



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 02:17 PM JST

PDB ID : 9UUS / pdb_00009uus
EMDB ID : EMD-64517
Title : The NuA3 histone acetyltransferase complex bound to acetyl-CoA and H3 tail
Authors : Wang, Y.R.; Zhang, H.Q.
Deposited on : 2025-05-08
Resolution : 3.20 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:

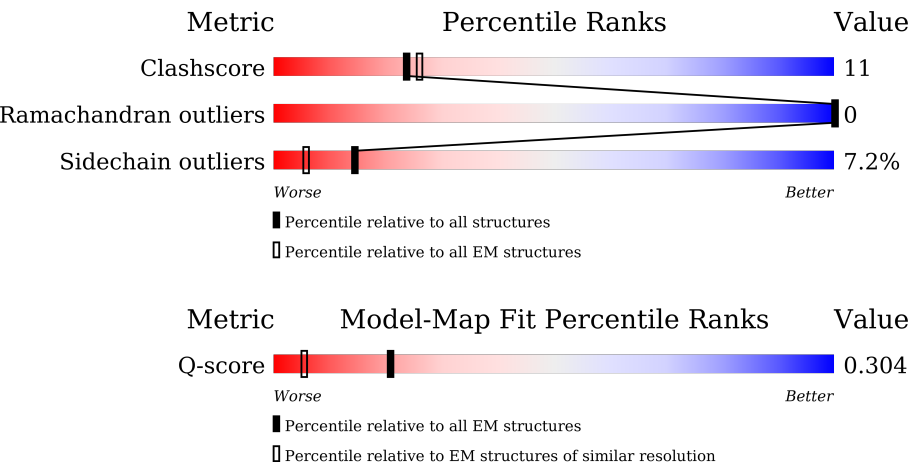
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	H	21	<div><div>48%</div><div><div></div><div></div><div></div><div></div></div><div>43%10%5%43%</div></div>
2	A	831	<div><div>23%</div><div><div></div><div></div><div></div><div></div></div><div>40%17%.41%</div></div>
3	B	738	<div><div>30%</div><div><div></div><div></div><div></div><div></div></div><div>52%20%.25%</div></div>
4	C	219	<div><div>19%</div><div><div></div><div></div><div></div><div></div></div><div>36%8%56%</div></div>

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Mol	Chain	Length	Quality of chain
5	E	244	<div><div><div></div><div></div><div></div></div><div>14%22%7%71%</div></div>
6	D	113	<div><div><div></div><div></div><div></div></div><div>61%63%16%•18%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10835 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	12	Total	C	N	O	S	0	0
			90	53	21	15	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	14	MET	LYS	conflict	UNP P61830

- Molecule 2 is a protein called Histone acetyltransferase SAS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	491	Total	C	N	O	S	0	0
			4117	2662	688	748	19		

- Molecule 3 is a protein called NuA3 HAT complex component NTO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	550	Total	C	N	O	S	0	0
			4462	2841	765	823	33		

- Molecule 4 is a protein called Protein YNG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	97	Total	C	N	O	S	0	0
			795	500	135	156	4		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	70	Total	C	N	O	S	0	0
			552	350	84	116	2		

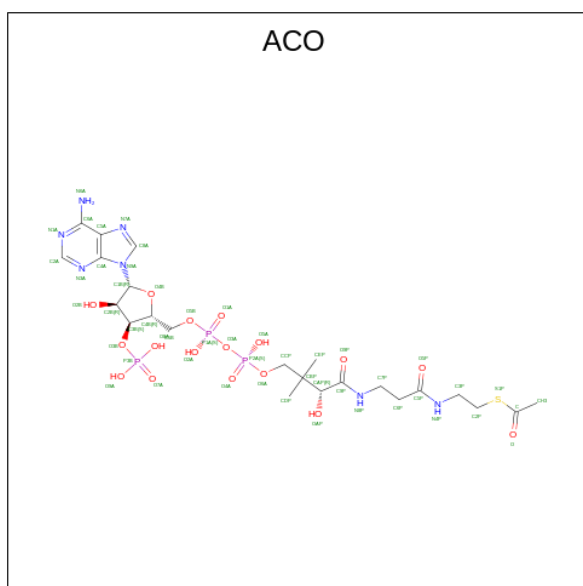
- Molecule 6 is a protein called Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	93	Total	C	N	O	0	0
			763	465	140	158		

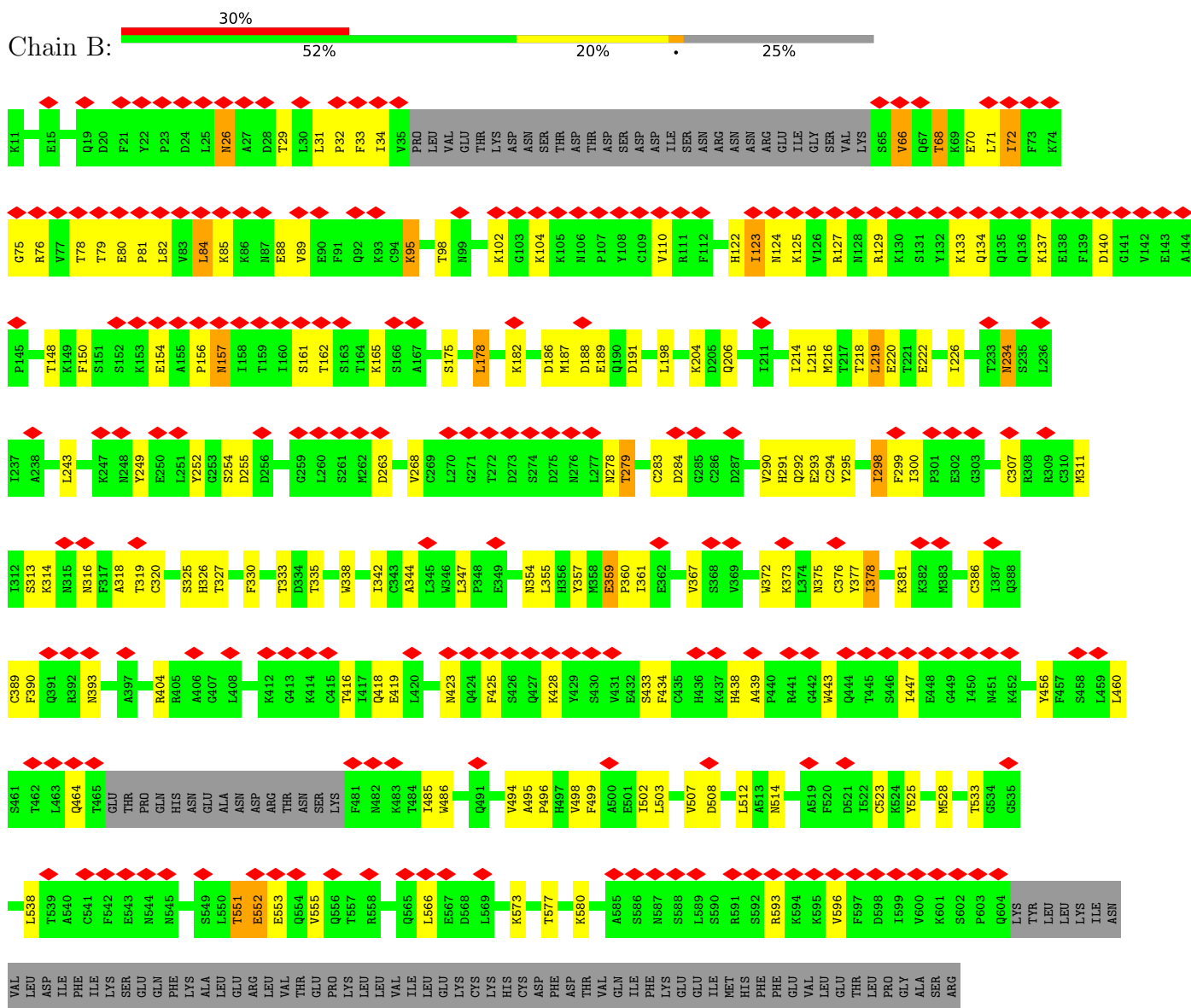
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	
7	B	4	Total	Zn	0
			4	4	

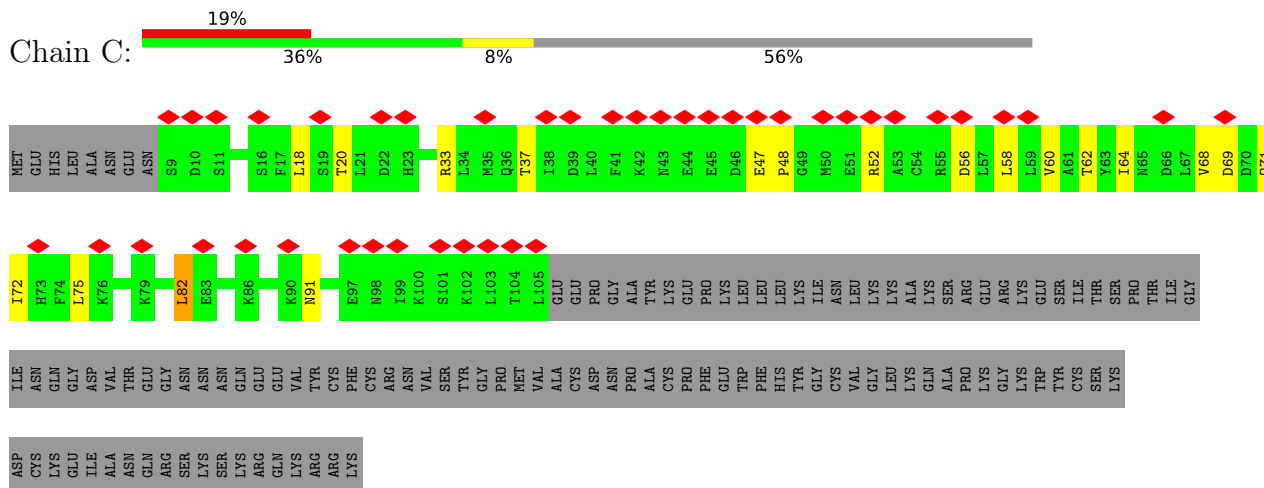
- Molecule 8 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



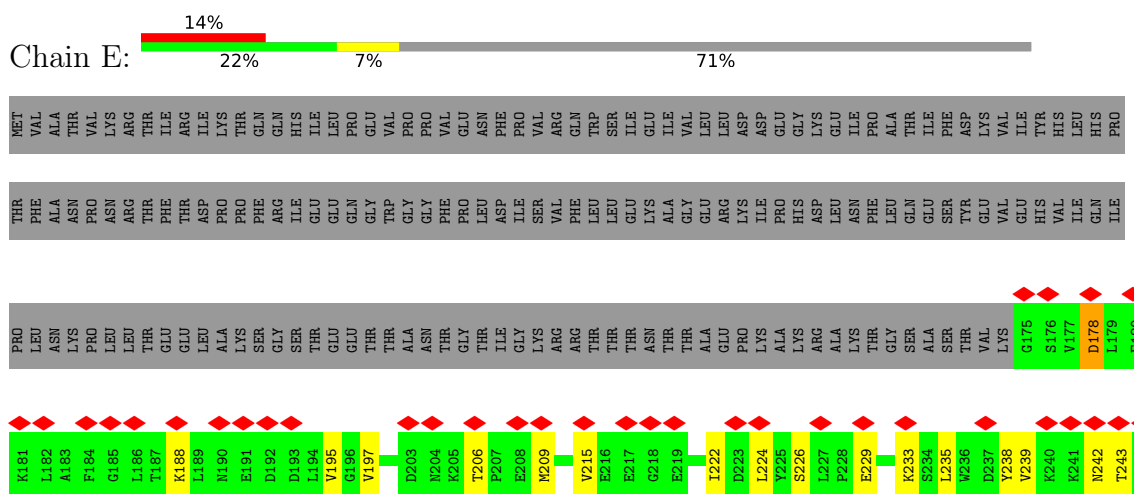
- Molecule 3: NuA3 HAT complex component NTO1



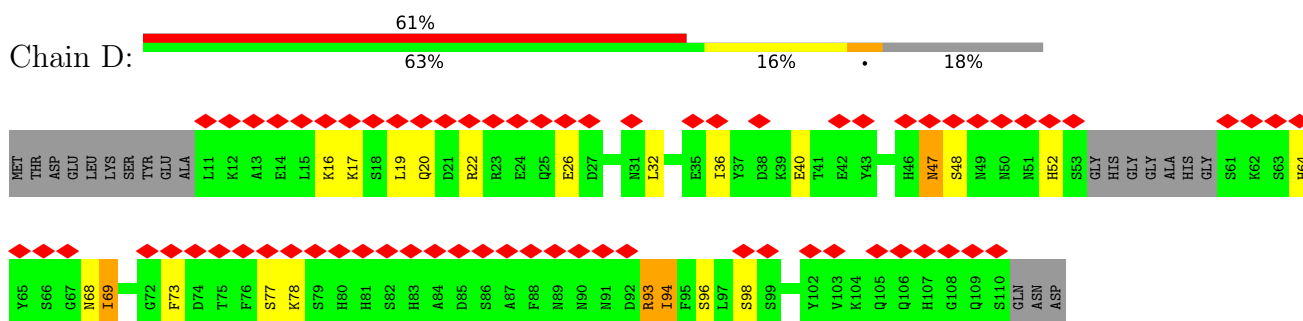
- Molecule 4: Protein YNG1



- Molecule 5: Transcription initiation factor TFIID subunit 14



- Molecule 6: Chromatin modification-related protein EAF6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.960	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.278	Depositor
Map size (Å)	279.647, 279.647, 279.647	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96430004, 0.96430004, 0.96430004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACO

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	H	0.21	0/90	0.48	0/116
2	A	0.49	6/4221 (0.1%)	0.49	5/5696 (0.1%)
3	B	0.21	0/4566	0.42	0/6162
4	C	0.23	0/805	0.41	0/1082
5	E	0.17	0/559	0.31	0/756
6	D	0.15	0/778	0.30	0/1041
All	All	0.34	6/11019 (0.1%)	0.43	5/14853 (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
3	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	366	SER	CA-CB	-18.48	1.28	1.53
2	A	366	SER	N-CA	11.55	1.59	1.46
2	A	367	LYS	CA-CB	10.02	1.71	1.53
2	A	367	LYS	CA-C	9.29	1.63	1.52
2	A	367	LYS	N-CA	-6.50	1.38	1.46
2	A	366	SER	CA-C	5.66	1.61	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	367	LYS	N-CA-CB	-8.07	97.69	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	366	SER	CA-C-N	-6.78	113.09	122.93
2	A	366	SER	C-N-CA	-6.78	113.09	122.93
2	A	367	LYS	CB-CA-C	-6.72	97.28	109.38
2	A	366	SER	CB-CA-C	5.58	119.71	111.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	359	GLU	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	H	90	0	98	4	0
2	A	4117	0	4083	103	0
3	B	4462	0	4400	116	0
4	C	795	0	804	17	0
5	E	552	0	545	9	0
6	D	763	0	694	16	0
7	A	1	0	0	0	0
7	B	4	0	0	0	0
8	A	51	0	33	2	0
All	All	10835	0	10657	229	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 11.

All (229) 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:H:17:ARG:HB3	3:B:72:ILE:HG23	1.57	0.83
2:A:667:MET:HG3	6:D:94:ILE:HG22	1.67	0.75
2:A:239:SER:HB3	2:A:299:MET:HE1	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:580:LYS:HE2	4:C:62:THR:HG22	1.76	0.68
2:A:203:MET:SD	2:A:203:MET:N	2.67	0.67
2:A:485:ARG:NH2	2:A:691:HIS:O	2.25	0.67
6:D:40:GLU:OE2	6:D:96:SER:OG	2.10	0.67
2:A:443:ARG:NH2	2:A:566:TYR:OH	2.27	0.67
1:H:17:ARG:HD3	3:B:72:ILE:HA	1.76	0.66
3:B:278:ASN:ND2	3:B:293:GLU:OE2	2.23	0.66
3:B:425:PHE:HD1	3:B:428:LYS:HE3	1.60	0.65
3:B:191:ASP:OD1	3:B:525:TYR:OH	2.14	0.65
2:A:496:GLN:NE2	3:B:29:THR:OG1	2.28	0.65
3:B:320:CYS:H	3:B:326:HIS:CD2	2.16	0.64
2:A:164:GLN:NE2	2:A:171:GLU:OE1	2.30	0.64
3:B:206:GLN:HB3	3:B:512:LEU:HD22	1.79	0.64
2:A:677:ARG:NH1	4:C:37:THR:OG1	2.31	0.63
8:A:902:ACO:OAP	8:A:902:ACO:O6A	2.17	0.63
2:A:408:LYS:NZ	2:A:581:GLY:O	2.28	0.63
4:C:20:THR:OG1	4:C:71:GLN:NE2	2.32	0.63
2:A:295:ASN:ND2	3:B:335:THR:O	2.32	0.62
2:A:310:MET:HE3	2:A:316:PHE:HD1	1.63	0.62
2:A:496:GLN:HB3	3:B:29:THR:HB	1.80	0.62
3:B:122:HIS:O	3:B:124:ASN:ND2	2.33	0.62
3:B:552:GLU:OE1	3:B:553:GLU:N	2.33	0.62
2:A:142:VAL:O	2:A:144:LYS:NZ	2.33	0.61
3:B:66:VAL:HG12	3:B:84:LEU:HD12	1.83	0.61
6:D:22:ARG:O	6:D:26:GLU:HG3	2.01	0.61
3:B:318:ALA:O	3:B:326:HIS:ND1	2.34	0.61
3:B:551:THR:OG1	3:B:552:GLU:N	2.31	0.60
2:A:237:ASN:OD1	2:A:297:ASN:ND2	2.35	0.60
3:B:123:ILE:O	3:B:127:ARG:NH2	2.22	0.60
3:B:219:LEU:HD23	3:B:499:PHE:HD2	1.66	0.60
2:A:487:ASN:ND2	2:A:488:ASN:OD1	2.35	0.59
3:B:307:CYS:O	3:B:311:MET:HB2	2.01	0.59
3:B:439:ALA:HB1	3:B:443:TRP:HB3	1.85	0.59
3:B:507:VAL:HG13	3:B:512:LEU:HD12	1.83	0.59
4:C:64:ILE:O	4:C:68:VAL:HG23	2.03	0.59
3:B:148:THR:HG22	3:B:150:PHE:H	1.68	0.59
2:A:318:ARG:HG2	3:B:187:MET:H	1.68	0.58
2:A:698:ARG:HH11	2:A:699:SER:HB3	1.68	0.58
2:A:178:SER:O	3:B:464:GLN:NE2	2.37	0.58
2:A:191:GLN:O	3:B:486:TRP:NE1	2.34	0.58
3:B:508:ASP:OD1	3:B:514:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:110:VAL:HG22	2:A:116:VAL:HG12	1.85	0.57
3:B:71:LEU:HD12	3:B:72:ILE:H	1.69	0.57
3:B:215:LEU:HD22	3:B:503:LEU:HD22	1.85	0.57
2:A:181:ASN:HD21	3:B:464:GLN:HA	1.70	0.57
3:B:460:LEU:O	3:B:464:GLN:HG2	2.05	0.56
2:A:199:THR:HG21	3:B:226:ILE:HG23	1.86	0.56
2:A:546:TRP:HE1	3:B:34:ILE:HG21	1.69	0.56
3:B:555:VAL:HG13	4:C:82:LEU:HD12	1.87	0.56
3:B:342:ILE:HD12	3:B:404:ARG:NH1	2.21	0.56
3:B:68:THR:HG23	3:B:84:LEU:HD23	1.88	0.55
2:A:453:LYS:O	2:A:455:LEU:N	2.39	0.55
2:A:125:PHE:CZ	2:A:234:ILE:HD11	2.42	0.55
2:A:542:LYS:HG3	3:B:33:PHE:CE1	2.42	0.54
3:B:290:VAL:HG11	3:B:295:TYR:CD2	2.42	0.54
2:A:368:THR:OG1	3:B:354:ASN:ND2	2.28	0.54
3:B:357:TYR:HB3	3:B:359:GLU:HG2	1.88	0.54
2:A:116:VAL:HG23	5:E:222:ILE:HG23	1.88	0.54
5:E:239:VAL:O	5:E:243:THR:OG1	2.17	0.54
2:A:335:ARG:HD3	3:B:140:ASP:OD2	2.08	0.53
3:B:376:CYS:SG	3:B:377:TYR:N	2.81	0.53
2:A:307:LEU:O	2:A:355:ASN:ND2	2.36	0.53
2:A:497:VAL:HG22	2:A:691:HIS:HE1	1.73	0.53
3:B:498:VAL:O	3:B:502:ILE:HG12	2.09	0.52
4:C:47:GLU:CD	4:C:47:GLU:H	2.18	0.52
3:B:75:GLY:O	3:B:76:ARG:NH1	2.42	0.52
2:A:425:TYR:HD2	2:A:427:ARG:H	1.57	0.52
3:B:157:ASN:OD1	3:B:157:ASN:N	2.40	0.52
3:B:330:PHE:HD2	3:B:338:TRP:HB3	1.74	0.52
3:B:70:GLU:HG2	3:B:71:LEU:H	1.74	0.52
3:B:214:ILE:O	3:B:218:THR:HG23	2.10	0.52
3:B:355:LEU:HD23	3:B:418:GLN:HB3	1.91	0.52
2:A:404:PHE:HD2	2:A:434:LEU:HD22	1.74	0.51
3:B:313:SER:OG	3:B:314:LYS:N	2.43	0.51
6:D:64:HIS:HB2	6:D:78:LYS:HD2	1.92	0.51
2:A:666:TYR:O	4:C:33:ARG:NE	2.40	0.51
6:D:48:SER:HB3	6:D:52:HIS:CE1	2.45	0.51
2:A:290:PHE:O	2:A:295:ASN:ND2	2.44	0.51
1:H:19:GLN:N	3:B:72:ILE:HG21	2.26	0.51
3:B:291:HIS:HB2	3:B:294:CYS:HB2	1.92	0.51
4:C:58:LEU:O	4:C:62:THR:HG23	2.10	0.51
3:B:188:ASP:OD1	3:B:189:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:48:PRO:O	4:C:52:ARG:HG2	2.11	0.50
2:A:158:ARG:HH21	3:B:533:THR:HA	1.77	0.50
2:A:500:ASN:OD1	3:B:26:ASN:ND2	2.33	0.50
2:A:203:MET:HA	2:A:206:PHE:CE1	2.47	0.49
3:B:319:THR:HA	3:B:326:HIS:CE1	2.47	0.49
2:A:124:LYS:NZ	5:E:195:VAL:HG21	2.27	0.49
2:A:206:PHE:CD1	2:A:206:PHE:C	2.89	0.49
2:A:163:LYS:HD3	2:A:170:THR:HG23	1.95	0.49
2:A:303:CYS:O	2:A:307:LEU:N	2.42	0.49
2:A:393:GLN:O	3:B:129:ARG:NE	2.45	0.49
3:B:359:GLU:HB3	3:B:360:PRO:CD	2.42	0.49
3:B:433:SER:OG	3:B:434:PHE:N	2.45	0.48
2:A:156:GLN:O	2:A:160:ASN:ND2	2.26	0.48
3:B:249:TYR:HD1	3:B:254:SER:HB3	1.78	0.48
4:C:60:VAL:O	4:C:64:ILE:HG12	2.13	0.48
6:D:16:LYS:HA	6:D:19:LEU:HD13	1.95	0.48
3:B:503:LEU:O	3:B:507:VAL:HG23	2.13	0.48
2:A:333:ILE:HD13	2:A:343:GLU:HB2	1.95	0.48
5:E:229:GLU:HG3	5:E:233:LYS:HE3	1.95	0.48
3:B:419:GLU:OE2	3:B:428:LYS:NZ	2.46	0.48
2:A:271:GLN:O	2:A:273:GLU:HG3	2.14	0.48
2:A:477:LYS:NZ	2:A:683:GLU:OE2	2.34	0.48
6:D:48:SER:O	6:D:52:HIS:ND1	2.47	0.48
2:A:405:SER:OG	2:A:406:LYS:N	2.47	0.48
2:A:658:ASP:OD1	2:A:659:THR:N	2.41	0.47
2:A:393:GLN:HG2	3:B:127:ARG:HD2	1.95	0.47
3:B:161:SER:OG	3:B:162:THR:N	2.47	0.47
6:D:47:ASN:HD21	6:D:68:ASN:HB2	1.79	0.47
6:D:68:ASN:OD1	6:D:69:ILE:N	2.46	0.47
2:A:537:PHE:HE2	2:A:700:LYS:HG3	1.79	0.47
3:B:359:GLU:HB3	3:B:360:PRO:HD3	1.95	0.47
3:B:234:ASN:OD1	3:B:234:ASN:N	2.46	0.47
2:A:509:ILE:O	2:A:513:VAL:HG23	2.15	0.47
2:A:292:GLU:O	2:A:296:GLN:HG2	2.15	0.47
2:A:410:ASN:ND2	2:A:414:TYR:HB2	2.30	0.47
3:B:314:LYS:HA	3:B:314:LYS:HD3	1.65	0.47
2:A:130:ARG:NH1	2:A:131:LEU:HD12	2.30	0.47
2:A:212:LEU:HD21	3:B:485:ILE:HD11	1.96	0.47
3:B:68:THR:HB	3:B:80:GLU:HB2	1.96	0.47
2:A:385:GLU:OE2	2:A:399:HIS:NE2	2.27	0.46
6:D:17:LYS:HA	6:D:20:GLN:HE22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:451:PRO:HG2	2:A:463:TYR:CE2	2.50	0.46
4:C:47:GLU:HB2	4:C:48:PRO:HD3	1.97	0.46
3:B:79:THR:HG22	3:B:81:PRO:HD3	1.97	0.46
3:B:344:ALA:HB2	3:B:361:ILE:HD13	1.98	0.46
2:A:408:LYS:HD3	2:A:581:GLY:HA3	1.98	0.46
2:A:668:CYS:HB3	2:A:671:LYS:HE3	1.97	0.46
4:C:69:ASP:O	4:C:72:ILE:HG22	2.16	0.46
2:A:130:ARG:HH12	2:A:131:LEU:HD12	1.81	0.46
6:D:32:LEU:O	6:D:36:ILE:HG13	2.16	0.46
2:A:587:ASN:OD1	2:A:587:ASN:N	2.49	0.45
3:B:102:LYS:HD2	3:B:102:LYS:HA	1.68	0.45
3:B:320:CYS:HA	3:B:338:TRP:O	2.15	0.45
2:A:439:TYR:CD2	2:A:466:PHE:HE2	2.35	0.45
2:A:457:ASP:HB2	3:B:84:LEU:HD22	1.99	0.45
3:B:279:THR:OG1	3:B:292:GLN:NE2	2.43	0.45
3:B:495:ALA:HB3	3:B:523:CYS:SG	2.57	0.45
2:A:127:ASN:OD1	2:A:128:PHE:N	2.49	0.45
2:A:301:PHE:O	2:A:309:TYR:HA	2.16	0.45
2:A:310:MET:HE3	2:A:316:PHE:CD1	2.48	0.45
3:B:416:THR:OG1	3:B:419:GLU:HG3	2.17	0.45
2:A:537:PHE:HZ	2:A:696:ILE:HG21	1.81	0.45
2:A:536:ASP:N	2:A:536:ASP:OD1	2.49	0.45
3:B:376:CYS:SG	3:B:378:ILE:HG22	2.57	0.45
3:B:573:LYS:O	3:B:577:THR:HG22	2.17	0.45
2:A:498:SER:HB3	2:A:501:ASP:OD2	2.17	0.44
5:E:178:ASP:OD1	5:E:178:ASP:N	2.47	0.44
2:A:166:TRP:HZ3	2:A:222:LEU:HG	1.82	0.44
2:A:192:TRP:CE3	3:B:485:ILE:HA	2.52	0.44
2:A:332:GLU:OE2	2:A:335:ARG:NH2	2.50	0.44
3:B:175:SER:HB3	3:B:178:LEU:HD12	2.00	0.44
3:B:216:MET:HE2	3:B:216:MET:HB2	1.80	0.44
3:B:389:CYS:SG	3:B:390:PHE:N	2.91	0.44
6:D:93:ARG:H	6:D:93:ARG:HG2	1.62	0.44
3:B:252:TYR:HB3	3:B:456:TYR:HB2	1.98	0.44
2:A:182:THR:HG21	2:A:185:ARG:HG3	1.98	0.44
3:B:496:PRO:HD2	3:B:499:PHE:CD1	2.53	0.44
2:A:286:TYR:CZ	2:A:365:ASN:HB2	2.52	0.44
2:A:384:ARG:HB2	2:A:398:PHE:CD1	2.53	0.44
3:B:255:ASP:HB2	3:B:404:ARG:HD3	2.00	0.44
3:B:538:LEU:HD12	3:B:538:LEU:H	1.83	0.44
3:B:566:LEU:HG	4:C:72:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:77:SER:OG	6:D:78:LYS:N	2.51	0.44
2:A:203:MET:HA	2:A:206:PHE:CD1	2.53	0.43
6:D:47:ASN:ND2	6:D:68:ASN:HB2	2.34	0.43
2:A:331:ASN:OD1	2:A:331:ASN:N	2.51	0.43
3:B:243:LEU:HD23	3:B:243:LEU:HA	1.72	0.43
2:A:292:GLU:OE2	3:B:338:TRP:NE1	2.45	0.43
2:A:212:LEU:HD11	3:B:485:ILE:HD11	2.00	0.43
3:B:268:VAL:HG21	3:B:294:CYS:HB3	1.99	0.43
5:E:235:LEU:HD23	5:E:235:LEU:HA	1.92	0.43
2:A:231:ALA:HA	2:A:234:ILE:HG22	2.01	0.43
3:B:283:CYS:SG	3:B:284:ASP:N	2.92	0.43
5:E:238:TYR:O	5:E:242:ASN:HB2	2.19	0.43
6:D:94:ILE:H	6:D:94:ILE:HG12	1.58	0.43
2:A:198:GLY:O	4:C:91:ASN:ND2	2.52	0.43
3:B:593:ARG:HA	3:B:596:VAL:HG12	2.01	0.43
3:B:133:LYS:HB2	3:B:133:LYS:HE2	1.75	0.42
3:B:373:LYS:HE3	3:B:373:LYS:HB3	1.89	0.42
2:A:459:GLY:O	2:A:463:TYR:HB3	2.19	0.42
3:B:204:LYS:HE2	3:B:204:LYS:HB3	1.82	0.42
5:E:188:LYS:HD2	5:E:188:LYS:HA	1.75	0.42
2:A:394:ASN:HB3	3:B:129:ARG:HB3	2.00	0.42
3:B:95:LYS:HE3	3:B:95:LYS:HB2	1.87	0.42
3:B:133:LYS:HG3	3:B:134:GLN:HG3	2.01	0.42
2:A:451:PRO:HD2	2:A:463:TYR:OH	2.19	0.42
3:B:381:LYS:HE3	3:B:381:LYS:HB2	1.87	0.42
2:A:463:TYR:O	2:A:463:TYR:CG	2.72	0.42
2:A:509:ILE:HD12	2:A:511:THR:HG23	2.01	0.42
2:A:344:ILE:HG23	2:A:349:ASN:OD1	2.19	0.42
3:B:254:SER:OG	3:B:255:ASP:N	2.53	0.42
2:A:493:THR:HB	2:A:695:GLY:HA3	2.02	0.42
3:B:123:ILE:HG13	3:B:125:LYS:HG3	2.02	0.42
3:B:566:LEU:HD23	4:C:72:ILE:HD11	2.01	0.42
2:A:676:ASP:OD2	2:A:681:GLN:HB3	2.19	0.41
4:C:56:ASP:O	4:C:60:VAL:HG23	2.20	0.41
2:A:144:LYS:HA	2:A:144:LYS:HD3	1.79	0.41
3:B:216:MET:O	3:B:220:GLU:HG2	2.21	0.41
3:B:222:GLU:OE1	3:B:502:ILE:HG13	2.20	0.41
3:B:298:ILE:HG22	3:B:299:PHE:HD1	1.84	0.41
2:A:453:LYS:HD2	2:A:453:LYS:HA	1.85	0.41
2:A:524:TYR:CD1	2:A:542:LYS:HB3	2.56	0.41
2:A:484:ARG:NH1	2:A:485:ARG:HB3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:209:MET:HA	5:E:226:SER:OG	2.21	0.41
2:A:283:LYS:HE3	2:A:283:LYS:HB3	1.88	0.41
3:B:137:LYS:HA	3:B:137:LYS:HD2	1.93	0.41
3:B:154:GLU:O	3:B:156:PRO:HD3	2.21	0.41
1:H:14:MET:HE1	8:A:902:ACO:S1P	2.61	0.41
2:A:374:GLU:HB2	2:A:375:PRO:HD3	2.03	0.41
2:A:451:PRO:HG2	2:A:463:TYR:CZ	2.55	0.41
2:A:661:SER:O	2:A:662:SER:OG	2.35	0.41
3:B:292:GLN:NE2	3:B:300:ILE:HD11	2.36	0.41
3:B:389:CYS:SG	3:B:438:HIS:HD2	2.44	0.41
4:C:72:ILE:HD12	4:C:72:ILE:HA	1.74	0.41
2:A:541:ILE:O	3:B:32:PRO:HA	2.21	0.41
2:A:574:ILE:HD11	2:A:576:LEU:HD21	2.03	0.41
6:D:93:ARG:HE	6:D:93:ARG:HB3	1.70	0.41
3:B:182:LYS:HE3	3:B:182:LYS:HB3	1.83	0.40
3:B:314:LYS:C	3:B:316:ASN:H	2.28	0.40
3:B:314:LYS:O	3:B:316:ASN:N	2.55	0.40
2:A:315:THR:HG23	3:B:186:ASP:HB3	2.03	0.40
2:A:546:TRP:O	2:A:550:GLU:HG2	2.22	0.40
2:A:321:LEU:HA	2:A:321:LEU:HD12	1.90	0.40
3:B:165:LYS:HA	3:B:165:LYS:HD2	1.85	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	H	10/21 (48%)	9 (90%)	1 (10%)	0	100	100
2	A	481/831 (58%)	446 (93%)	35 (7%)	0	100	100
3	B	544/738 (74%)	499 (92%)	45 (8%)	0	100	100
4	C	95/219 (43%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	68/244 (28%)	66 (97%)	2 (3%)	0	100	100
6	D	89/113 (79%)	86 (97%)	3 (3%)	0	100	100
All	All	1287/2166 (59%)	1198 (93%)	89 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	9/15 (60%)	8 (89%)	1 (11%)	5	22
2	A	462/777 (60%)	429 (93%)	33 (7%)	12	42
3	B	500/675 (74%)	460 (92%)	40 (8%)	10	37
4	C	94/201 (47%)	91 (97%)	3 (3%)	34	65
5	E	64/219 (29%)	59 (92%)	5 (8%)	10	38
6	D	86/100 (86%)	80 (93%)	6 (7%)	12	42
All	All	1215/1987 (61%)	1127 (93%)	88 (7%)	14	41

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	MET
2	A	116	VAL
2	A	131	LEU
2	A	132	ILE
2	A	135	SER
2	A	137	VAL
2	A	144	LYS
2	A	179	SER
2	A	182	THR
2	A	206	PHE
2	A	210	ARG
2	A	268	TRP

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Mol	Chain	Res	Type
2	A	287	THR
2	A	310	MET
2	A	320	GLN
2	A	349	ASN
2	A	350	VAL
2	A	351	LEU
2	A	427	ARG
2	A	442	SER
2	A	453	LYS
2	A	460	LEU
2	A	463	TYR
2	A	479	ARG
2	A	491	GLU
2	A	495	GLN
2	A	506	THR
2	A	511	THR
2	A	519	GLN
2	A	522	VAL
2	A	538	ASN
2	A	574	ILE
2	A	575	ILE
2	A	698	ARG
3	B	26	ASN
3	B	31	LEU
3	B	66	VAL
3	B	68	THR
3	B	72	ILE
3	B	78	THR
3	B	82	LEU
3	B	84	LEU
3	B	85	LYS
3	B	88	GLU
3	B	89	VAL
3	B	95	LYS
3	B	98	THR
3	B	104	LYS
3	B	110	VAL
3	B	123	ILE
3	B	157	ASN
3	B	178	LEU
3	B	198	LEU
3	B	219	LEU

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Mol	Chain	Res	Type
3	B	234	ASN
3	B	263	ASP
3	B	279	THR
3	B	298	ILE
3	B	325	SER
3	B	327	THR
3	B	333	THR
3	B	347	LEU
3	B	367	VAL
3	B	372	TRP
3	B	375	ASN
3	B	378	ILE
3	B	386	CYS
3	B	393	ASN
3	B	423	ASN
3	B	447	ILE
3	B	494	VAL
3	B	528	MET
3	B	551	THR
3	B	552	GLU
4	C	18	LEU
4	C	75	LEU
4	C	82	LEU
5	E	178	ASP
5	E	197	VAL
5	E	206	THR
5	E	215	VAL
5	E	224	LEU
6	D	47	ASN
6	D	69	ILE
6	D	73	PHE
6	D	93	ARG
6	D	94	ILE
6	D	98	SER

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

Mol	Chain	Res	Type
1	H	19	GLN
2	A	181	ASN
2	A	235	ASN
2	A	295	ASN

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Mol	Chain	Res	Type
2	A	393	GLN
2	A	490	ASN
2	A	496	GLN
2	A	691	HIS
3	B	124	ASN
3	B	190	GLN
3	B	209	HIS
3	B	240	HIS
3	B	423	ASN
3	B	424	GLN
3	B	451	ASN
3	B	565	GLN
4	C	71	GLN
5	E	204	ASN
5	E	214	ASN
5	E	242	ASN
6	D	52	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](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACO	A	902	-	45,53,53	3.42	16 (35%)	56,79,79	2.46	10 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ACO	A	902	-	-	18/47/67/67	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	902	ACO	O4B-C1B	12.95	1.59	1.41
8	A	902	ACO	C2B-C3B	-9.14	1.32	1.52
8	A	902	ACO	C9P-N8P	7.95	1.51	1.33
8	A	902	ACO	C5P-N4P	6.28	1.47	1.33
8	A	902	ACO	O4B-C4B	-6.26	1.31	1.45
8	A	902	ACO	C3B-C4B	4.40	1.64	1.52
8	A	902	ACO	C7P-C6P	3.72	1.63	1.51
8	A	902	ACO	P2A-O6A	3.61	1.73	1.59
8	A	902	ACO	C2A-N3A	3.26	1.37	1.32
8	A	902	ACO	C6P-C5P	3.19	1.57	1.51
8	A	902	ACO	OAP-CAP	-3.16	1.36	1.42
8	A	902	ACO	C5A-C4A	-2.81	1.33	1.40
8	A	902	ACO	O9P-C9P	-2.40	1.18	1.23
8	A	902	ACO	O2B-C2B	2.27	1.48	1.43
8	A	902	ACO	O5P-C5P	-2.20	1.18	1.23
8	A	902	ACO	C6A-N6A	2.04	1.41	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	902	ACO	C1B-N9A-C4A	14.07	151.36	126.64
8	A	902	ACO	N3A-C2A-N1A	-5.52	120.05	128.68
8	A	902	ACO	C5A-C6A-N6A	4.80	127.64	120.35
8	A	902	ACO	N6A-C6A-N1A	-3.31	111.71	118.57
8	A	902	ACO	CAP-C9P-N8P	2.66	121.87	116.58
8	A	902	ACO	P2A-O3A-P1A	-2.61	123.87	132.83
8	A	902	ACO	C6P-C5P-N4P	2.49	120.61	116.42
8	A	902	ACO	CEP-CBP-CAP	2.44	113.06	108.82
8	A	902	ACO	O4B-C1B-C2B	-2.32	103.54	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	902	ACO	C3P-N4P-C5P	-2.01	119.11	122.84

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	902	ACO	C3B-C4B-C5B-O5B
8	A	902	ACO	C5B-O5B-P1A-O1A
8	A	902	ACO	C5B-O5B-P1A-O2A
8	A	902	ACO	CCP-O6A-P2A-O3A
8	A	902	ACO	S1P-C2P-C3P-N4P
8	A	902	ACO	O-C-S1P-C2P
8	A	902	ACO	O4B-C4B-C5B-O5B
8	A	902	ACO	CH3-C-S1P-C2P
8	A	902	ACO	C5P-C6P-C7P-N8P
8	A	902	ACO	P2A-O3A-P1A-O2A
8	A	902	ACO	CCP-O6A-P2A-O4A
8	A	902	ACO	CAP-CBP-CCP-O6A
8	A	902	ACO	CDP-CBP-CCP-O6A
8	A	902	ACO	CEP-CBP-CCP-O6A
8	A	902	ACO	C6P-C7P-N8P-C9P
8	A	902	ACO	N8P-C9P-CAP-OAP
8	A	902	ACO	C3B-O3B-P3B-O9A
8	A	902	ACO	C5B-O5B-P1A-O3A

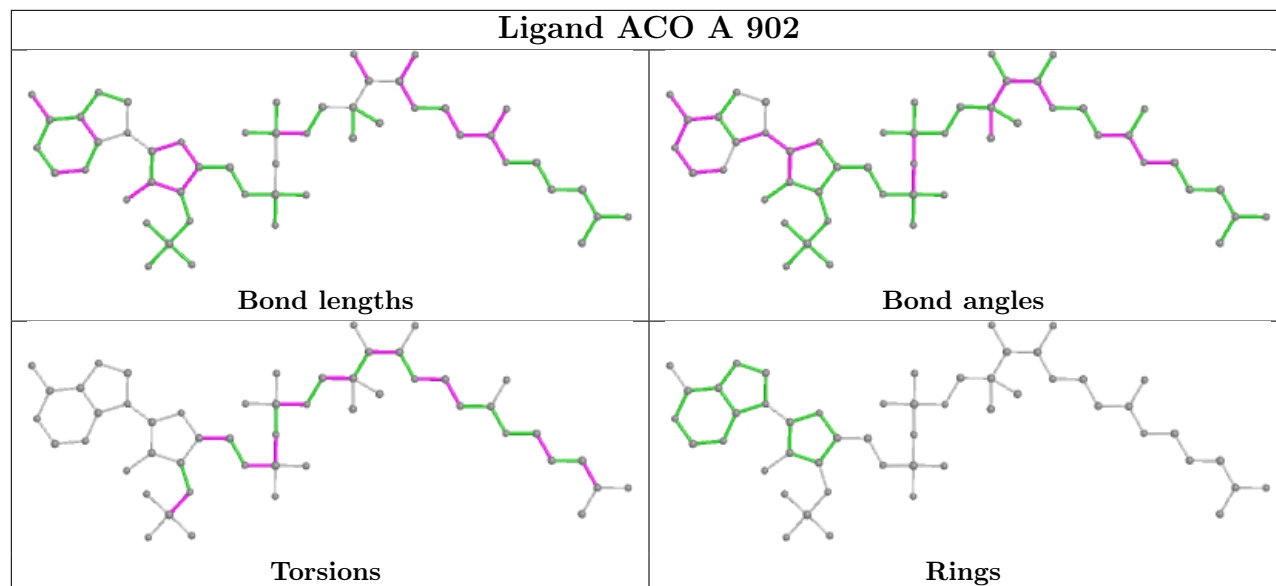
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	902	ACO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



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.

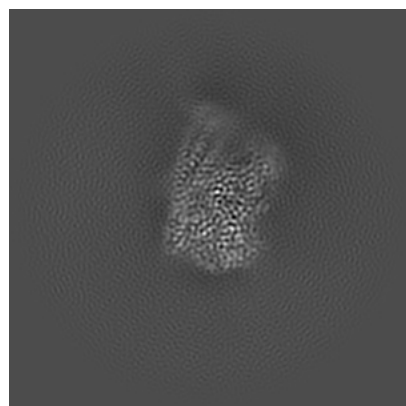
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64517. These allow visual inspection of the internal detail of the map and identification of artifacts.

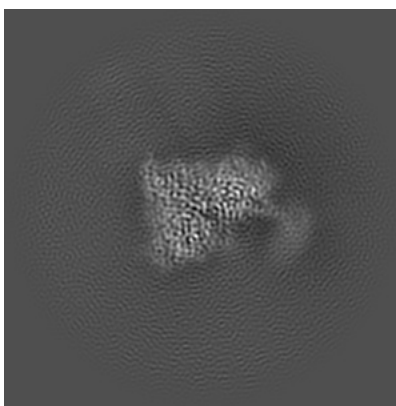
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

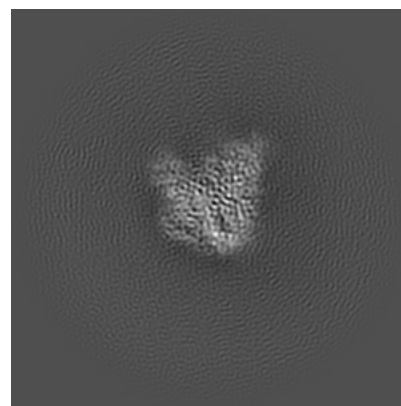
6.1.1 Primary map



X

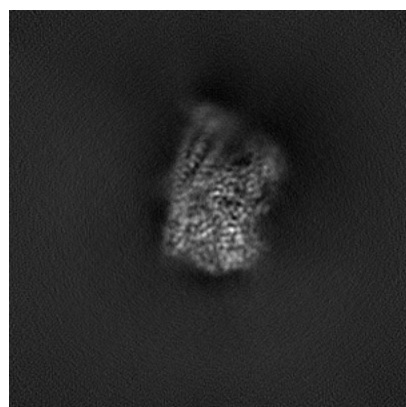


Y

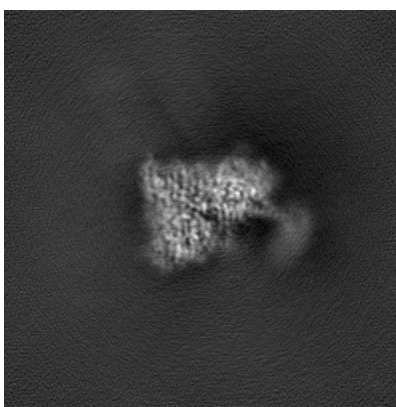


Z

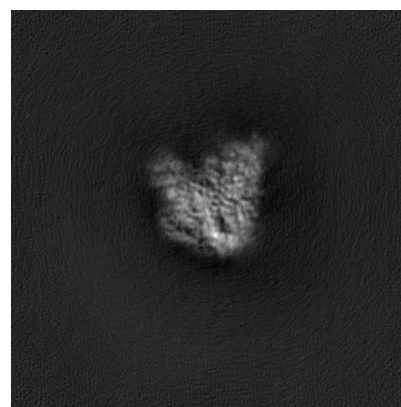
6.1.2 Raw map



X



Y

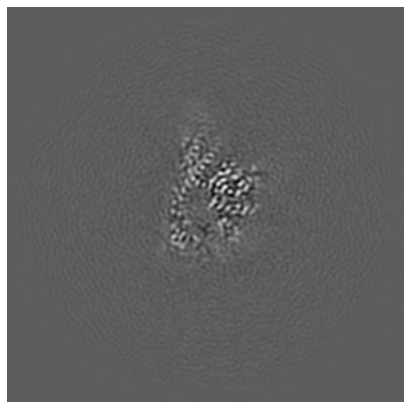


Z

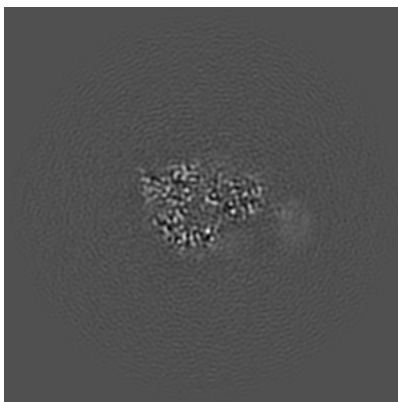
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

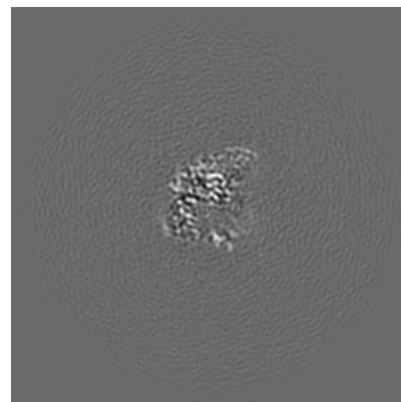
6.2.1 Primary map



X Index: 145

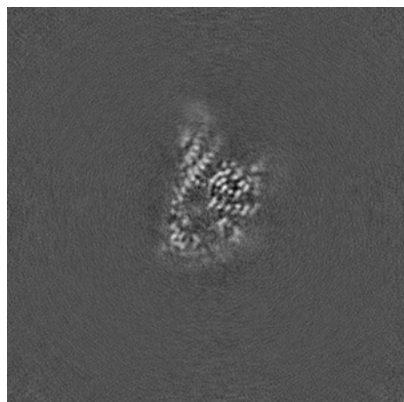


Y Index: 145

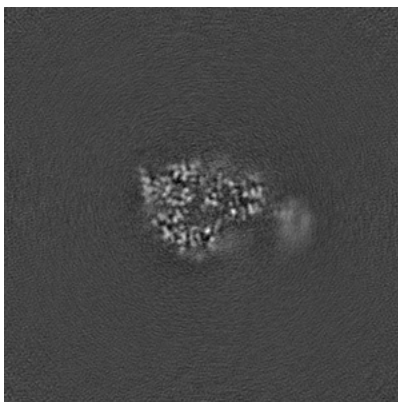


Z Index: 145

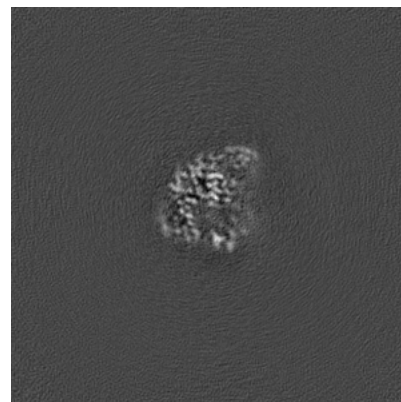
6.2.2 Raw map



X Index: 145



Y Index: 145

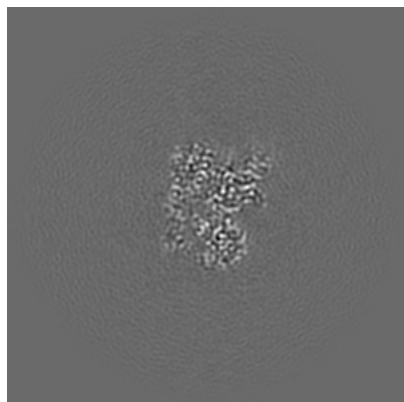


Z Index: 145

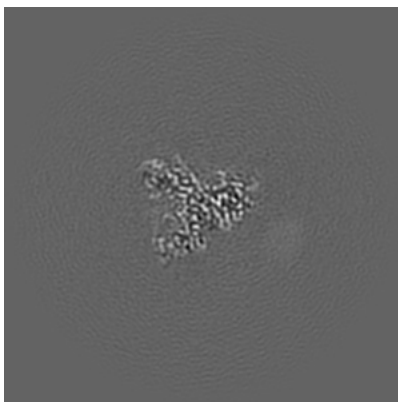
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

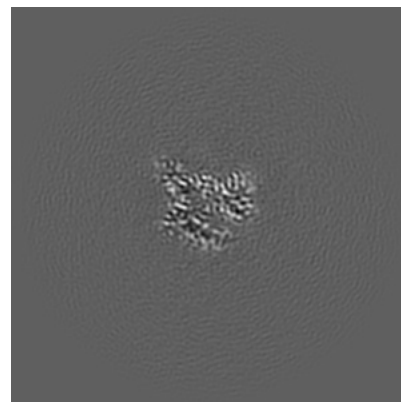
6.3.1 Primary map



X Index: 157

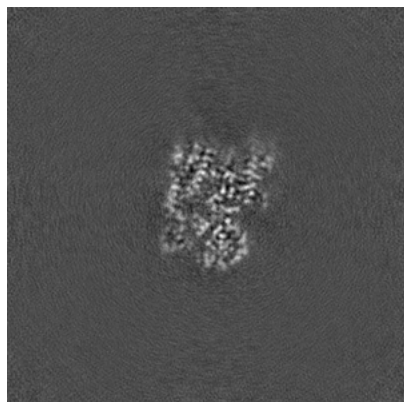


Y Index: 160

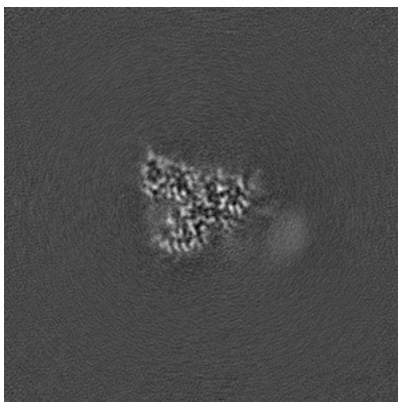


Z Index: 130

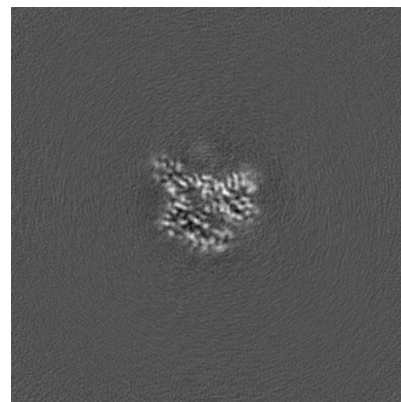
6.3.2 Raw map



X Index: 157



Y Index: 156

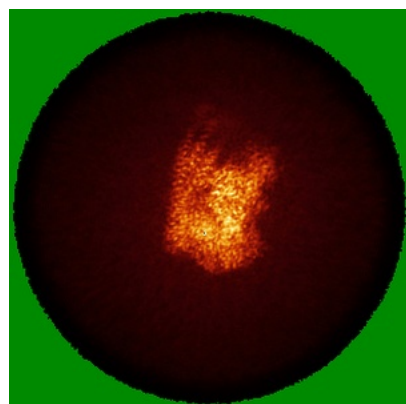


Z Index: 130

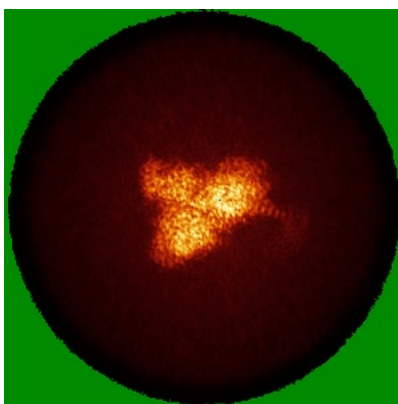
The images above show the largest variance slices of the map in three orthogonal directions.

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

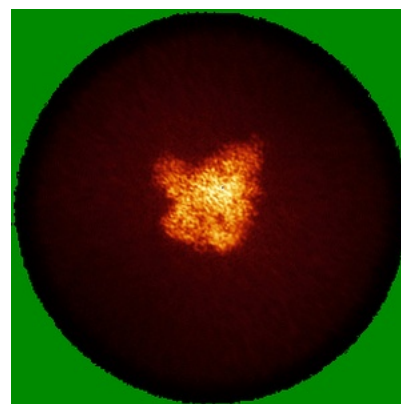
6.4.1 Primary map



X

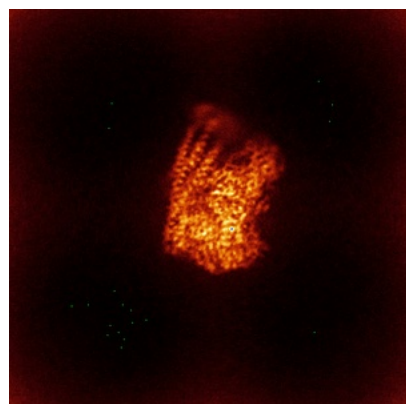


Y

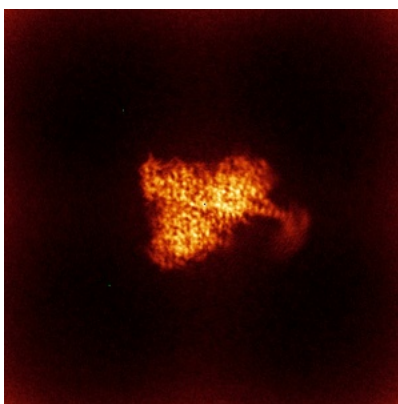


Z

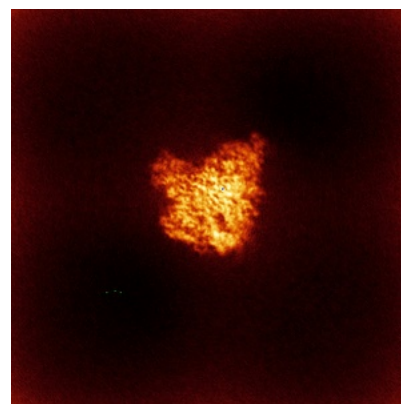
6.4.2 Raw map



X



Y

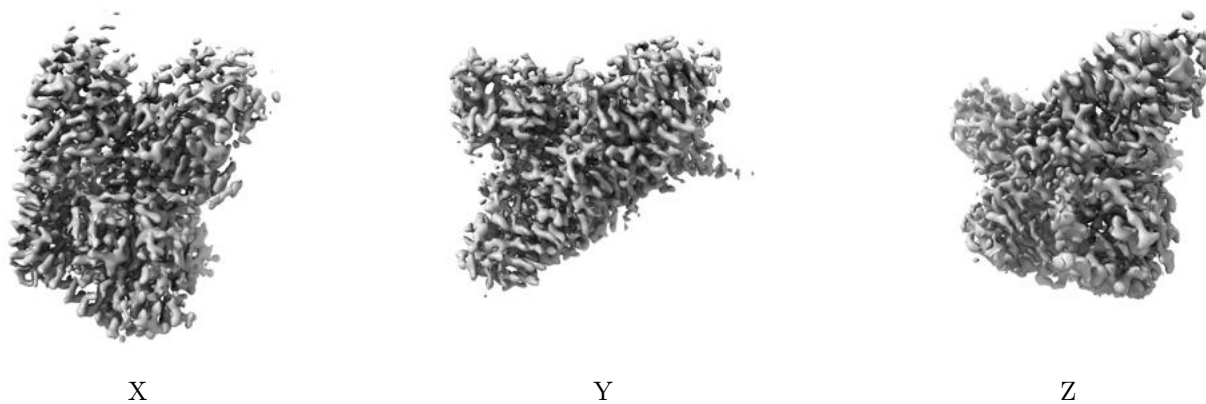


Z

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

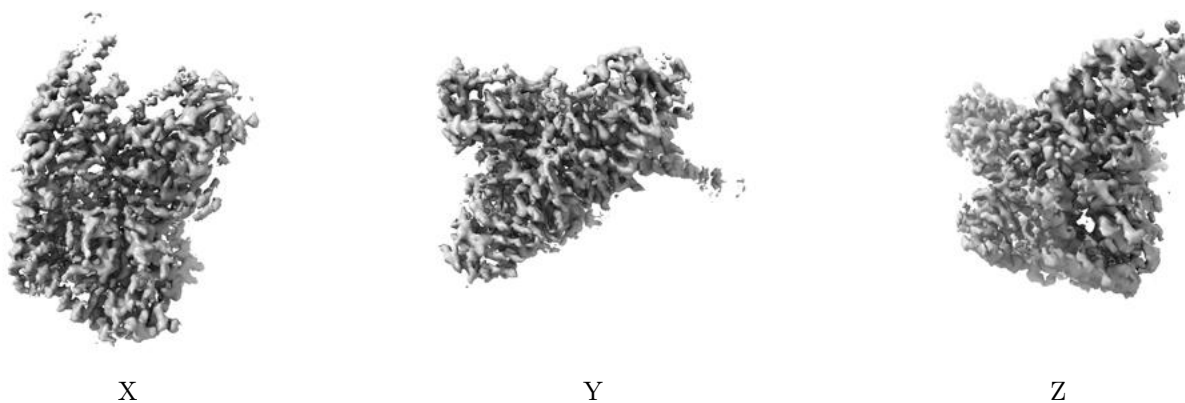
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.278. 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.

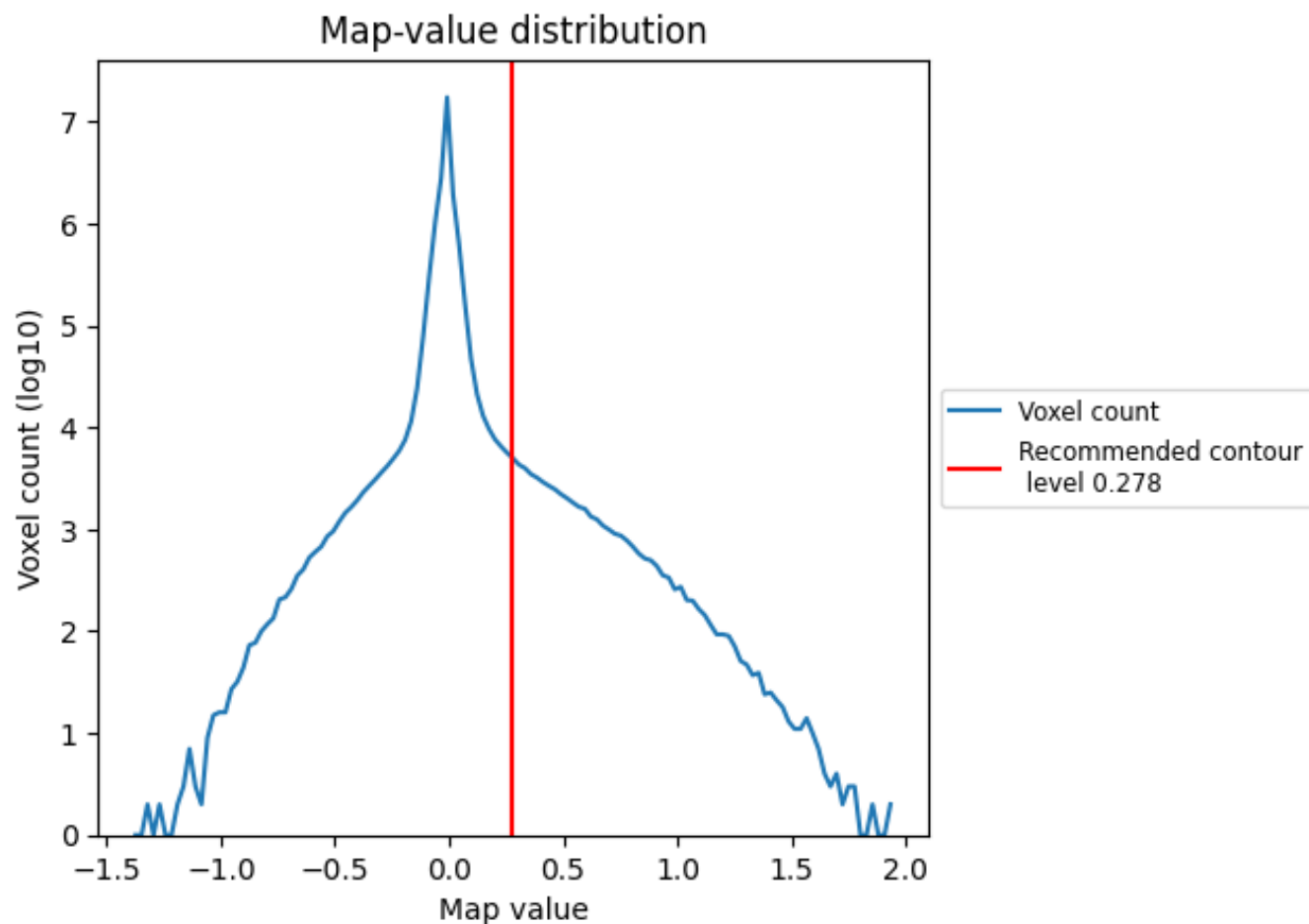
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

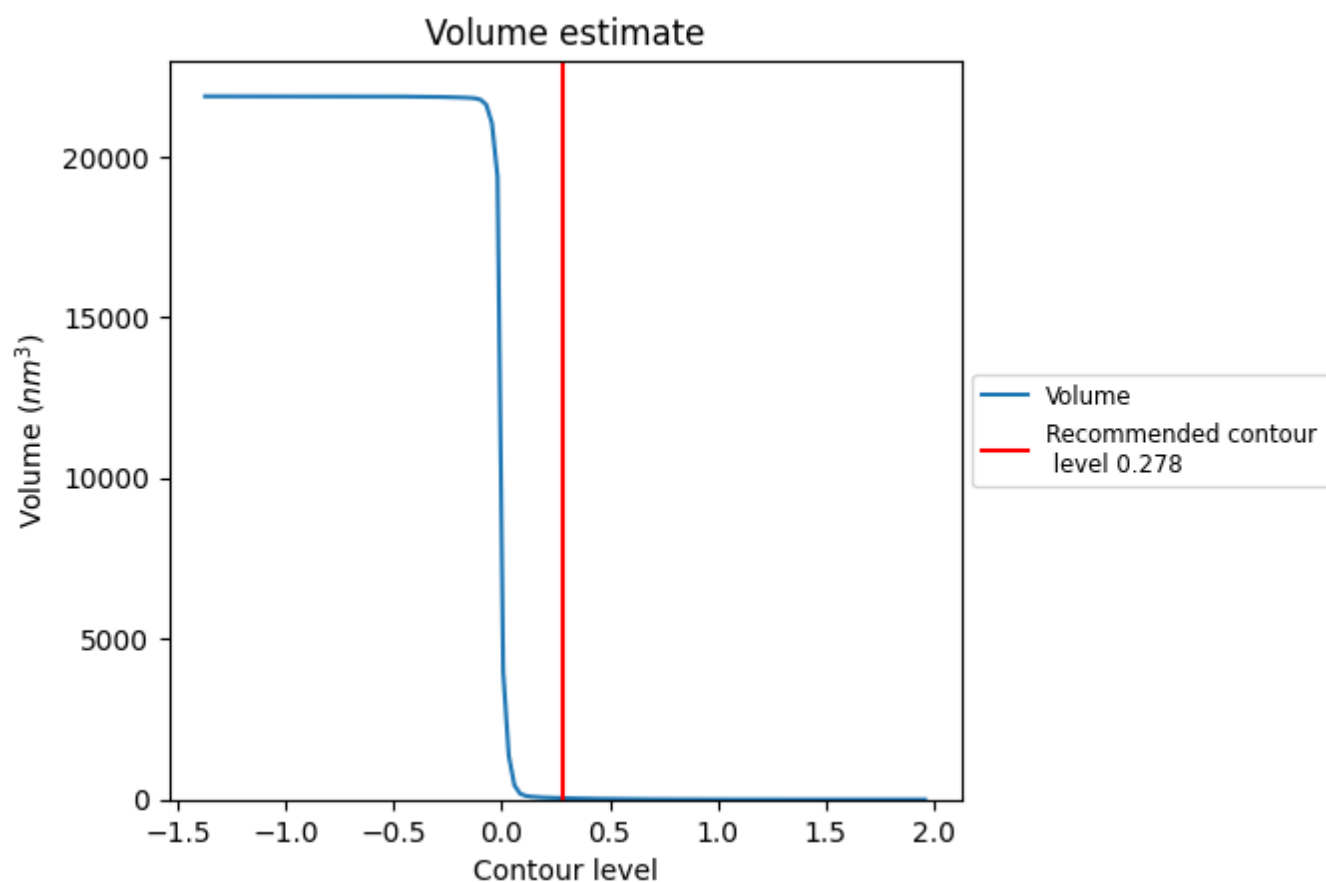
This section contains the results of statistical analysis of the map.

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.

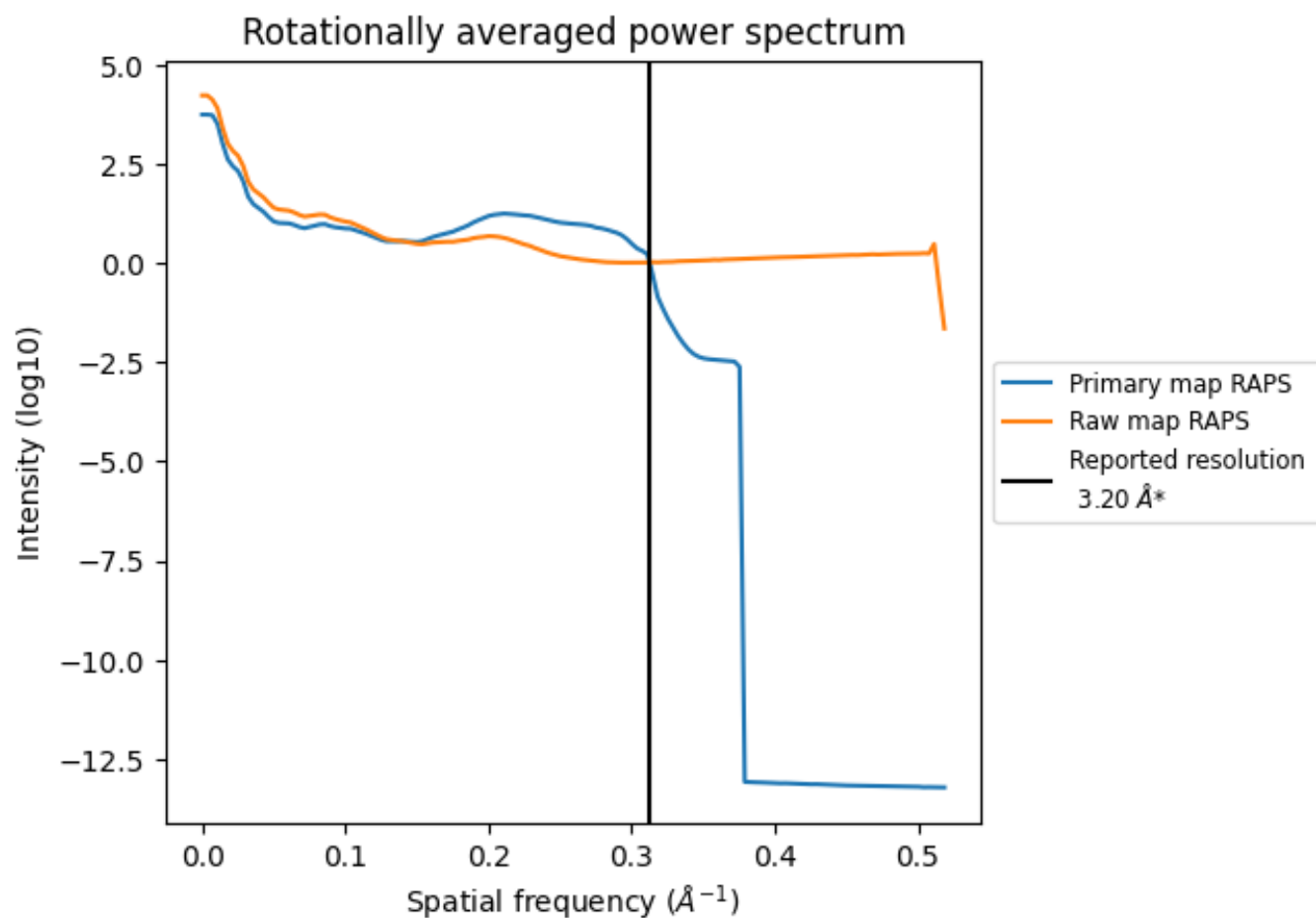
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 ⓘ

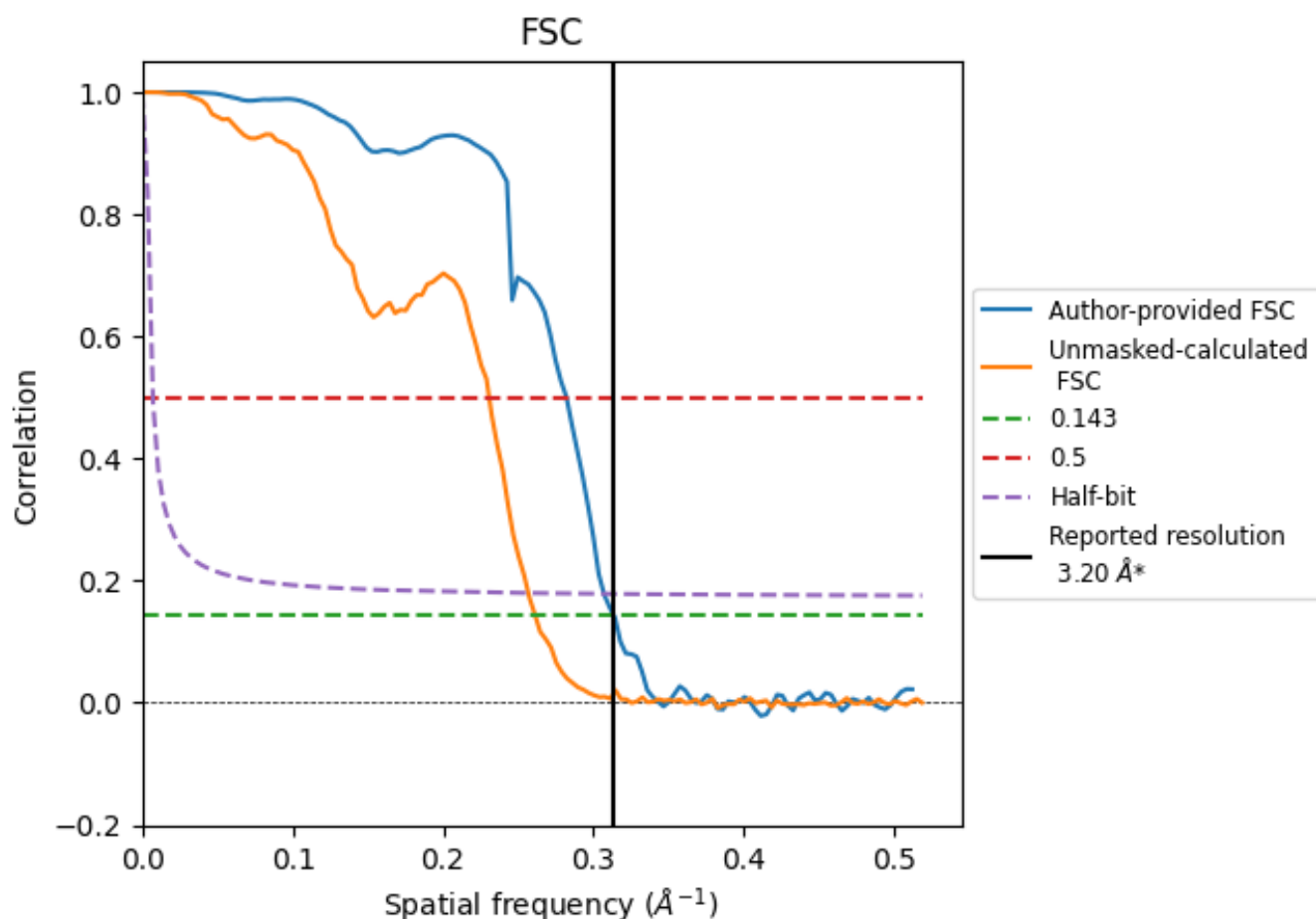


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

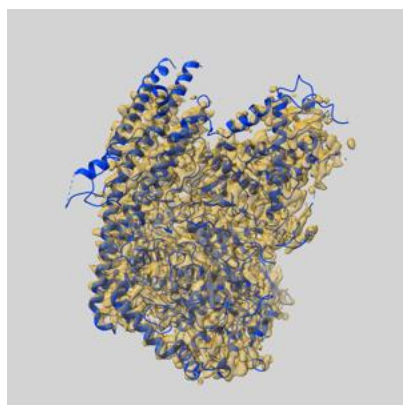
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.55	3.26
Unmasked-calculated*	3.83	4.33	3.90

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

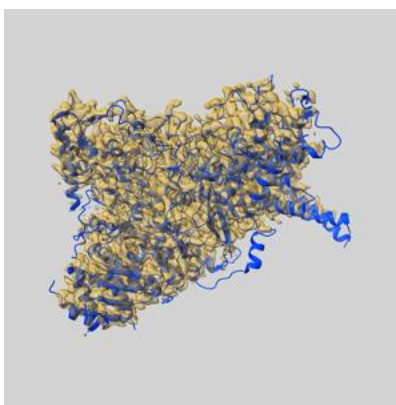
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64517 and PDB model 9UUS. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

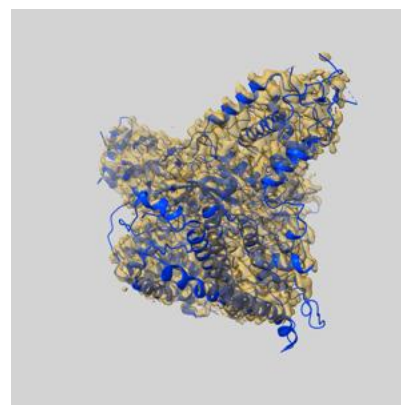
9.1 Map-model overlay [i](#)



X



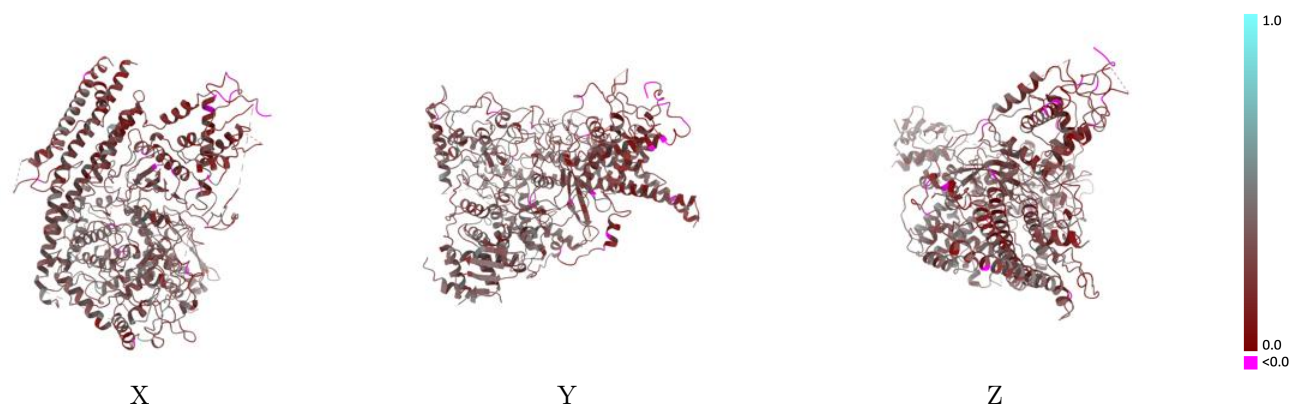
Y



Z

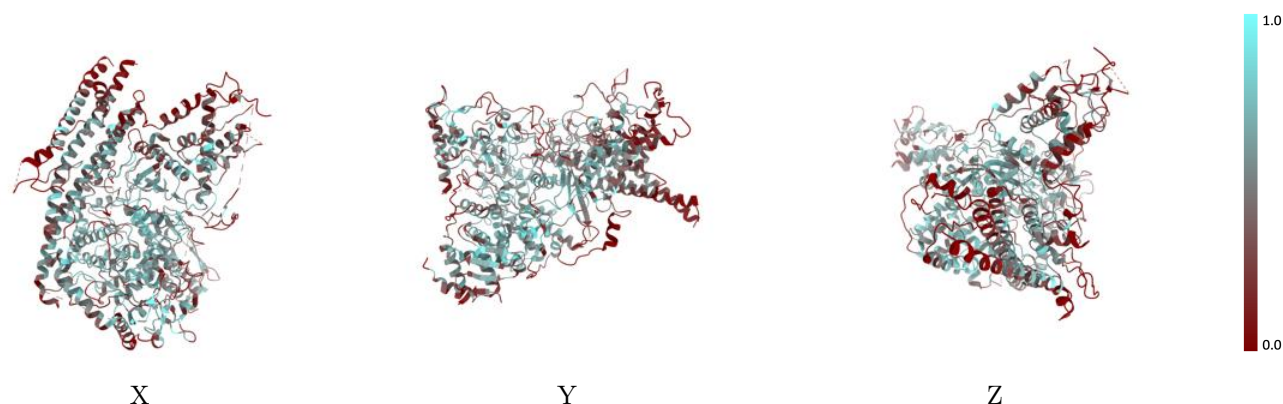
The images above show the 3D surface view of the map at the recommended contour level 0.278 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



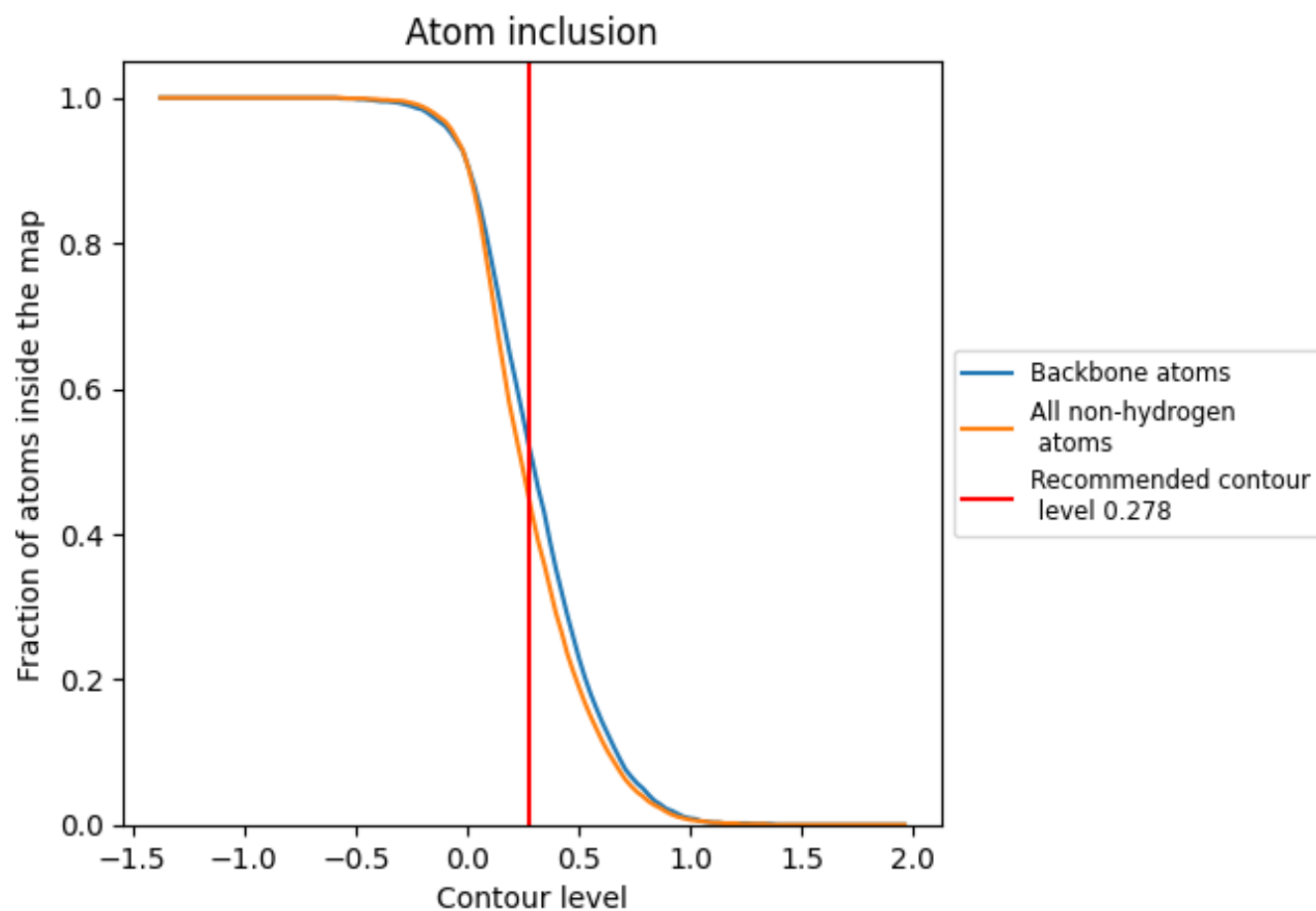
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.278).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 45% 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 (0.278) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4470	<div></div> 0.3040
A	<div></div> 0.4760	<div></div> 0.2930
B	<div></div> 0.4650	<div></div> 0.3180
C	<div></div> 0.4430	<div></div> 0.2960
D	<div></div> 0.2340	<div></div> 0.2700
E	<div></div> 0.4280	<div></div> 0.3400
H	<div></div> 0.2330	<div></div> 0.2930

1.0

0.0

<0.0