:409:LEU:HD22	2.51	0.46
4:G1:490:HIS:CE1	4:H1:512:LYS:HA	2.51	0.46
1:B1:142:LYS:O	1:B1:146:ILE:HG13	2.15	0.46
1:B1:343:ILE:HD12	1:B1:392:PHE:CE2	2.51	0.46
4:H1:513:LEU:HD12	4:H1:530:ASN:O	2.15	0.46
1:B1:585:LEU:HB2	1:B1:623:LEU:HD13	1.98	0.46
1:B1:866:ASN:HA	1:B1:887:LYS:HD2	1.97	0.46
3:E1:53:THR:CG2	3:F1:67:THR:HB	2.46	0.46
3:E1:13:MET:HE1	3:E1:18:GLN:HB3	1.98	0.46
4:G1:449:LYS:HA	4:G1:452:GLU:CD	2.40	0.46
2:C1:59:ILE:O	2:C1:63:THR:HG23	2.15	0.46
1:A1:290:PHE:HB3	1:A1:341:ILE:HG12	1.98	0.45
1:B1:366:LEU:HD13	1:B1:371:ARG:NH1	2.31	0.45
1:A1:37:LEU:HD22	1:B1:14:PHE:HZ	1.80	0.45
1:A1:390:VAL:HB	1:A1:417:PHE:CE1	2.51	0.45
1:A1:317:GLU:HG2	1:A1:320:VAL:HG23	1.98	0.45
1:A1:463:PHE:HB2	1:A1:511:ALA:HB2	1.98	0.45
1:A1:563:SER:HB2	1:A1:726:HIS:O	2.16	0.45
1:A1:668:PRO:HA	1:B1:833:PRO:HG3	1.97	0.45
1:B1:367:ARG:O	1:B1:371:ARG:HG2	2.16	0.45
1:B1:724:ARG:HD2	1:B1:741:ILE:HD13	1.98	0.45
1:B1:802:PHE:HZ	1:B1:858:ILE:HG23	1.81	0.45
3:F1:28:ALA:HB2	3:F1:41:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:14:PHE:HZ	1:B1:37:LEU:HD22	1.81	0.45
3:E1:13:MET:CE	3:E1:18:GLN:HB3	2.47	0.45
1:A1:22:GLN:O	1:A1:25:GLN:HG3	2.16	0.45
1:A1:63:GLN:HB2	1:B1:70:MET:HE1	1.98	0.45
1:B1:297:ILE:HG21	1:B1:344:PHE:CE2	2.52	0.45
3:F1:20:ASP:O	3:F1:23:GLU:HG3	2.16	0.45
1:A1:573:GLU:O	1:A1:576:GLN:HG3	2.17	0.45
1:B1:328:LEU:HA	1:B1:331:LYS:HG2	1.98	0.45
3:E1:10:ASN:HD21	4:G1:431:ILE:HD11	1.81	0.45
1:A1:420:PRO:HG3	1:A1:435:TRP:CE2	2.51	0.45
3:E1:25:ALA:HA	3:E1:42:ILE:HD11	1.98	0.45
4:G1:487:ILE:HG13	4:H1:510:MET:HE1	1.99	0.45
1:A1:319:SER:HB2	1:B1:785:ILE:O	2.16	0.45
1:A1:400:GLU:HB3	1:B1:724:ARG:HH12	1.82	0.45
1:B1:717:LEU:HG	1:B1:744:ILE:HG22	1.98	0.45
3:E1:67:THR:HG22	4:G1:428:LYS:HG3	1.98	0.45
1:A1:113:GLU:HB2	1:A1:138:TYR:OH	2.17	0.45
1:A1:25:GLN:NE2	1:A1:26:GLU:HG3	2.32	0.45
1:A1:409:LEU:HB3	1:A1:417:PHE:CE2	2.52	0.45
4:G1:460:GLN:HA	4:G1:463:MET:HG2	1.99	0.45
1:A1:480:LYS:NZ	1:B1:837:THR:HA	2.32	0.44
1:B1:371:ARG:HA	1:B1:371:ARG:HD2	1.73	0.44
1:B1:463:PHE:HD1	1:B1:836:ARG:HH11	1.64	0.44
1:A1:681:ILE:HG22	1:A1:684:PHE:H	1.82	0.44
1:A1:467:THR:O	1:A1:471:VAL:HG23	2.18	0.44
1:A1:808:GLU:HG2	1:B1:682:PRO:CG	2.43	0.44
1:B1:815:LEU:HB3	1:B1:822:LEU:HD11	1.99	0.44
1:B1:22:GLN:O	1:B1:25:GLN:HG3	2.17	0.44
1:A1:292:LEU:HD22	1:A1:329:ILE:HD11	2.00	0.44
1:A1:794:HIS:H	1:A1:808:GLU:H	1.65	0.44
1:A1:423:ILE:HG21	1:B1:719:LEU:HD23	1.99	0.44
1:A1:671:LEU:HD13	1:B1:831:HIS:HB3	1.99	0.44
1:A1:758:ILE:HG23	1:B1:832:THR:HG21	2.00	0.44
3:E1:26:THR:O	3:E1:30:GLU:OE1	2.35	0.44
1:A1:354:LEU:HG	1:A1:355:LEU:HG	1.99	0.44
1:B1:614:ILE:HG12	4:G1:517:THR:HG21	2.00	0.44
1:B1:145:TYR:O	1:B1:149:VAL:HG22	2.18	0.44
1:B1:722:ALA:O	1:B1:725:LEU:HB3	2.17	0.44
3:F1:18:GLN:O	3:F1:22:VAL:HG13	2.17	0.44
1:B1:729:ALA:HA	1:B1:734:ARG:HD3	2.00	0.43
1:B1:802:PHE:CZ	1:B1:858:ILE:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:25:VAL:HA	2:C1:28:LYS:HG2	1.99	0.43
1:A1:424:ALA:H	1:B1:718:ASN:ND2	2.16	0.43
1:A1:574:LEU:CD1	1:A1:719:LEU:HB3	2.48	0.43
1:B1:365:LEU:O	1:B1:371:ARG:HD3	2.18	0.43
1:B1:401:ALA:O	1:B1:405:VAL:HG23	2.18	0.43
1:A1:831:HIS:HB2	1:B1:671:LEU:HD13	2.00	0.43
4:H1:479:TYR:O	4:H1:483:GLN:HG2	2.17	0.43
1:A1:28:VAL:HG22	1:B1:46:PHE:HD1	1.83	0.43
1:A1:302:MET:HG2	1:A1:496:PHE:CE2	2.53	0.43
1:A1:424:ALA:HB3	1:B1:718:ASN:ND2	2.31	0.43
1:B1:240:LEU:O	1:B1:243:GLN:HG3	2.18	0.43
4:G1:513:LEU:HD12	4:G1:530:ASN:O	2.18	0.43
1:A1:435:TRP:CG	1:A1:444:PRO:HD2	2.53	0.43
1:B1:688:LEU:HB3	1:B1:692:ASP:OD2	2.19	0.43
1:A1:136:ASN:O	1:B1:138:TYR:HB2	2.19	0.43
2:C1:126:MET:HE1	2:C1:139:PHE:CE1	2.53	0.43
1:A1:486:ILE:HG12	1:A1:489:ARG:HH12	1.84	0.42
1:A1:568:ALA:O	1:A1:572:ARG:HG3	2.18	0.42
1:B1:395:PRO:HD3	1:B1:430:HIS:NE2	2.34	0.42
1:A1:457:TRP:CE2	1:A1:461:THR:HG22	2.54	0.42
1:A1:462:ASP:CA	1:A1:836:ARG:HH12	2.32	0.42
1:A1:502:THR:HG22	1:A1:514:LEU:HD13	2.01	0.42
2:D1:57:LYS:HD3	2:D1:103:LEU:HD21	2.01	0.42
3:F1:52:PRO:HA	3:F1:53:THR:HA	1.79	0.42
1:A1:614:ILE:HG22	1:A1:615:ILE:HD13	2.01	0.42
3:E1:67:THR:HG23	4:G1:429:ARG:C	2.45	0.42
1:A1:43:ARG:HD2	1:B1:58:GLN:NE2	2.34	0.42
1:A1:632:ASN:C	1:A1:632:ASN:HD22	2.27	0.42
1:B1:361:GLY:O	1:B1:365:LEU:HG	2.18	0.42
1:B1:392:PHE:O	1:B1:420:PRO:HD3	2.19	0.42
1:B1:445:SER:HB2	1:B1:454:LEU:HD21	2.00	0.42
4:G1:494:TYR:CB	4:H1:513:LEU:HD23	2.49	0.42
1:A1:700:LEU:HD22	1:A1:704:GLU:CD	2.45	0.42
3:F1:55:HIS:HB2	3:F1:86:PHE:CE1	2.55	0.42
1:B1:35:PHE:HA	1:B1:38:TRP:CE3	2.55	0.42
1:B1:686:THR:HA	1:B1:689:LYS:HG2	2.01	0.42
1:A1:77:PHE:HB2	1:A1:81:LEU:HD12	2.02	0.42
1:B1:57:SER:O	1:B1:60:ARG:HG3	2.19	0.42
1:B1:307:VAL:HG22	1:B1:449:PHE:CE1	2.54	0.42
1:B1:724:ARG:HD2	1:B1:741:ILE:CD1	2.50	0.42
4:H1:512:LYS:H	4:H1:512:LYS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:452:SER:O	1:B1:455:GLN:HG3	2.20	0.42
1:B1:469:LYS:O	1:B1:472:ARG:HG2	2.20	0.42
1:A1:689:LYS:HA	1:A1:689:LYS:HD3	1.81	0.42
1:A1:303:VAL:O	1:A1:307:VAL:HG23	2.20	0.42
1:A1:698:LYS:HD3	1:B1:455:GLN:OE1	2.19	0.42
1:A1:830:SER:HA	1:B1:675:GLU:OE2	2.20	0.42
1:B1:106:TRP:HB3	1:B1:107:PRO:HD3	2.02	0.42
1:B1:888:PHE:HD2	1:B1:889:LEU:HD23	1.85	0.42
4:G1:484:LEU:HD11	4:H1:491:LEU:HG	2.02	0.42
4:G1:491:LEU:CD1	4:H1:484:LEU:HD22	2.49	0.42
4:G1:512:LYS:HA	4:G1:512:LYS:HD2	1.85	0.42
1:A1:134:THR:HG23	1:B1:136:ASN:C	2.45	0.41
1:B1:360:ILE:HD13	1:B1:374:TRP:CH2	2.45	0.41
1:B1:663:PHE:HE1	1:B1:706:LEU:HD11	1.84	0.41
3:E1:15:GLU:HA	3:E1:18:GLN:NE2	2.35	0.41
1:B1:607:LEU:HD11	1:B1:684:PHE:CE1	2.56	0.41
1:B1:676:LYS:O	1:B1:680:MET:HG2	2.20	0.41
1:A1:71:GLN:OE1	2:C1:98:GLY:HA3	2.19	0.41
1:A1:129:LEU:HD23	1:A1:133:PRO:HG3	2.02	0.41
1:B1:587:ILE:HG21	1:B1:697:THR:HA	2.02	0.41
3:E1:53:THR:HG23	3:F1:67:THR:HB	2.01	0.41
4:G1:487:ILE:HG12	4:H1:531:TYR:CE2	2.47	0.41
1:A1:95:PRO:HG3	1:A1:121:LYS:HD3	2.00	0.41
1:A1:93:LEU:HB3	1:A1:97:ASP:HB2	2.02	0.41
1:A1:290:PHE:CE2	1:A1:329:ILE:HD12	2.55	0.41
1:A1:398:ALA:O	1:B1:722:ALA:HA	2.20	0.41
1:B1:891:LEU:O	1:B1:895:ARG:HG3	2.20	0.41
1:A1:27:ARG:HA	1:A1:30:LEU:HG	2.02	0.41
2:C1:7:GLN:HE21	2:C1:7:GLN:HB2	1.73	0.41
4:G1:513:LEU:HD23	4:H1:494:TYR:CG	2.56	0.41
1:A1:424:ALA:HB2	1:A1:430:HIS:ND1	2.36	0.41
2:D1:90:GLN:O	2:D1:94:LYS:HG2	2.21	0.41
3:F1:60:ARG:HH21	3:F1:80:GLN:HE21	1.68	0.41
3:F1:71:LYS:O	3:F1:71:LYS:HG3	2.21	0.41
3:F1:73:PHE:CZ	3:F1:75:TYR:HB2	2.55	0.41
1:A1:326:LEU:HG	1:A1:373:PHE:CD2	2.55	0.41
1:A1:339:GLN:O	1:A1:388:GLY:HA2	2.20	0.41
1:A1:517:GLY:HA2	1:A1:520:GLU:HG2	2.03	0.41
1:B1:366:LEU:HA	1:B1:371:ARG:HH11	1.85	0.41
3:E1:10:ASN:ND2	4:G1:431:ILE:HD11	2.36	0.41
3:E1:35:GLU:HG3	3:F1:63:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E1:80:GLN:NE2	4:G1:438:LEU:HD22	2.36	0.41
3:F1:27:GLN:O	3:F1:30:GLU:HG3	2.21	0.41
1:A1:58:GLN:NE2	1:B1:43:ARG:HD2	2.36	0.41
1:A1:754:MET:SD	1:B1:834:PHE:CD1	3.14	0.41
1:B1:70:MET:HB3	1:B1:71:GLN:H	1.77	0.41
1:B1:113:GLU:HA	1:B1:118:TRP:HE1	1.85	0.41
1:B1:890:TRP:CZ2	1:B1:894:LEU:HD21	2.56	0.41
3:E1:9:LYS:HE3	3:E1:75:TYR:HD2	1.85	0.41
3:F1:38:ILE:HG22	3:F1:58:VAL:HG21	2.03	0.41
1:A1:349:SER:HB2	1:A1:395:PRO:O	2.20	0.41
1:A1:350:ARG:CG	1:B1:721:TYR:CD1	2.96	0.41
1:A1:571:VAL:HA	1:A1:574:LEU:HD13	2.01	0.41
1:A1:874:LYS:HG3	1:A1:875:TYR:CD2	2.56	0.41
1:B1:292:LEU:HD12	1:B1:314:VAL:HG13	2.03	0.41
2:D1:133:GLU:HB3	2:D1:137:LYS:HZ1	1.86	0.41
4:J1:278:LEU:HD23	4:J1:278:LEU:HA	1.81	0.41
1:A1:664:PHE:CB	1:B1:834:PHE:HE1	2.34	0.40
1:B1:883:ILE:HG22	1:B1:885:ASP:N	2.34	0.40
3:F1:13:MET:HE1	3:F1:72:HIS:HA	2.02	0.40
1:A1:297:ILE:HG21	1:A1:344:PHE:CE2	2.55	0.40
1:B1:370:VAL:O	1:B1:374:TRP:HE3	2.04	0.40
1:B1:616:PHE:HA	1:B1:619:ILE:HG22	2.04	0.40
3:F1:60:ARG:HE	4:G1:443:GLY:HA3	1.87	0.40
1:A1:464:LEU:O	1:A1:468:LEU:HG	2.20	0.40
1:B1:714:GLU:HG3	1:B1:748:LYS:HE2	2.04	0.40
2:D1:149:GLU:HA	2:D1:152:GLN:CD	2.45	0.40
4:H1:513:LEU:HD13	4:H1:531:TYR:HE1	1.87	0.40
1:A1:47:LEU:HD13	1:B1:62:VAL:HG21	2.02	0.40
1:A1:110:PHE:HE2	1:B1:106:TRP:CZ3	2.40	0.40
1:B1:302:MET:HA	1:B1:305:GLU:OE1	2.22	0.40
1:B1:370:VAL:HG13	1:B1:374:TRP:CE3	2.55	0.40
1:B1:420:PRO:HG3	1:B1:435:TRP:CZ2	2.57	0.40
1:B1:611:ASN:O	1:B1:615:ILE:HD12	2.22	0.40
1:B1:802:PHE:CE2	1:B1:859:PRO:HD2	2.56	0.40
2:C1:20:ILE:HD11	2:C1:66:LYS:HD3	2.03	0.40
1:A1:693:LYS:HA	1:A1:699:MET:C	2.47	0.40
1:A1:810:ILE:HG22	1:A1:811:HIS:CE1	2.57	0.40
2:D1:57:LYS:HE3	2:D1:95:VAL:HG11	2.04	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	A1	741/904 (82%)	721 (97%)	20 (3%)	0	100	100
1	B1	688/904 (76%)	671 (98%)	16 (2%)	1 (0%)	48	83
2	C1	161/163 (99%)	160 (99%)	1 (1%)	0	100	100
2	D1	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
3	E1	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
3	F1	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
4	G1	100/752 (13%)	99 (99%)	1 (1%)	0	100	100
4	H1	64/752 (8%)	62 (97%)	2 (3%)	0	100	100
4	I1	11/752 (2%)	11 (100%)	0	0	100	100
4	J1	72/752 (10%)	63 (88%)	9 (12%)	0	100	100
All	All	2172/5320 (41%)	2110 (97%)	61 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B1	148	CYS

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	A1	673/820 (82%)	673 (100%)	0	100	100
1	B1	630/820 (77%)	629 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C1	150/150 (100%)	149 (99%)	1 (1%)	76	81
2	D1	150/150 (100%)	150 (100%)	0	100	100
3	E1	78/78 (100%)	77 (99%)	1 (1%)	61	74
3	F1	78/78 (100%)	78 (100%)	0	100	100
4	G1	89/641 (14%)	89 (100%)	0	100	100
4	H1	56/641 (9%)	56 (100%)	0	100	100
4	I1	10/641 (2%)	10 (100%)	0	100	100
4	J1	61/641 (10%)	61 (100%)	0	100	100
All	All	1975/4660 (42%)	1972 (100%)	3 (0%)	85	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B1	628	GLN
2	C1	7	GLN
3	E1	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	411	GLN
1	A1	493	GLN
1	A1	626	ASN
1	A1	768	GLN
1	A1	788	GLN
1	B1	336	GLN
1	B1	389	HIS
1	B1	611	ASN
1	B1	621	GLN
1	B1	628	GLN
1	B1	632	ASN
1	B1	718	ASN
2	C1	64	HIS
2	D1	23	GLN
3	E1	61	ASN
3	F1	19	GLN
3	F1	33	ASN
3	F1	55	HIS

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Mol	Chain	Res	Type
4	G1	483	GLN
4	H1	486	HIS
4	H1	498	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

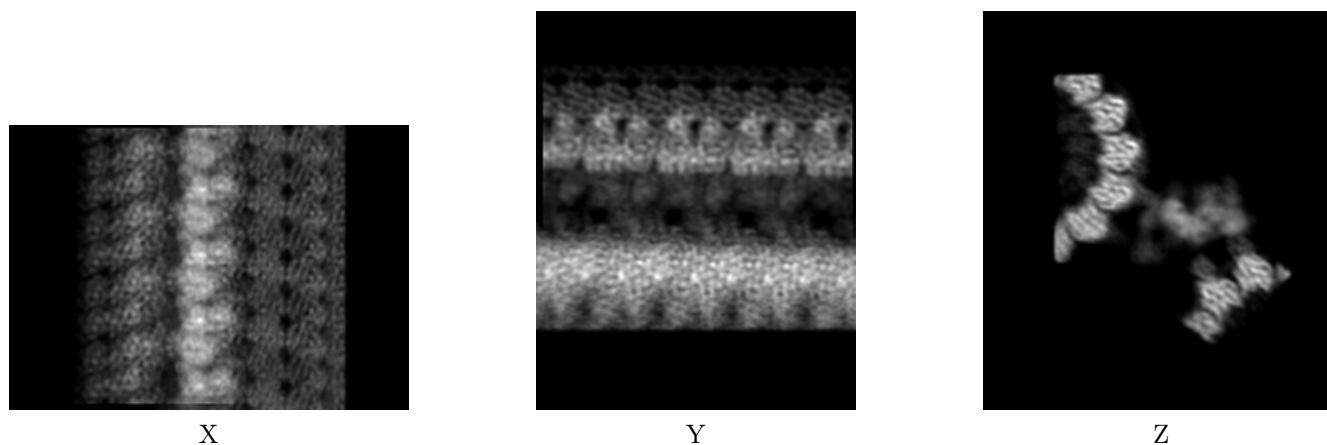
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76173. 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](#)

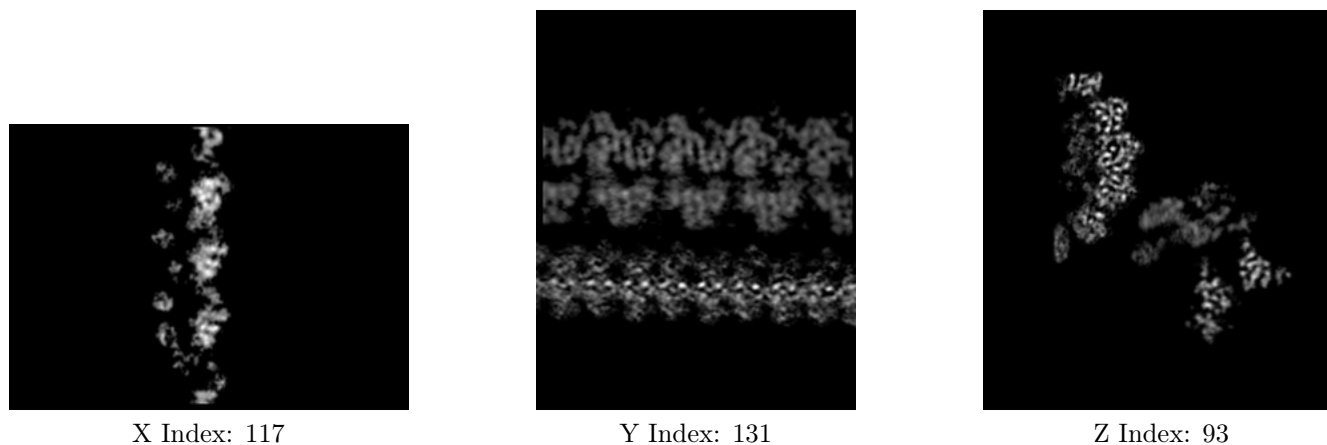
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



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: 85



Y Index: 83

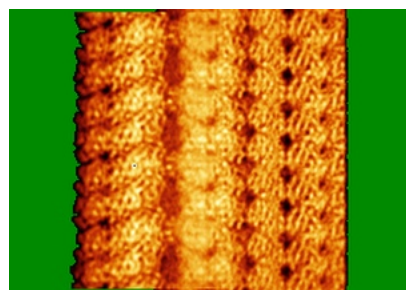


Z Index: 102

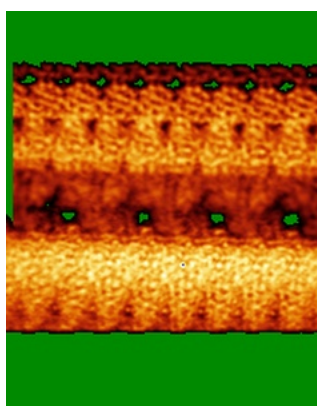
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

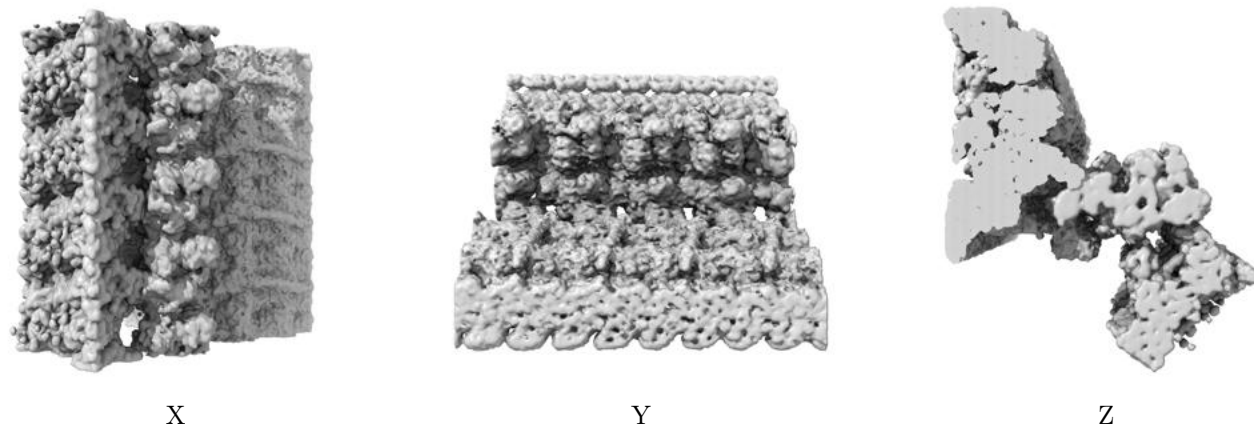


Z

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 0.0005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

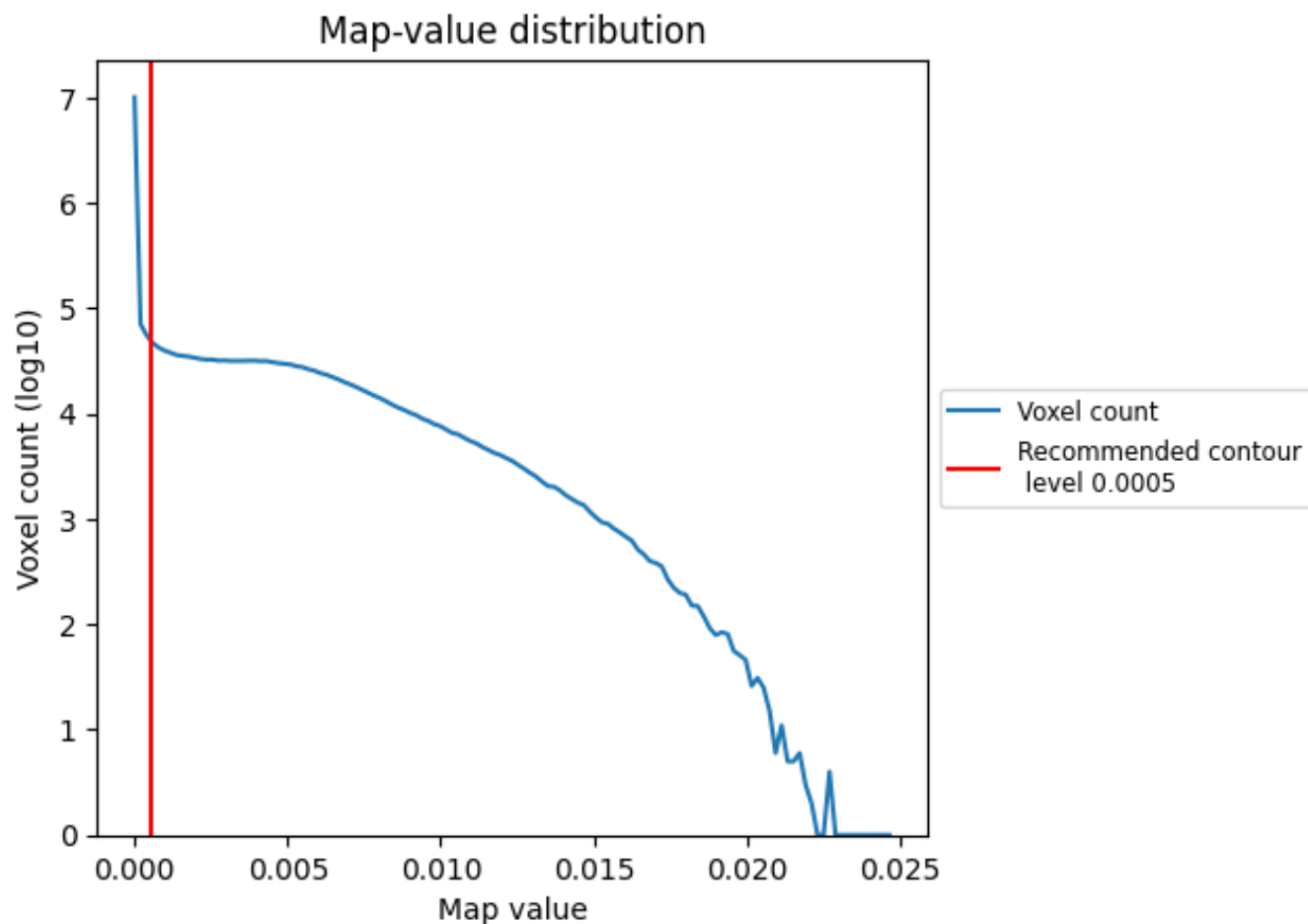
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

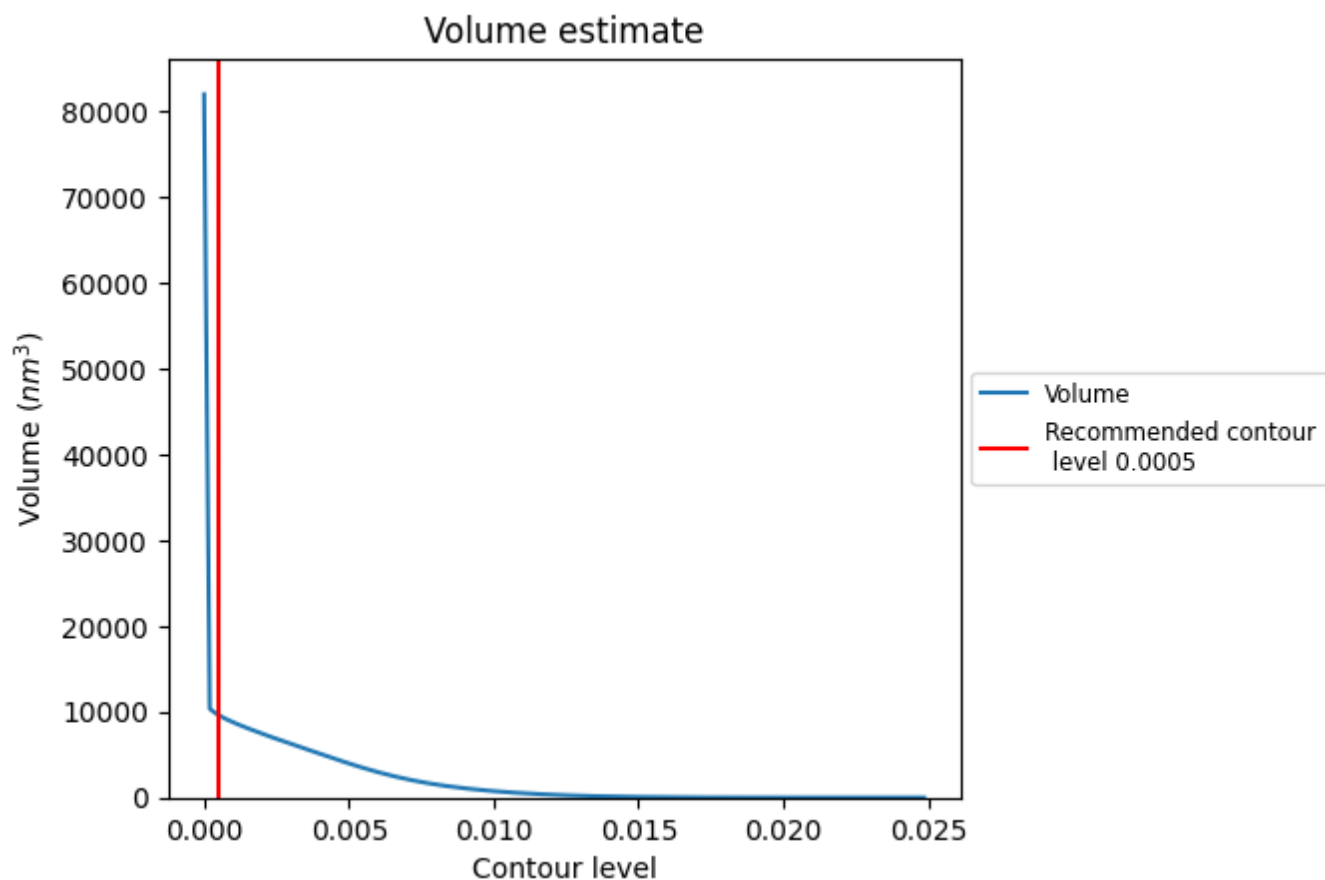
This section contains the results of statistical analysis of the map.

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 9620 nm³; this corresponds to an approximate mass of 8690 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

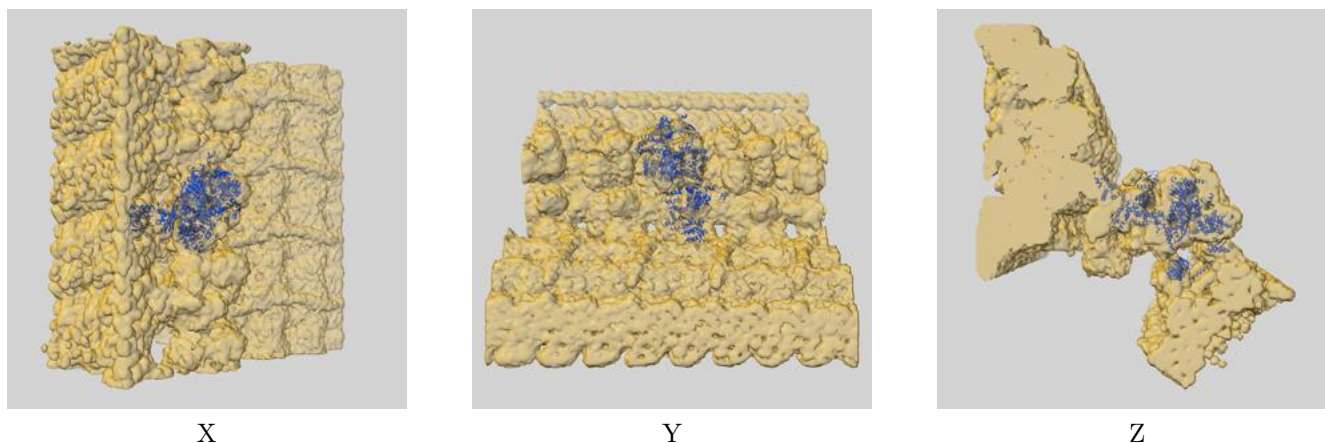
8 Fourier-Shell correlation ⓘ

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-76173 and PDB model 11XU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0005 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](#)



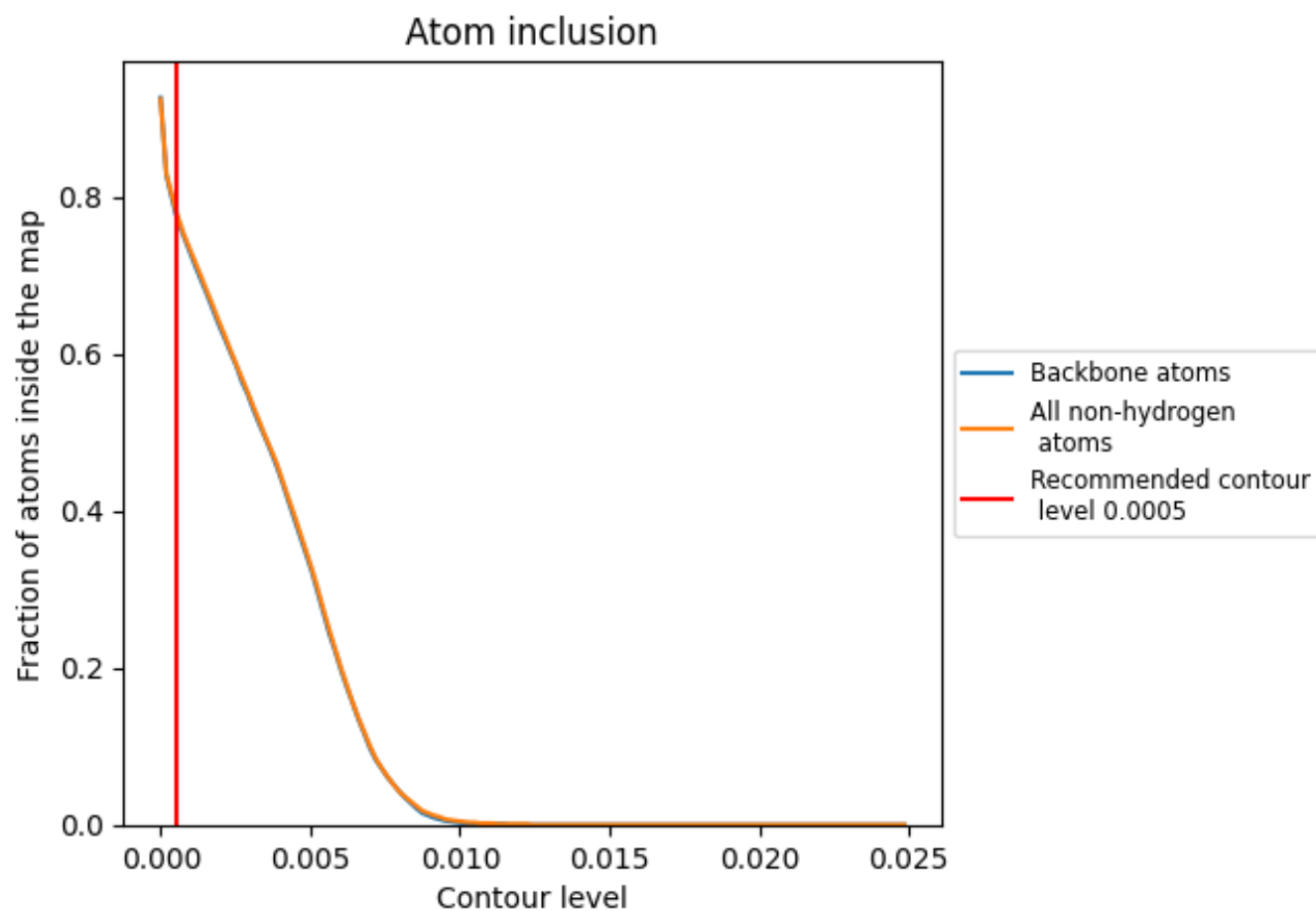
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.0005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7840	 -0.0180
A1	 0.8110	 -0.0140
B1	 0.8530	 -0.0080
C1	 0.6130	 -0.0110
D1	 0.8480	 -0.0000
E1	 0.7660	 -0.0540
F1	 0.5400	 -0.0600
G1	 0.6450	 -0.0450
H1	 0.5710	 -0.0550
I1	 0.2670	 -0.1700
J1	 0.8550	 -0.0190

