



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 09:45 AM EDT

PDB ID : 8GH9  
EMDB ID : EMD-40038  
Title : Cryo-EM structure of hSlo1 in total membrane vesicles  
Authors : Tao, X.; Zhao, C.; MacKinnon, R.  
Deposited on : 2023-03-09  
Resolution : 3.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

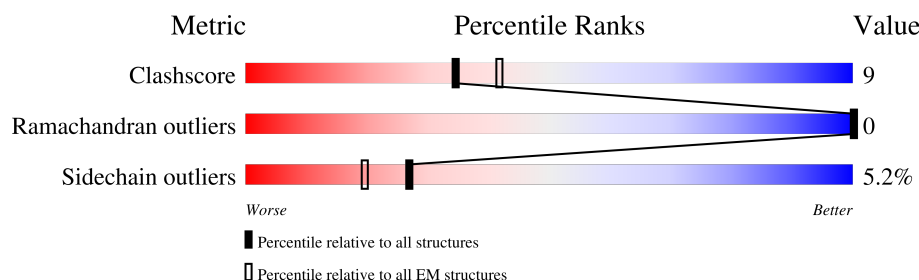
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1072	<div> <div>9%</div> <div>56%</div> <div>20%</div> <div>•</div> <div>23%</div> </div>
1	B	1072	<div> <div>9%</div> <div>58%</div> <div>19%</div> <div>•</div> <div>22%</div> </div>
1	C	1072	<div> <div>12%</div> <div>61%</div> <div>18%</div> <div>•</div> <div>19%</div> </div>
1	D	1072	<div> <div>11%</div> <div>62%</div> <div>17%</div> <div>•</div> <div>20%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27066 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	830	Total	C	N	O	S	1	0
			6644	4314	1077	1208	45		
1	C	866	Total	C	N	O	S	1	0
			6900	4477	1125	1254	44		
1	B	831	Total	C	N	O	S	1	0
			6651	4319	1078	1209	45		
1	D	862	Total	C	N	O	S	1	0
			6871	4459	1121	1247	44		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q12791
A	-14	ALA	-	expression tag	UNP Q12791
A	-13	PRO	-	expression tag	UNP Q12791
A	-12	SER	-	expression tag	UNP Q12791
A	-11	ARG	-	expression tag	UNP Q12791
A	-10	LEU	-	expression tag	UNP Q12791
A	-9	GLU	-	expression tag	UNP Q12791
A	-8	GLU	-	expression tag	UNP Q12791
A	-7	GLU	-	expression tag	UNP Q12791
A	-6	LEU	-	expression tag	UNP Q12791
A	-5	ARG	-	expression tag	UNP Q12791
A	-4	ARG	-	expression tag	UNP Q12791
A	-3	ARG	-	expression tag	UNP Q12791
A	-2	LEU	-	expression tag	UNP Q12791
A	-1	THR	-	expression tag	UNP Q12791
A	0	GLU	-	expression tag	UNP Q12791
A	1	PRO	-	expression tag	UNP Q12791
C	-15	MET	-	expression tag	UNP Q12791
C	-14	ALA	-	expression tag	UNP Q12791
C	-13	PRO	-	expression tag	UNP Q12791
C	-12	SER	-	expression tag	UNP Q12791
C	-11	ARG	-	expression tag	UNP Q12791

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	LEU	-	expression tag	UNP Q12791
C	-9	GLU	-	expression tag	UNP Q12791
C	-8	GLU	-	expression tag	UNP Q12791
C	-7	GLU	-	expression tag	UNP Q12791
C	-6	LEU	-	expression tag	UNP Q12791
C	-5	ARG	-	expression tag	UNP Q12791
C	-4	ARG	-	expression tag	UNP Q12791
C	-3	ARG	-	expression tag	UNP Q12791
C	-2	LEU	-	expression tag	UNP Q12791
C	-1	THR	-	expression tag	UNP Q12791
C	0	GLU	-	expression tag	UNP Q12791
C	1	PRO	-	expression tag	UNP Q12791
B	-15	MET	-	expression tag	UNP Q12791
B	-14	ALA	-	expression tag	UNP Q12791
B	-13	PRO	-	expression tag	UNP Q12791
B	-12	SER	-	expression tag	UNP Q12791
B	-11	ARG	-	expression tag	UNP Q12791
B	-10	LEU	-	expression tag	UNP Q12791
B	-9	GLU	-	expression tag	UNP Q12791
B	-8	GLU	-	expression tag	UNP Q12791
B	-7	GLU	-	expression tag	UNP Q12791
B	-6	LEU	-	expression tag	UNP Q12791
B	-5	ARG	-	expression tag	UNP Q12791
B	-4	ARG	-	expression tag	UNP Q12791
B	-3	ARG	-	expression tag	UNP Q12791
B	-2	LEU	-	expression tag	UNP Q12791
B	-1	THR	-	expression tag	UNP Q12791
B	0	GLU	-	expression tag	UNP Q12791
B	1	PRO	-	expression tag	UNP Q12791
D	-15	MET	-	expression tag	UNP Q12791
D	-14	ALA	-	expression tag	UNP Q12791
D	-13	PRO	-	expression tag	UNP Q12791
D	-12	SER	-	expression tag	UNP Q12791
D	-11	ARG	-	expression tag	UNP Q12791
D	-10	LEU	-	expression tag	UNP Q12791
D	-9	GLU	-	expression tag	UNP Q12791
D	-8	GLU	-	expression tag	UNP Q12791
D	-7	GLU	-	expression tag	UNP Q12791
D	-6	LEU	-	expression tag	UNP Q12791
D	-5	ARG	-	expression tag	UNP Q12791
D	-4	ARG	-	expression tag	UNP Q12791
D	-3	ARG	-	expression tag	UNP Q12791

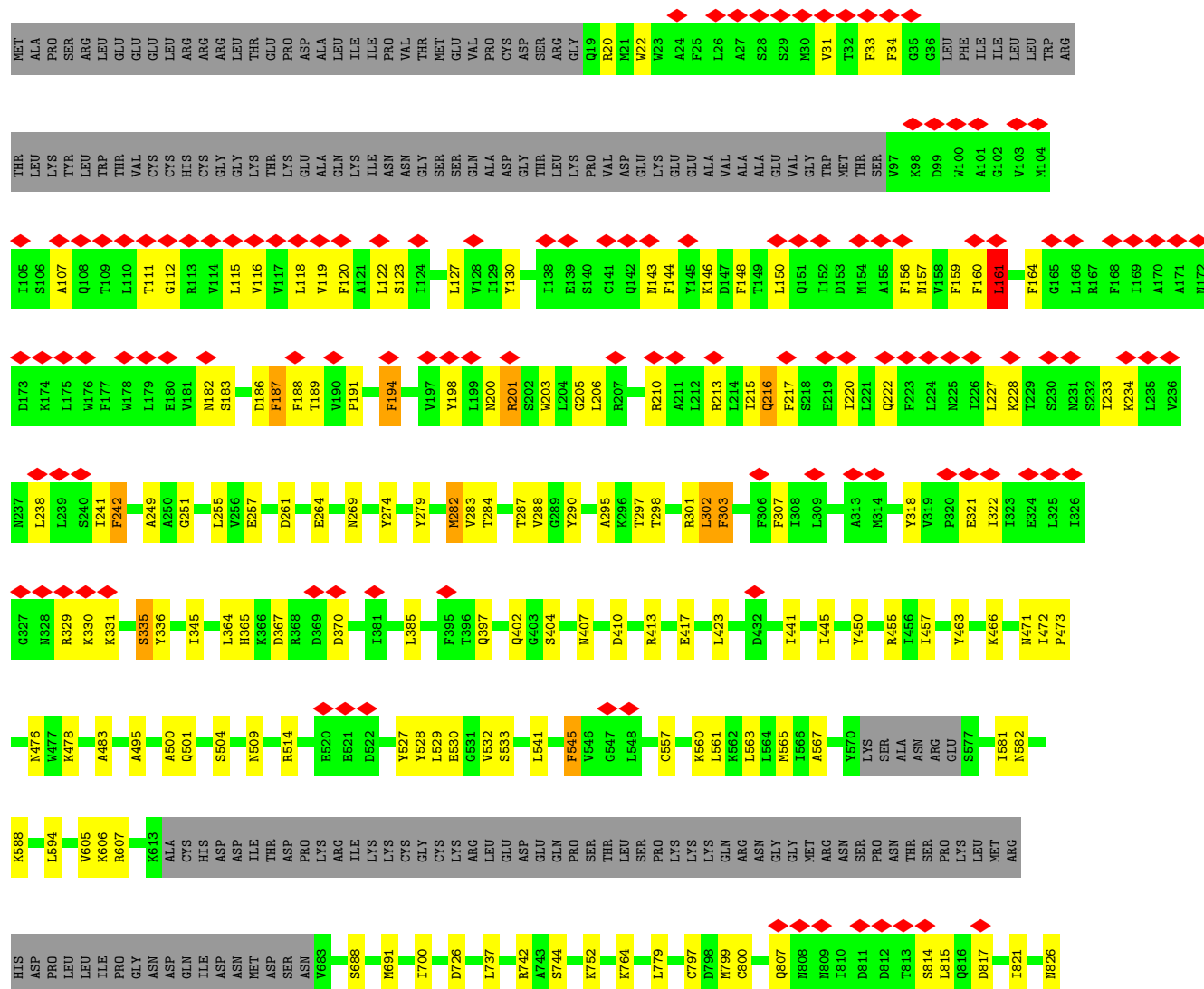
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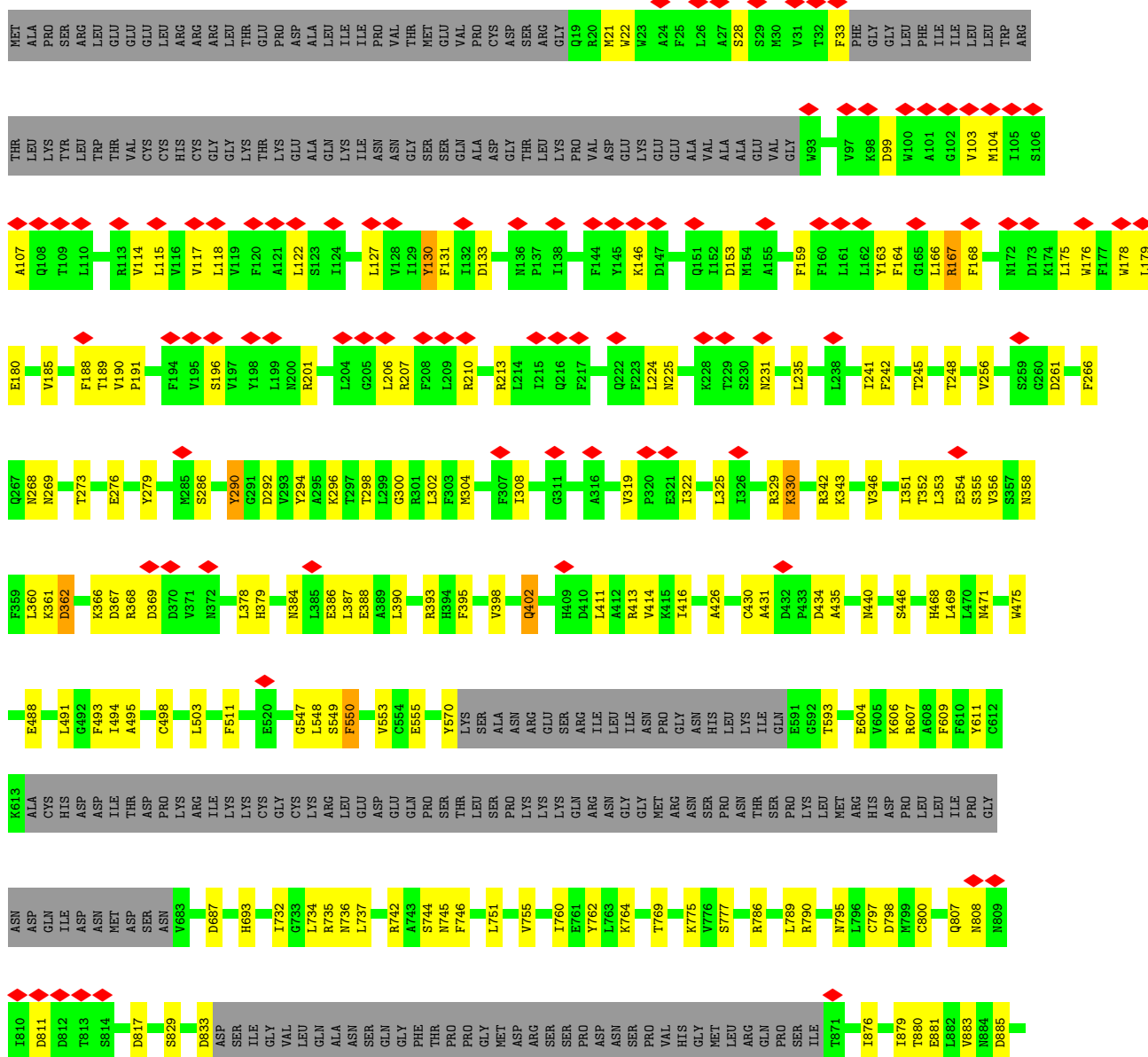
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP Q12791
D	-1	THR	-	expression tag	UNP Q12791
D	0	GLU	-	expression tag	UNP Q12791
D	1	PRO	-	expression tag	UNP Q12791



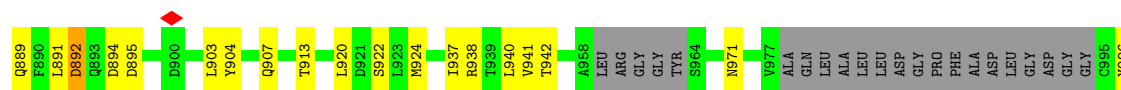
- Molecule 1: Calcium-activated potassium channel subunit alpha-1



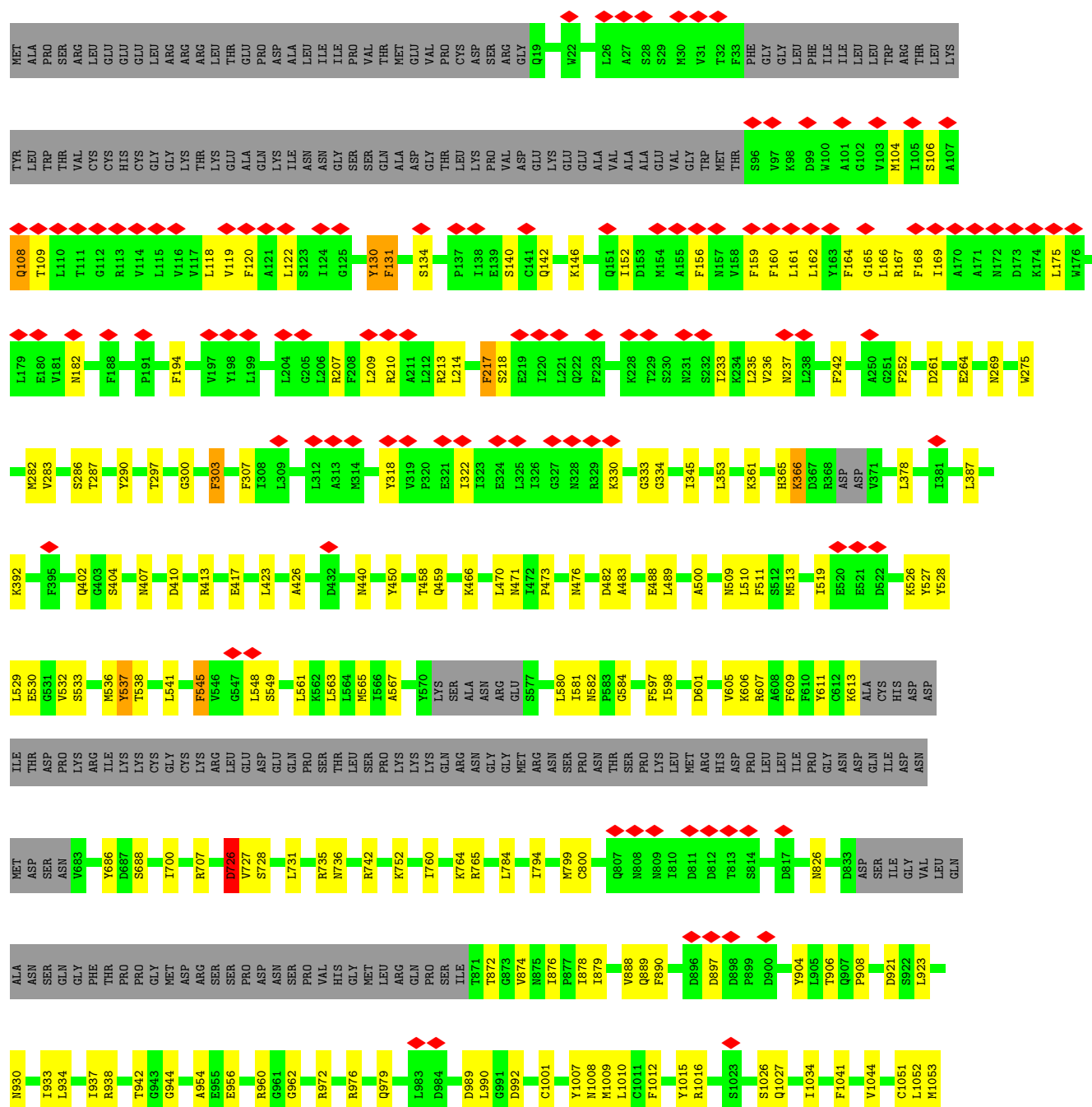
- Molecule 1: Calcium-activated potassium channel subunit alpha-1







● Molecule 1: Calcium-activated potassium channel subunit alpha-1



Q1054  
F1055  
D1056

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	85135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.660	Depositor
Minimum map value	-1.035	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.29	0/6796	0.54	1/9219 (0.0%)
1	B	0.28	0/6803	0.52	0/9229
1	C	0.28	0/7058	0.54	5/9575 (0.1%)
1	D	0.28	0/7027	0.54	3/9532 (0.0%)
All	All	0.28	0/27684	0.53	9/37555 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	LEU	CA-CB-CG	7.18	131.83	115.30
1	C	206	LEU	CA-CB-CG	7.13	131.70	115.30
1	D	235	LEU	CA-CB-CG	6.50	130.24	115.30
1	D	209	LEU	CA-CB-CG	6.32	129.83	115.30
1	D	726	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	302	LEU	CA-CB-CG	5.65	128.30	115.30
1	C	115	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	726	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	214	LEU	CA-CB-CG	5.34	127.57	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6644	0	6608	138	0
1	B	6651	0	6617	115	0
1	C	6900	0	6872	124	0
1	D	6871	0	6853	112	0
All	All	27066	0	26950	475	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 9.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD12	1:A:737:LEU:HB2	1.58	0.83
1:B:411:LEU:HD12	1:B:416:ILE:HD13	1.67	0.77
1:A:827:ILE:HD13	1:A:878:ILE:HD11	1.67	0.76
1:B:164:PHE:HA	1:B:167:ARG:HE	1.51	0.76
1:D:538:THR:HG23	1:D:930:ASN:HD21	1.50	0.75
1:C:161:LEU:HA	1:C:164:PHE:HB3	1.69	0.73
1:A:500:ALA:HA	1:A:1050:PHE:HD2	1.53	0.72
1:B:488:GLU:HA	1:B:736:ASN:HD22	1.57	0.69
1:B:807:GLN:NE2	1:B:808:ASN:OD1	2.27	0.68
1:D:119:VAL:HB	1:D:213:ARG:HD2	1.76	0.68
1:B:971:ASN:H	1:B:1056:ASP:HB2	1.59	0.67
1:A:305:VAL:HG23	1:C:282:MET:HG2	1.74	0.67
1:A:241:ILE:HD11	1:A:318:TYR:HE2	1.60	0.66
1:C:330:LYS:HZ3	1:C:331:LYS:H	1.41	0.66
1:A:512:SER:OG	1:A:514:ARG:NH2	2.29	0.65
1:A:484:ILE:HG22	1:A:934:LEU:HD11	1.77	0.65
1:B:755:VAL:HG12	1:B:777:SER:HB2	1.77	0.65
1:A:273:THR:HG23	1:A:275:TRP:H	1.60	0.65
1:C:295:ALA:O	1:C:301:ARG:NH2	2.30	0.64
1:A:742:ARG:NH2	1:A:774:PRO:O	2.31	0.64
1:D:727:VAL:O	1:D:765:ARG:NH1	2.29	0.64
1:A:378:LEU:HD11	1:A:414:VAL:HG21	1.79	0.63
1:A:471:ASN:ND2	1:C:826[B]:ASN:OD1	2.31	0.63
1:C:799:MET:SD	1:C:800:CYS:N	2.71	0.63
1:D:541:LEU:HD12	1:D:545:PHE:HD2	1.63	0.63
1:C:284:THR:OG1	1:B:290:TYR:OH	2.17	0.62
1:A:339:VAL:HB	1:A:342:ARG:HH21	1.64	0.62
1:A:1017:LEU:HB3	1:A:1031:ARG:HD3	1.80	0.62
1:B:471:ASN:ND2	1:D:826[B]:ASN:OD1	2.33	0.62
1:D:402:GLN:O	1:D:413:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ARG:HD3	1:B:751:LEU:HD11	1.82	0.61
1:A:892:ASP:OD2	1:A:1030:LYS:NZ	2.34	0.61
1:C:471:ASN:OD1	1:B:786:ARG:NH2	2.34	0.61
1:C:1018:ARG:NH1	1:C:1028:CYS:SG	2.74	0.60
1:C:1044:VAL:HG12	1:C:1046:THR:H	1.65	0.60
1:C:222:GLN:NE2	1:C:227:LEU:O	2.33	0.60
1:A:528:TYR:HE2	1:A:905:LEU:HA	1.67	0.60
1:C:1010:LEU:HD23	1:C:1052:LEU:HD12	1.82	0.60
1:C:410:ASP:OD1	1:C:413:ARG:NH2	2.31	0.60
1:A:756:PHE:HB2	1:A:778:ILE:HD13	1.83	0.59
1:C:367:ASP:OD1	1:C:367:ASP:N	2.35	0.59
1:B:189:THR:HG23	1:B:190:VAL:HG23	1.82	0.59
1:C:976:ARG:NH2	1:C:1053:MET:SD	2.75	0.59
1:C:123:SER:HA	1:C:127:LEU:HD23	1.83	0.59
1:C:365:HIS:ND1	1:C:367:ASP:OD1	2.36	0.59
1:D:565:MET:HE2	1:D:597:PHE:HE1	1.66	0.59
1:A:190:VAL:HG23	1:A:191:PRO:HD3	1.85	0.59
1:A:560:LYS:HD3	1:A:1000:PHE:HE2	1.67	0.59
1:C:118:LEU:HB2	1:C:159:PHE:HD2	1.65	0.59
1:D:159:PHE:HA	1:D:162:LEU:HD12	1.85	0.59
1:D:582:ASN:HD22	1:D:1010:LEU:HD22	1.68	0.58
1:D:1010:LEU:HD23	1:D:1052:LEU:HD12	1.85	0.58
1:D:482:ASP:HB3	1:D:934:LEU:HD23	1.83	0.58
1:D:214:LEU:HA	1:D:217:PHE:HB2	1.84	0.58
1:A:689:THR:HG21	1:A:949:LEU:HD21	1.84	0.58
1:C:157:ASN:O	1:C:161:LEU:HD12	2.04	0.58
1:A:735:ARG:NH1	1:A:769:THR:OG1	2.36	0.58
1:B:351:ILE:HD11	1:B:379:HIS:HB2	1.86	0.58
1:D:992:ASP:OD1	1:D:992:ASP:N	2.35	0.58
1:C:335:SER:OG	1:C:336:TYR:N	2.37	0.58
1:A:488:GLU:OE2	1:A:938:ARG:NH1	2.37	0.57
1:C:606:LYS:NZ	1:C:606:LYS:O	2.37	0.57
1:C:529:LEU:HA	1:C:532:VAL:HG12	1.86	0.57
1:D:161:LEU:HA	1:D:164:PHE:HB3	1.86	0.57
1:D:611:TYR:O	1:D:613:LYS:NZ	2.37	0.57
1:A:351:ILE:HD11	1:A:379:HIS:HB2	1.85	0.57
1:B:471:ASN:ND2	1:D:826[A]:ASN:OD1	2.36	0.57
1:C:527:TYR:HB3	1:C:1034:ILE:HD11	1.86	0.57
1:C:876:ILE:HD12	1:C:876:ILE:H	1.69	0.57
1:D:606:LYS:O	1:D:606:LYS:NZ	2.36	0.57
1:D:261:ASP:HB3	1:D:264:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:HIS:O	1:A:258:ASN:ND2	2.38	0.57
1:C:989:ASP:OD1	1:C:989:ASP:N	2.36	0.57
1:B:547:GLY:HA2	1:B:553:VAL:HG11	1.87	0.57
1:C:567:ALA:HB2	1:C:581:ILE:HD13	1.86	0.57
1:C:33:PHE:HB2	1:C:187:PHE:HZ	1.69	0.56
1:D:140:SER:O	1:D:142:GLN:NE2	2.38	0.56
1:B:892:ASP:OD2	1:B:1030:LYS:NZ	2.36	0.56
1:A:113:ARG:NH2	1:A:223:PHE:O	2.38	0.56
1:A:149:THR:HG22	1:A:151:GLN:H	1.69	0.56
1:A:871:THR:OG1	1:A:872:THR:N	2.36	0.56
1:C:370:ASP:N	1:C:370:ASP:OD1	2.39	0.56
1:C:445:ILE:HD13	1:C:472:ILE:HD12	1.86	0.56
1:C:541:LEU:HD12	1:C:545:PHE:HD2	1.71	0.56
1:B:390:LEU:HA	1:B:393:ARG:NH1	2.21	0.56
1:D:166:LEU:HA	1:D:169:ILE:HG22	1.87	0.56
1:A:342:ARG:NH1	1:A:343:LYS:O	2.38	0.56
1:C:563:LEU:HD21	1:C:605:VAL:HA	1.87	0.56
1:D:164:PHE:HA	1:D:167:ARG:HB2	1.88	0.56
1:D:426:ALA:HB2	1:D:440:ASN:HD21	1.70	0.56
1:A:833:ASP:N	1:A:833:ASP:OD1	2.36	0.56
1:B:261:ASP:OD2	1:B:268:ASN:ND2	2.40	0.55
1:D:942:THR:HG22	1:D:944:GLY:H	1.71	0.55
1:D:410:ASP:OD1	1:D:413:ARG:NH2	2.32	0.55
1:A:786:ARG:NH2	1:D:471:ASN:OD1	2.38	0.55
1:C:814:SER:OG	1:C:815:LEU:N	2.40	0.55
1:B:99:ASP:O	1:B:103:VAL:HG13	2.06	0.55
1:B:1015:TYR:HB3	1:B:1048:LEU:HB2	1.89	0.55
1:D:104:MET:HA	1:D:109:THR:HG21	1.88	0.55
1:A:139:GLU:OE1	1:A:204:LEU:N	2.40	0.55
1:D:106:SER:OG	1:D:108:GLN:NE2	2.40	0.55
1:C:191:PRO:HA	1:C:194:PHE:HB2	1.88	0.55
1:D:233:ILE:O	1:D:237:ASN:ND2	2.40	0.55
1:B:469:LEU:HD21	1:B:475:TRP:CZ2	2.42	0.55
1:B:997:GLY:HA3	1:B:1039:TYR:CZ	2.41	0.55
1:C:407:ASN:OD1	1:C:410:ASP:N	2.33	0.54
1:C:561:LEU:HD12	1:C:607:ARG:HB2	1.88	0.54
1:C:402:GLN:O	1:C:413:ARG:NH2	2.40	0.54
1:A:140:SER:OG	1:A:141:CYS:N	2.41	0.54
1:A:147:ASP:OD1	1:A:147:ASP:N	2.40	0.54
1:A:287:THR:OG1	1:C:287:THR:O	2.26	0.54
1:D:210:ARG:HA	1:D:213:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:CYS:SG	1:B:798:ASP:N	2.81	0.54
1:B:292:ASP:OD1	1:B:292:ASP:N	2.40	0.54
1:C:364:LEU:HD11	1:C:397:GLN:HE21	1.72	0.54
1:B:378:LEU:HD21	1:B:414:VAL:HG21	1.88	0.54
1:A:175:LEU:HA	1:A:178:TRP:HD1	1.73	0.54
1:A:455:ARG:NH2	1:A:931:ASP:OD1	2.41	0.54
1:A:471:ASN:ND2	1:C:826[A]:ASN:OD1	2.41	0.54
1:A:707:ARG:NH2	1:A:788:ASP:OD1	2.40	0.54
1:C:283:VAL:HG23	1:C:288:VAL:HG23	1.89	0.54
1:A:292:ASP:OD1	1:A:292:ASP:N	2.39	0.54
1:D:976:ARG:NH2	1:D:1053:MET:SD	2.81	0.53
1:A:186:ASP:HA	1:A:189:THR:HG22	1.89	0.53
1:B:342:ARG:NH1	1:B:343:LYS:O	2.41	0.53
1:D:527:TYR:HB3	1:D:1034:ILE:HD11	1.89	0.53
1:C:186:ASP:HA	1:C:189:THR:HG22	1.91	0.53
1:C:217:PHE:HA	1:C:220:ILE:HD12	1.90	0.53
1:B:742:ARG:NH2	1:B:775:LYS:O	2.40	0.53
1:A:315:PHE:O	1:A:319:VAL:HG23	2.08	0.53
1:B:491:LEU:HD12	1:B:737:LEU:HB2	1.90	0.53
1:D:417:GLU:OE2	1:D:450:TYR:OH	2.26	0.53
1:C:143:ASN:HD22	1:C:146:LYS:HG2	1.74	0.53
1:D:686:TYR:OH	1:D:972:ARG:NH2	2.42	0.53
1:A:367:ASP:OD1	1:A:367:ASP:N	2.42	0.52
1:B:745:ASN:HD22	1:B:1053:MET:HB3	1.73	0.52
1:B:494:ILE:HG23	1:B:879:ILE:HD11	1.91	0.52
1:D:511:PHE:HE2	1:D:933:ILE:HG23	1.73	0.52
1:C:466:LYS:HE2	1:C:483:ALA:HB3	1.92	0.52
1:C:257:GLU:OE1	1:C:297:THR:OG1	2.27	0.52
1:B:28:SER:HB2	1:B:191:PRO:HB2	1.91	0.52
1:B:570:TYR:HA	1:B:593:THR:HG22	1.92	0.52
1:D:561:LEU:HD23	1:D:607:ARG:HB3	1.92	0.52
1:A:795:ASN:OD1	1:A:795:ASN:N	2.43	0.52
1:C:261:ASP:HB3	1:C:264:GLU:HB2	1.92	0.52
1:D:536:MET:HB2	1:D:598:ILE:HG12	1.92	0.51
1:A:286:SER:O	1:A:286:SER:OG	2.25	0.51
1:B:736:ASN:OD1	1:B:736:ASN:N	2.33	0.51
1:A:799:MET:SD	1:A:801:VAL:HG23	2.50	0.51
1:B:503:LEU:HD21	1:B:1052:LEU:HD11	1.92	0.51
1:D:989:ASP:OD1	1:D:989:ASP:N	2.44	0.51
1:C:279:TYR:O	1:C:283:VAL:HG12	2.11	0.51
1:B:224:LEU:O	1:B:225:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:OE2	1:A:321:GLU:N	2.44	0.51
1:D:269:ASN:OD1	1:D:269:ASN:N	2.44	0.51
1:C:269:ASN:N	1:C:269:ASN:OD1	2.42	0.51
1:C:495:ALA:HB2	1:C:737:LEU:HD12	1.92	0.50
1:D:530:GLU:O	1:D:533:SER:OG	2.28	0.50
1:A:257:GLU:OE2	1:A:272:LEU:N	2.41	0.50
1:A:346:VAL:HG21	1:A:416:ILE:HG22	1.93	0.50
1:A:697:PRO:HB3	1:A:771:HIS:HD2	1.74	0.50
1:A:907:GLN:HE22	1:A:1018:ARG:HH21	1.58	0.50
1:C:744:SER:HB3	1:C:972:ARG:HG2	1.93	0.50
1:A:812:ASP:N	1:A:812:ASP:OD1	2.44	0.50
1:C:119:VAL:HG22	1:C:213:ARG:HD3	1.94	0.50
1:C:182:ASN:OD1	1:C:213:ARG:NH2	2.45	0.50
1:C:980:LEU:HD11	1:C:1009:MET:HE1	1.93	0.50
1:A:219:GLU:OE1	1:A:219:GLU:N	2.45	0.49
1:A:402:GLN:O	1:A:413:ARG:NH2	2.45	0.49
1:D:541:LEU:H	1:D:541:LEU:HD23	1.77	0.49
1:D:794:ILE:HG13	1:D:876:ILE:HD11	1.94	0.49
1:A:301:ARG:HG3	1:C:279:TYR:CD2	2.47	0.49
1:A:829:SER:HB2	1:D:473:PRO:HG3	1.93	0.49
1:A:319:VAL:HA	1:A:322:ILE:HG12	1.94	0.49
1:C:457:ILE:HD13	1:C:927:THR:HG23	1.94	0.49
1:A:520:GLU:OE1	1:A:520:GLU:N	2.45	0.49
1:A:564:LEU:HB3	1:A:598:ILE:HG23	1.94	0.49
1:A:601:ASP:OD1	1:A:602:ALA:N	2.44	0.49
1:B:604:GLU:HG2	1:B:607:ARG:HD2	1.95	0.49
1:B:273:THR:OG1	1:B:276:GLU:OE1	2.21	0.49
1:B:362:ASP:O	1:B:368:ARG:NH2	2.34	0.49
1:D:1026:SER:OG	1:D:1027:GLN:N	2.45	0.49
1:C:205:GLY:HA3	1:C:255:LEU:HD13	1.95	0.49
1:C:330:LYS:HZ3	1:C:331:LYS:N	2.09	0.49
1:B:894:ASP:OD1	1:B:894:ASP:N	2.46	0.49
1:A:95:THR:HG22	1:A:98:LYS:HE3	1.95	0.49
1:B:118:LEU:O	1:B:122:LEU:HG	2.13	0.49
1:A:560:LYS:HD3	1:A:1000:PHE:CE2	2.48	0.48
1:A:906:THR:HG22	1:A:908:PRO:HD2	1.94	0.48
1:C:251:GLY:HA2	1:C:274:TYR:HE1	1.78	0.48
1:D:407:ASN:OD1	1:D:410:ASP:N	2.34	0.48
1:C:238:LEU:HD13	1:C:322:ILE:HG12	1.94	0.48
1:B:130:TYR:CE2	1:B:207:ARG:HG2	2.48	0.48
1:D:799:MET:SD	1:D:800:CYS:N	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:GLU:OE2	1:D:960:ARG:NH1	2.43	0.48
1:A:392:LYS:HD2	1:A:392:LYS:HA	1.54	0.48
1:A:975:CYS:HB2	1:A:1052:LEU:HB2	1.95	0.48
1:A:534:ASN:HD21	1:A:1036:ASN:HD22	1.61	0.48
1:A:103:VAL:HG21	1:A:109:THR:H	1.78	0.48
1:A:115:LEU:HG	1:A:163:TYR:OH	2.13	0.48
1:B:735:ARG:NH1	1:B:769:THR:OG1	2.46	0.48
1:A:687:ASP:N	1:A:692:PHE:O	2.45	0.48
1:C:817:ASP:O	1:C:821:ILE:HD12	2.13	0.48
1:C:992:ASP:OD1	1:C:992:ASP:N	2.35	0.48
1:B:353:LEU:HD11	1:B:386:GLU:HB2	1.95	0.48
1:B:358:ASN:OD1	1:B:361:LYS:NZ	2.38	0.48
1:D:466:LYS:HE3	1:D:938:ARG:HH22	1.79	0.48
1:A:563:LEU:HD21	1:A:605:VAL:HA	1.95	0.48
1:A:996:TYR:CZ	1:A:1037:PRO:HG2	2.49	0.48
1:B:304:MET:O	1:B:308:ILE:HG22	2.14	0.48
1:B:319:VAL:HA	1:B:322:ILE:HG22	1.95	0.48
1:C:183:SER:O	1:C:187:PHE:HB3	2.14	0.47
1:C:222:GLN:O	1:C:228:LYS:NZ	2.47	0.47
1:B:196:SER:OG	1:B:201:ARG:O	2.32	0.47
1:B:235:LEU:HB2	1:B:325:LEU:HD12	1.97	0.47
1:D:611:TYR:HD2	1:D:613:LYS:HZ2	1.62	0.47
1:A:261:ASP:HB2	1:A:264:GLU:HB2	1.95	0.47
1:A:797:CYS:SG	1:A:798:ASP:N	2.88	0.47
1:A:924:MET:HA	1:A:927:THR:HG22	1.96	0.47
1:C:118:LEU:HD22	1:C:159:PHE:HB3	1.96	0.47
1:A:261:ASP:OD2	1:A:268:ASN:ND2	2.47	0.47
1:C:417:GLU:OE1	1:C:417:GLU:N	2.46	0.47
1:B:998:ASP:O	1:B:1002:LYS:HG2	2.14	0.47
1:A:880:THR:HG21	1:A:891:LEU:HD11	1.97	0.47
1:C:530:GLU:O	1:C:533:SER:OG	2.32	0.47
1:B:795:ASN:HA	1:B:876:ILE:HD11	1.95	0.47
1:B:176:TRP:HA	1:B:179:LEU:HB2	1.96	0.47
1:D:303:PHE:O	1:D:307:PHE:HD1	1.96	0.47
1:D:582:ASN:O	1:D:1054:GLN:NE2	2.48	0.47
1:C:215:ILE:HG12	1:C:241:ILE:HG22	1.96	0.47
1:C:385:LEU:H	1:C:385:LEU:HD23	1.79	0.47
1:C:455:ARG:HH22	1:C:928:TYR:HA	1.80	0.47
1:C:700:ILE:HD13	1:C:764:LYS:HE3	1.97	0.47
1:B:175:LEU:HA	1:B:178:TRP:CE2	2.49	0.47
1:B:330:LYS:HA	1:B:330:LYS:HD2	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:THR:O	1:B:356:VAL:HG22	2.14	0.47
1:A:555:GLU:HB3	1:A:1004:LEU:HD12	1.96	0.47
1:C:345:ILE:HD12	1:C:423:LEU:HD13	1.97	0.47
1:D:509:ASN:HB3	1:D:532:VAL:HG23	1.95	0.47
1:A:534:ASN:ND2	1:A:1036:ASN:HD22	2.13	0.47
1:C:330:LYS:HD2	1:C:330:LYS:HA	1.56	0.47
1:C:560:LYS:HD3	1:C:560:LYS:HA	1.69	0.47
1:B:127:LEU:HG	1:B:131:PHE:CZ	2.50	0.47
1:C:122:LEU:HA	1:C:156:PHE:HE1	1.79	0.47
1:D:330:LYS:HD2	1:D:333:GLY:HA3	1.97	0.46
1:A:503:LEU:HD21	1:A:1052:LEU:HD11	1.97	0.46
1:A:603:LYS:HE3	1:A:603:LYS:HB3	1.78	0.46
1:B:346:VAL:HG21	1:B:416:ILE:HG22	1.97	0.46
1:B:1008:ASN:OD1	1:B:1008:ASN:N	2.48	0.46
1:D:700:ILE:HG21	1:D:764:LYS:NZ	2.29	0.46
1:D:726:ASP:OD2	1:D:728:SER:N	2.47	0.46
1:A:410:ASP:OD2	1:A:413:ARG:NH2	2.46	0.46
1:C:1026:SER:OG	1:C:1027:GLN:N	2.48	0.46
1:D:283:VAL:HG11	1:D:290:TYR:HB2	1.98	0.46
1:A:335:SER:OG	1:A:336:TYR:N	2.48	0.46
1:A:1016:ARG:NH2	1:A:1047:ASP:OD2	2.44	0.46
1:C:157:ASN:HA	1:C:160:PHE:HD1	1.80	0.46
1:C:476:ASN:OD1	1:C:476:ASN:N	2.48	0.46
1:B:426:ALA:HB2	1:B:440:ASN:HD21	1.80	0.46
1:C:249:ALA:HB1	1:C:307:PHE:HE1	1.81	0.46
1:C:509:ASN:ND2	1:C:528:TYR:OH	2.43	0.46
1:D:584:GLY:HA3	1:D:1008:ASN:ND2	2.31	0.46
1:C:872:THR:OG1	1:C:873:GLY:N	2.49	0.46
1:B:493:PHE:HE2	1:B:920:LEU:HD21	1.80	0.46
1:C:111:THR:O	1:C:116:VAL:HB	2.16	0.46
1:B:390:LEU:HA	1:B:393:ARG:HH12	1.80	0.46
1:A:139:GLU:HB3	1:A:204:LEU:H	1.80	0.46
1:A:324:GLU:HG2	1:A:325:LEU:HD22	1.96	0.46
1:C:417:GLU:OE2	1:C:450:TYR:OH	2.25	0.46
1:B:402:GLN:O	1:B:413:ARG:NH2	2.48	0.46
1:C:20:ARG:HE	1:C:22:TRP:HB3	1.80	0.46
1:B:245:THR:HA	1:B:248:THR:HG22	1.97	0.46
1:B:606:LYS:HA	1:B:606:LYS:HD3	1.71	0.46
1:B:811:ASP:OD1	1:B:811:ASP:N	2.49	0.46
1:D:488:GLU:HA	1:D:736:ASN:HD21	1.80	0.46
1:C:473:PRO:HG3	1:B:829:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1017:LEU:HA	1:B:1031:ARG:HG2	1.98	0.45
1:D:1016:ARG:NH2	1:D:1044:VAL:H	2.14	0.45
1:C:303:PHE:O	1:C:307:PHE:HD2	1.99	0.45
1:B:256:VAL:HG11	1:B:300:GLY:HA2	1.99	0.45
1:A:410:ASP:O	1:A:414:VAL:HG23	2.17	0.45
1:A:181:VAL:HA	1:A:184:VAL:HG22	1.98	0.45
1:A:731:LEU:HD23	1:A:731:LEU:H	1.81	0.45
1:C:298:THR:O	1:C:302:LEU:HG	2.17	0.45
1:C:122:LEU:HD22	1:C:210:ARG:HD2	1.99	0.45
1:C:1016:ARG:HH21	1:C:1044:VAL:H	1.63	0.45
1:A:360:LEU:HD13	1:A:364:LEU:HD23	1.99	0.45
1:A:747:HIS:CE1	1:A:971:ASN:HD21	2.33	0.45
1:A:823:ALA:O	1:A:827:ILE:HG22	2.17	0.45
1:C:441:ILE:HD12	1:C:441:ILE:HA	1.83	0.45
1:C:742:ARG:NH2	1:C:752:LYS:O	2.39	0.45
1:D:417:GLU:OE1	1:D:417:GLU:N	2.47	0.45
1:A:894:ASP:OD1	1:A:894:ASP:N	2.44	0.45
1:B:153:ASP:N	1:B:153:ASP:OD2	2.50	0.45
1:D:353:LEU:HD21	1:D:387:LEU:HB2	1.99	0.45
1:A:490:LYS:NZ	1:A:881:GLU:OE2	2.37	0.45
1:A:785:SER:HB3	1:A:788:ASP:HB2	1.99	0.45
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.79	0.45
1:B:352:THR:HG22	1:B:353:LEU:H	1.82	0.45
1:C:233:ILE:HG13	1:C:234:LYS:N	2.31	0.44
1:C:318:TYR:O	1:C:321:GLU:HG2	2.17	0.44
1:B:298:THR:O	1:B:302:LEU:HG	2.17	0.44
1:D:799:MET:HE3	1:D:879:ILE:HG13	2.00	0.44
1:A:966:PRO:HG2	1:A:967:GLN:HE21	1.82	0.44
1:C:201:ARG:HD3	1:C:203:TRP:HB2	1.98	0.44
1:B:176:TRP:O	1:B:180:GLU:HG3	2.16	0.44
1:D:1007:TYR:HB2	1:D:1009:MET:HG2	1.99	0.44
1:A:795:ASN:HA	1:A:876:ILE:HD11	1.98	0.44
1:D:297:THR:HG23	1:D:300:GLY:H	1.81	0.44
1:D:345:ILE:HD12	1:D:423:LEU:HD13	1.98	0.44
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.85	0.44
1:D:519:ILE:HB	1:D:526:LYS:HB3	2.00	0.44
1:D:742:ARG:NH2	1:D:752:LYS:O	2.38	0.44
1:C:238:LEU:HA	1:C:241:ILE:HG12	2.00	0.44
1:C:906:THR:HG22	1:C:908:PRO:HD2	1.98	0.44
1:B:261:ASP:H	1:B:266:PHE:HA	1.82	0.44
1:D:567:ALA:HB2	1:D:581:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:CYS:SG	1:B:431:ALA:N	2.91	0.44
1:C:898:ASP:O	1:C:901:THR:OG1	2.35	0.44
1:C:691:MET:HG2	1:C:974:ARG:HH22	1.82	0.44
1:D:888:VAL:HG13	1:D:908:PRO:HG2	2.00	0.44
1:A:933:ILE:O	1:A:937:ILE:HG12	2.18	0.44
1:C:894:ASP:OD1	1:C:894:ASP:N	2.40	0.44
1:B:114:VAL:HA	1:B:117:VAL:HB	2.00	0.44
1:B:833:ASP:OD1	1:B:833:ASP:N	2.51	0.44
1:B:880:THR:HG21	1:B:891:LEU:HD11	1.99	0.44
1:D:392:LYS:O	1:D:392:LYS:NZ	2.43	0.44
1:D:488:GLU:HA	1:D:736:ASN:ND2	2.33	0.44
1:C:582:ASN:ND2	1:C:1010:LEU:HB2	2.33	0.43
1:B:241:ILE:HG13	1:B:242:PHE:N	2.33	0.43
1:B:938:ARG:HA	1:B:938:ARG:HD2	1.85	0.43
1:A:606:LYS:HD3	1:A:606:LYS:HA	1.79	0.43
1:A:880:THR:OG1	1:A:881:GLU:N	2.51	0.43
1:A:888:VAL:HG21	1:A:903:LEU:HD13	2.00	0.43
1:B:296:LYS:O	1:B:296:LYS:NZ	2.41	0.43
1:D:286:SER:OG	1:D:287:THR:N	2.51	0.43
1:C:122:LEU:HB3	1:C:210:ARG:HD2	2.00	0.43
1:B:789:LEU:HD23	1:B:789:LEU:HA	1.82	0.43
1:A:131:PHE:O	1:A:135:SER:N	2.39	0.43
1:A:253:ILE:HD11	1:A:303:PHE:CD2	2.52	0.43
1:C:478:LYS:H	1:C:478:LYS:HG2	1.65	0.43
1:D:476:ASN:OD1	1:D:476:ASN:N	2.49	0.43
1:D:489:LEU:HD11	1:D:937:ILE:HG21	2.01	0.43
1:D:601:ASP:O	1:D:605:VAL:HG23	2.18	0.43
1:A:354:GLU:HG2	1:A:355:SER:N	2.33	0.43
1:C:557:CYS:O	1:C:561:LEU:HD23	2.18	0.43
1:C:1051:CYS:SG	1:C:1052:LEU:N	2.92	0.43
1:B:760:ILE:HG13	1:B:764:LYS:HZ2	1.84	0.43
1:A:379:HIS:CE1	1:A:381:ILE:HG12	2.54	0.43
1:A:884:ASN:OD1	1:A:887:ASN:ND2	2.52	0.43
1:B:495:ALA:HB2	1:B:737:LEU:HD12	2.00	0.43
1:B:1049:ILE:HD12	1:B:1049:ILE:HA	1.85	0.43
1:D:131:PHE:O	1:D:134:SER:OG	2.26	0.43
1:C:938:ARG:O	1:C:942:THR:HB	2.18	0.43
1:A:297:THR:HG23	1:A:300:GLY:HA3	2.01	0.43
1:A:428:LYS:HA	1:A:461:LEU:HD21	2.00	0.43
1:B:269:ASN:OD1	1:B:269:ASN:N	2.52	0.43
1:B:807:GLN:HB2	1:B:883:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HD12	1:D:169:ILE:HA	1.94	0.43
1:D:466:LYS:HE2	1:D:483:ALA:HB3	2.01	0.43
1:A:469:LEU:HD21	1:A:475:TRP:CZ2	2.54	0.43
1:C:144:PHE:CG	1:C:200:ASN:HB3	2.53	0.43
1:B:732:ILE:HG22	1:B:762:TYR:OH	2.17	0.43
1:D:1051:CYS:SG	1:D:1052:LEU:N	2.92	0.43
1:A:159:PHE:O	1:A:162:LEU:HG	2.19	0.43
1:C:120:PHE:HD1	1:C:216:GLN:HE22	1.67	0.43
1:B:360:LEU:HD11	1:B:398:VAL:HG11	1.99	0.43
1:B:940:LEU:HD12	1:B:940:LEU:HA	1.82	0.43
1:D:872:THR:HG23	1:D:874:VAL:HG22	2.00	0.43
1:A:243:ILE:HD13	1:A:243:ILE:HA	1.88	0.42
1:A:352:THR:O	1:A:356:VAL:HG22	2.18	0.42
1:A:453:LYS:HA	1:A:453:LYS:HD2	1.80	0.42
1:A:499:LEU:HD11	1:A:746:PHE:CZ	2.53	0.42
1:A:560:LYS:HA	1:A:563:LEU:O	2.19	0.42
1:B:146:LYS:HA	1:B:146:LYS:HD2	1.77	0.42
1:B:468:HIS:HE1	1:D:784:LEU:HD13	1.84	0.42
1:D:122:LEU:HD22	1:D:152:ILE:HG21	1.99	0.42
1:A:895:ASP:OD1	1:A:895:ASP:N	2.53	0.42
1:C:31:VAL:HA	1:C:34:PHE:CD2	2.54	0.42
1:B:446:SER:HB3	1:D:890:PHE:HE1	1.84	0.42
1:B:941:VAL:HG23	1:B:942:THR:HG22	2.00	0.42
1:A:195:VAL:HA	1:A:198:TYR:CD1	2.54	0.42
1:B:356:VAL:HG21	1:B:387:LEU:HD13	2.01	0.42
1:B:548:LEU:H	1:B:553:VAL:HG21	1.83	0.42
1:D:165:GLY:HA2	1:D:168:PHE:CE2	2.54	0.42
1:D:218:SER:OG	1:D:236:VAL:HG22	2.19	0.42
1:D:888:VAL:HG11	1:D:906:THR:HG21	2.01	0.42
1:C:606:LYS:HA	1:C:606:LYS:HD2	1.95	0.42
1:D:130:TYR:CD1	1:D:207:ARG:HB3	2.54	0.42
1:D:760:ILE:O	1:D:764:LYS:HG2	2.19	0.42
1:A:745:ASN:OD1	1:A:745:ASN:N	2.52	0.42
1:C:33:PHE:HB2	1:C:187:PHE:CZ	2.53	0.42
1:D:122:LEU:HD22	1:D:152:ILE:HG13	2.01	0.42
1:C:588:LYS:HA	1:C:588:LYS:HD3	1.81	0.42
1:D:500:ALA:HB1	1:D:979:GLN:HE21	1.85	0.42
1:B:1052:LEU:HA	1:B:1052:LEU:HD23	1.84	0.42
1:A:110:LEU:HD12	1:A:113:ARG:HB3	2.02	0.42
1:B:549:SER:OG	1:B:550:PHE:N	2.53	0.42
1:D:458:THR:OG1	1:D:459:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HA	1:A:198:TYR:HD1	1.85	0.42
1:A:769:THR:OG1	1:A:769:THR:O	2.34	0.42
1:A:799:MET:HB2	1:A:877:PRO:HB2	2.01	0.42
1:B:693:HIS:CE1	1:B:744:SER:HA	2.55	0.42
1:A:1015:TYR:CD2	1:A:1031:ARG:HB2	2.55	0.42
1:B:104:MET:HE1	1:B:115:LEU:HD12	2.01	0.42
1:B:913:THR:O	1:B:913:THR:OG1	2.34	0.42
1:B:511:PHE:HZ	1:B:937:ILE:HD11	1.84	0.41
1:D:545:PHE:HA	1:D:548:LEU:HD23	2.00	0.41
1:A:191:PRO:HA	1:A:194:PHE:HB3	2.02	0.41
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.87	0.41
1:C:118:LEU:O	1:C:122:LEU:HG	2.19	0.41
1:C:501:GLN:HE22	1:C:877:PRO:HB3	1.85	0.41
1:B:286:SER:O	1:B:286:SER:OG	2.35	0.41
1:D:322:ILE:H	1:D:322:ILE:HG13	1.69	0.41
1:A:493:PHE:HE2	1:A:920:LEU:HD21	1.85	0.41
1:A:562:LYS:HE2	1:A:562:LYS:HB2	1.67	0.41
1:C:241:ILE:HG13	1:C:242:PHE:N	2.35	0.41
1:C:283:VAL:HG21	1:C:290:TYR:H	1.84	0.41
1:D:509:ASN:ND2	1:D:528:TYR:OH	2.53	0.41
1:D:529:LEU:HA	1:D:532:VAL:HG12	2.02	0.41
1:A:804:SER:O	1:A:807:GLN:NE2	2.53	0.41
1:C:980:LEU:HB2	1:C:1049:ILE:HG23	2.03	0.41
1:B:21:MET:H	1:B:21:MET:HG2	1.61	0.41
1:D:365:HIS:O	1:D:366:LYS:HG2	2.20	0.41
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.85	0.41
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.87	0.41
1:C:923:LEU:HD23	1:C:923:LEU:HA	1.81	0.41
1:A:127:LEU:HD21	1:A:210:ARG:HB2	2.03	0.41
1:A:514:ARG:HD3	1:A:514:ARG:HA	1.70	0.41
1:B:384:ASN:O	1:B:388:GLU:HG2	2.20	0.41
1:D:365:HIS:CD2	1:D:513:MET:HG3	2.54	0.41
1:D:1012:PHE:HE1	1:D:1052:LEU:HD21	1.85	0.41
1:A:1017:LEU:HA	1:A:1031:ARG:HA	2.03	0.41
1:B:354:GLU:HG2	1:B:355:SER:N	2.36	0.41
1:A:369:ASP:N	1:A:369:ASP:OD1	2.54	0.41
1:A:495:ALA:O	1:A:498:CYS:HB3	2.21	0.41
1:A:812:ASP:O	1:A:816:GLN:HB2	2.21	0.41
1:C:107:ALA:HA	1:C:112:GLY:HA3	2.03	0.41
1:C:807:GLN:HB2	1:C:883:VAL:HG11	2.02	0.41
1:B:163:TYR:HD1	1:B:166:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASP:OD1	1:B:435:ALA:N	2.54	0.41
1:B:895:ASP:OD1	1:B:895:ASP:N	2.53	0.41
1:B:996:TYR:OH	1:B:1011:CYS:HB2	2.21	0.41
1:D:167:ARG:HH21	1:D:182:ASN:HB3	1.86	0.41
1:D:510:LEU:HD23	1:D:510:LEU:HA	1.90	0.41
1:D:580:LEU:HD13	1:D:580:LEU:HA	1.93	0.41
1:D:731:LEU:HD21	1:D:765:ARG:HE	1.86	0.41
1:A:241:ILE:HG13	1:A:242:PHE:N	2.35	0.41
1:C:937:ILE:HD13	1:C:937:ILE:HA	1.92	0.41
1:B:175:LEU:HD12	1:B:178:TRP:HE1	1.86	0.41
1:B:367:ASP:N	1:B:367:ASP:OD1	2.54	0.41
1:B:817:ASP:OD1	1:B:817:ASP:N	2.54	0.41
1:D:334:GLY:O	1:D:413:ARG:HD2	2.21	0.41
1:D:563:LEU:HD21	1:D:597:PHE:CD1	2.56	0.41
1:D:923:LEU:HD12	1:D:923:LEU:HA	1.79	0.41
1:A:205:GLY:O	1:A:207:ARG:HG3	2.21	0.40
1:A:322:ILE:O	1:A:326:ILE:HG12	2.21	0.40
1:A:390:LEU:HA	1:A:393:ARG:NE	2.36	0.40
1:B:103:VAL:O	1:B:107:ALA:N	2.51	0.40
1:D:511:PHE:CZ	1:D:937:ILE:HD11	2.56	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.89	0.40
1:C:500:ALA:HB1	1:C:979:GLN:HE21	1.84	0.40
1:B:907:GLN:HE22	1:B:1018:ARG:HH11	1.68	0.40
1:D:537:TYR:HD2	1:D:605:VAL:HG21	1.85	0.40
1:B:185:VAL:O	1:B:189:THR:HG22	2.22	0.40
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.91	0.40
1:D:470:LEU:HD13	1:D:954:ALA:HB2	2.02	0.40
1:D:878:ILE:HD12	1:D:878:ILE:HA	1.89	0.40
1:A:476:ASN:OD1	1:A:476:ASN:N	2.53	0.40
1:C:688:SER:HA	1:C:962:GLY:HA3	2.02	0.40
1:C:905:LEU:HD12	1:C:905:LEU:HA	1.88	0.40
1:B:885:ASP:HB3	1:B:903:LEU:HD22	2.03	0.40
1:A:1016:ARG:HG2	1:A:1032:TYR:CZ	2.57	0.40
1:D:118:LEU:HD12	1:D:118:LEU:HA	1.94	0.40
1:D:688:SER:HA	1:D:962:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	817/1072 (76%)	748 (92%)	69 (8%)	0	100	100
1	B	818/1072 (76%)	755 (92%)	63 (8%)	0	100	100
1	C	857/1072 (80%)	803 (94%)	54 (6%)	0	100	100
1	D	851/1072 (79%)	799 (94%)	52 (6%)	0	100	100
All	All	3343/4288 (78%)	3105 (93%)	238 (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	A	736/943 (78%)	693 (94%)	43 (6%)	20	51
1	B	737/943 (78%)	691 (94%)	46 (6%)	18	49
1	C	759/943 (80%)	727 (96%)	32 (4%)	30	58
1	D	758/943 (80%)	725 (96%)	33 (4%)	28	57
All	All	2990/3772 (79%)	2836 (95%)	154 (5%)	27	54

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	22	TRP

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Mol	Chain	Res	Type
1	A	100	TRP
1	A	128	VAL
1	A	154	MET
1	A	178	TRP
1	A	187	PHE
1	A	194	PHE
1	A	198	TYR
1	A	201	ARG
1	A	217	PHE
1	A	242	PHE
1	A	252	PHE
1	A	279	TYR
1	A	285	MET
1	A	286	SER
1	A	290	TYR
1	A	294	TYR
1	A	306	PHE
1	A	307	PHE
1	A	315	PHE
1	A	348	CYS
1	A	362	ASP
1	A	384	ASN
1	A	498	CYS
1	A	512	SER
1	A	514	ARG
1	A	548	LEU
1	A	550	PHE
1	A	558	PHE
1	A	562	LYS
1	A	565	MET
1	A	731	LEU
1	A	745	ASN
1	A	746	PHE
1	A	881	GLU
1	A	886	THR
1	A	892	ASP
1	A	904	TYR
1	A	936	LEU
1	A	1000	PHE
1	A	1041	PHE
1	A	1055	PHE
1	C	130	TYR

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Mol	Chain	Res	Type
1	C	148	PHE
1	C	161	LEU
1	C	187	PHE
1	C	188	PHE
1	C	194	PHE
1	C	198	TYR
1	C	201	ARG
1	C	216	GLN
1	C	242	PHE
1	C	282	MET
1	C	303	PHE
1	C	329	ARG
1	C	335	SER
1	C	404	SER
1	C	463	TYR
1	C	504	SER
1	C	514	ARG
1	C	545	PHE
1	C	565	MET
1	C	594	LEU
1	C	779	LEU
1	C	797	CYS
1	C	892	ASP
1	C	921	ASP
1	C	931	ASP
1	C	982	LEU
1	C	990	LEU
1	C	1001	CYS
1	C	1011	CYS
1	C	1015	TYR
1	C	1041	PHE
1	B	22	TRP
1	B	33	PHE
1	B	130	TYR
1	B	133	ASP
1	B	159	PHE
1	B	167	ARG
1	B	168	PHE
1	B	188	PHE
1	B	206	LEU
1	B	210	ARG
1	B	213	ARG

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	279	TYR
1	B	290	TYR
1	B	294	TYR
1	B	329	ARG
1	B	330	LYS
1	B	362	ASP
1	B	366	LYS
1	B	369	ASP
1	B	395	PHE
1	B	402	GLN
1	B	498	CYS
1	B	550	PHE
1	B	555	GLU
1	B	609	PHE
1	B	611	TYR
1	B	687	ASP
1	B	734	LEU
1	B	746	PHE
1	B	790	ARG
1	B	800	CYS
1	B	881	GLU
1	B	889	GLN
1	B	892	ASP
1	B	904	TYR
1	B	922	SER
1	B	924	MET
1	B	1000	PHE
1	B	1001	CYS
1	B	1009	MET
1	B	1011	CYS
1	B	1015	TYR
1	B	1051	CYS
1	B	1052	LEU
1	B	1056	ASP
1	D	108	GLN
1	D	120	PHE
1	D	130	TYR
1	D	131	PHE
1	D	146	LYS
1	D	156	PHE
1	D	160	PHE

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Mol	Chain	Res	Type
1	D	194	PHE
1	D	217	PHE
1	D	242	PHE
1	D	252	PHE
1	D	275	TRP
1	D	282	MET
1	D	303	PHE
1	D	318	TYR
1	D	361	LYS
1	D	366	LYS
1	D	404	SER
1	D	537	TYR
1	D	545	PHE
1	D	549	SER
1	D	609	PHE
1	D	707	ARG
1	D	726	ASP
1	D	735	ARG
1	D	889	GLN
1	D	897	ASP
1	D	904	TYR
1	D	921	ASP
1	D	990	LEU
1	D	1001	CYS
1	D	1015	TYR
1	D	1041	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	200	ASN
1	A	222	GLN
1	A	258	ASN
1	A	384	ASN
1	A	440	ASN
1	A	462	GLN
1	A	534	ASN
1	A	749	HIS
1	A	887	ASN
1	A	907	GLN
1	A	967	GLN

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Mol	Chain	Res	Type
1	C	143	ASN
1	C	397	GLN
1	C	449	ASN
1	C	462	GLN
1	C	464	HIS
1	C	534	ASN
1	C	1036	ASN
1	B	225	ASN
1	B	440	ASN
1	B	464	HIS
1	B	465	ASN
1	B	468	HIS
1	B	496	GLN
1	B	509	ASN
1	B	534	ASN
1	B	745	ASN
1	B	807	GLN
1	D	108	GLN
1	D	225	ASN
1	D	365	HIS
1	D	397	GLN
1	D	402	GLN
1	D	440	ASN
1	D	449	ASN
1	D	462	GLN
1	D	534	ASN
1	D	582	ASN
1	D	736	ASN
1	D	979	GLN
1	D	1021	HIS
1	D	1054	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

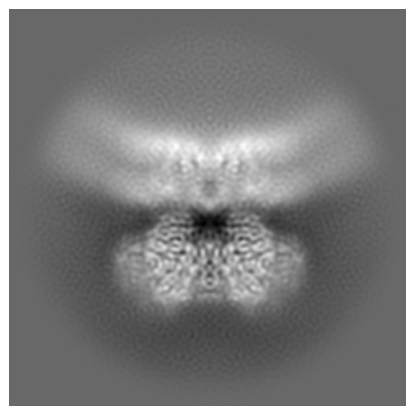
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40038. These allow visual inspection of the internal detail of the map and identification of artifacts.

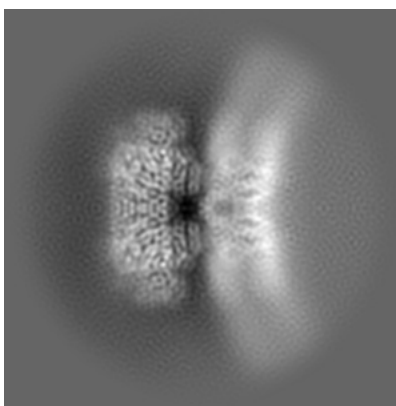
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

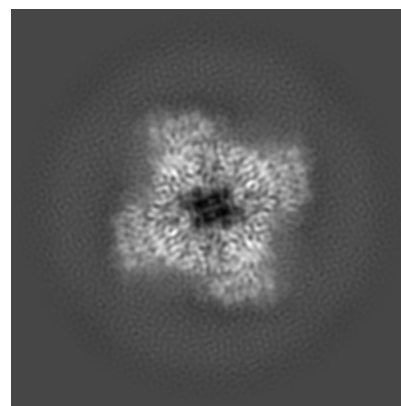
#### 6.1.1 Primary map



X

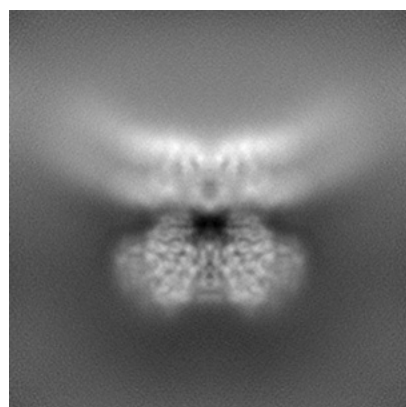


Y

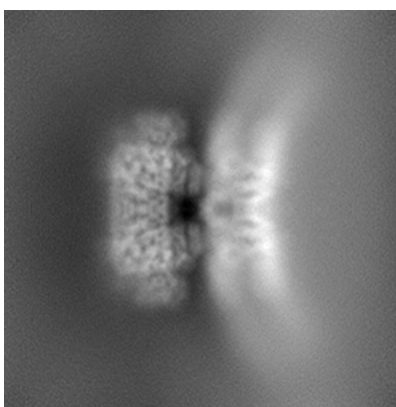


Z

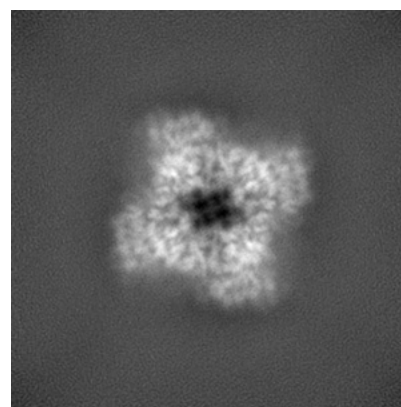
#### 6.1.2 Raw map



X



Y



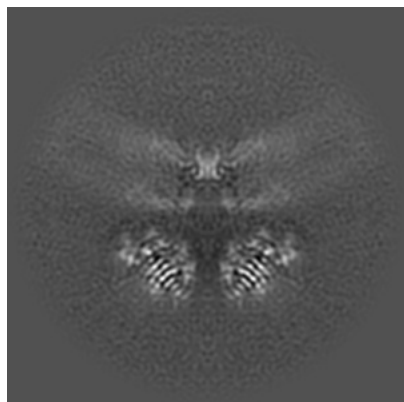
Z

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

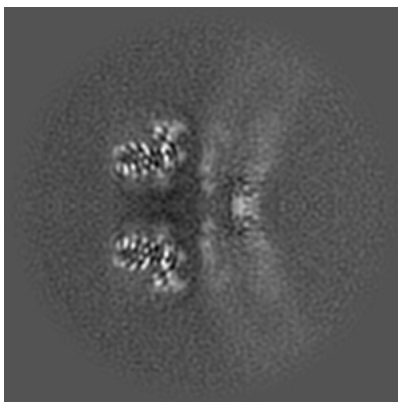


## 6.2 Central slices [i](#)

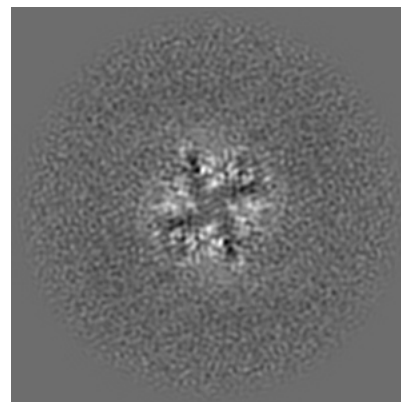
### 6.2.1 Primary map



X Index: 128

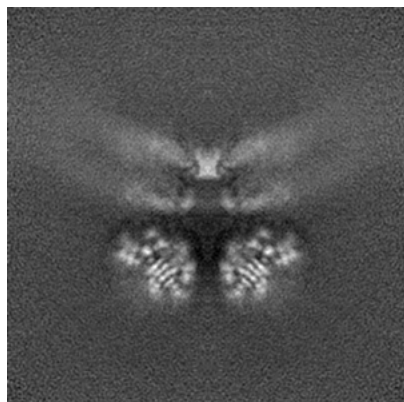


Y Index: 128

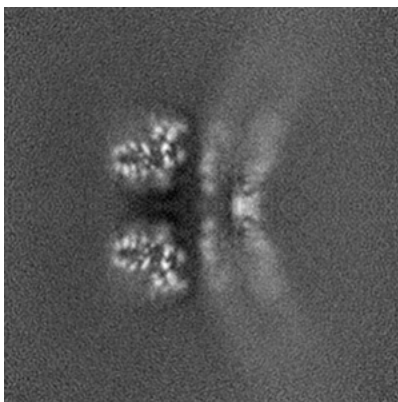


Z Index: 128

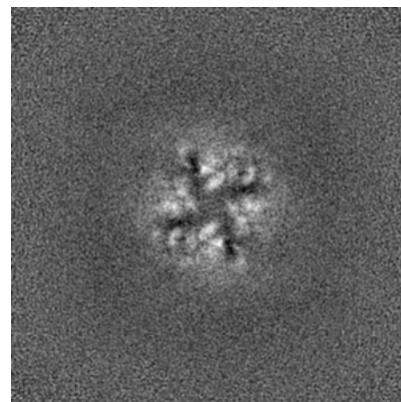
### 6.2.2 Raw map



X Index: 128



Y Index: 128

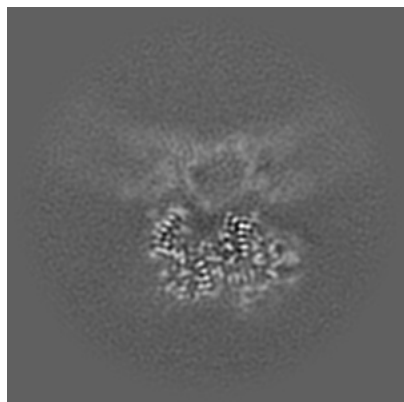


Z Index: 128

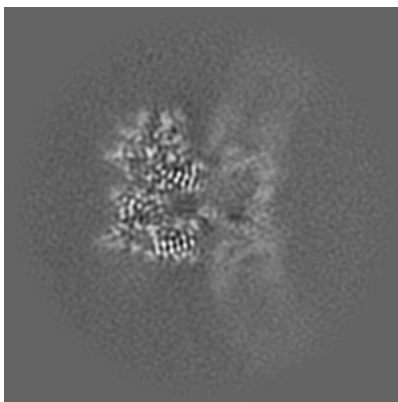
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

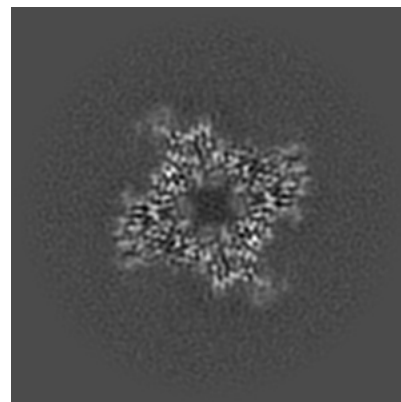
### 6.3.1 Primary map



X Index: 103

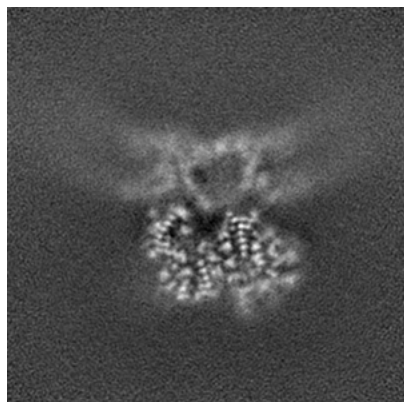


Y Index: 151

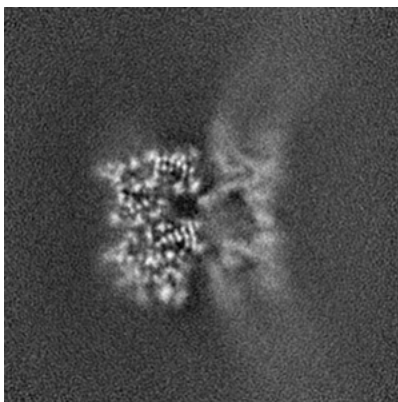


Z Index: 102

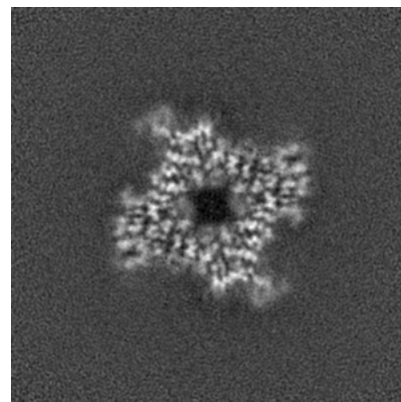
### 6.3.2 Raw map



X Index: 104



Y Index: 104

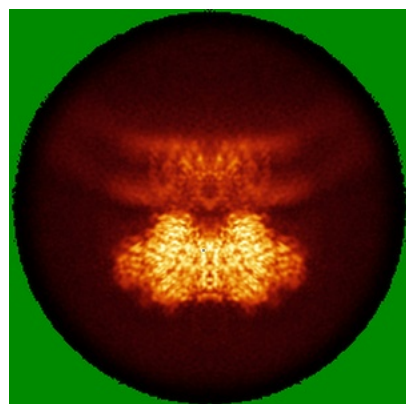


Z Index: 102

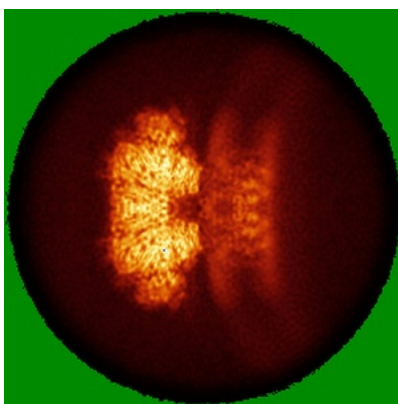
The images above show the largest variance slices of the map in three orthogonal directions.

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

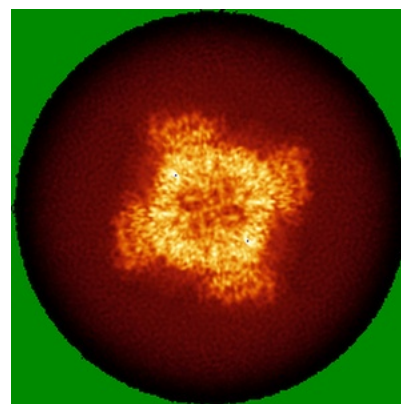
### 6.4.1 Primary map



X

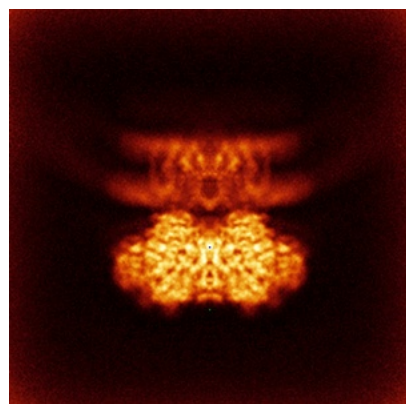


Y

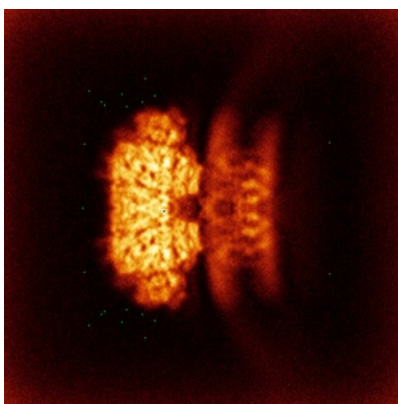


Z

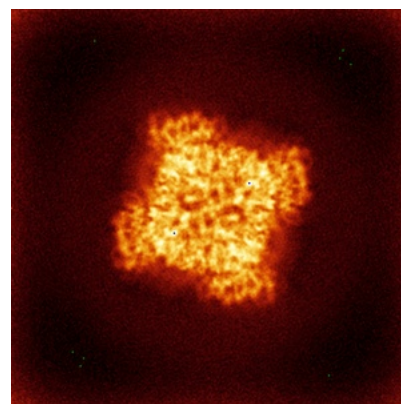
### 6.4.2 Raw map



X



Y

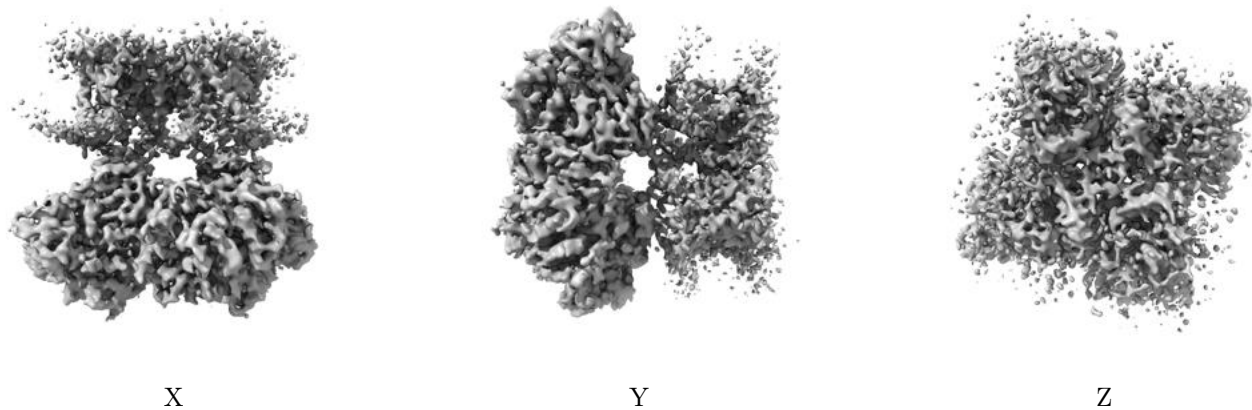


Z

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 0.25. 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.

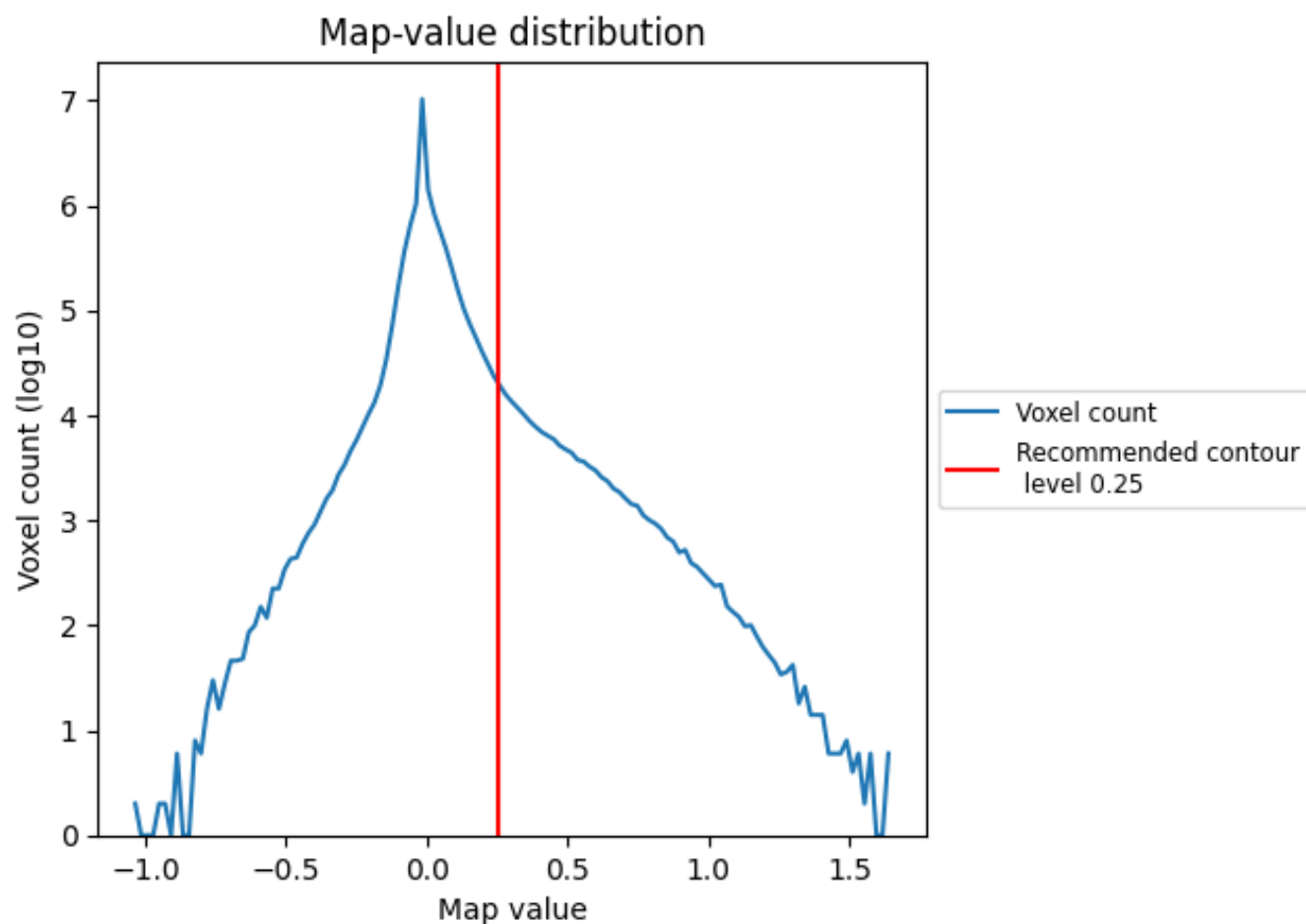
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

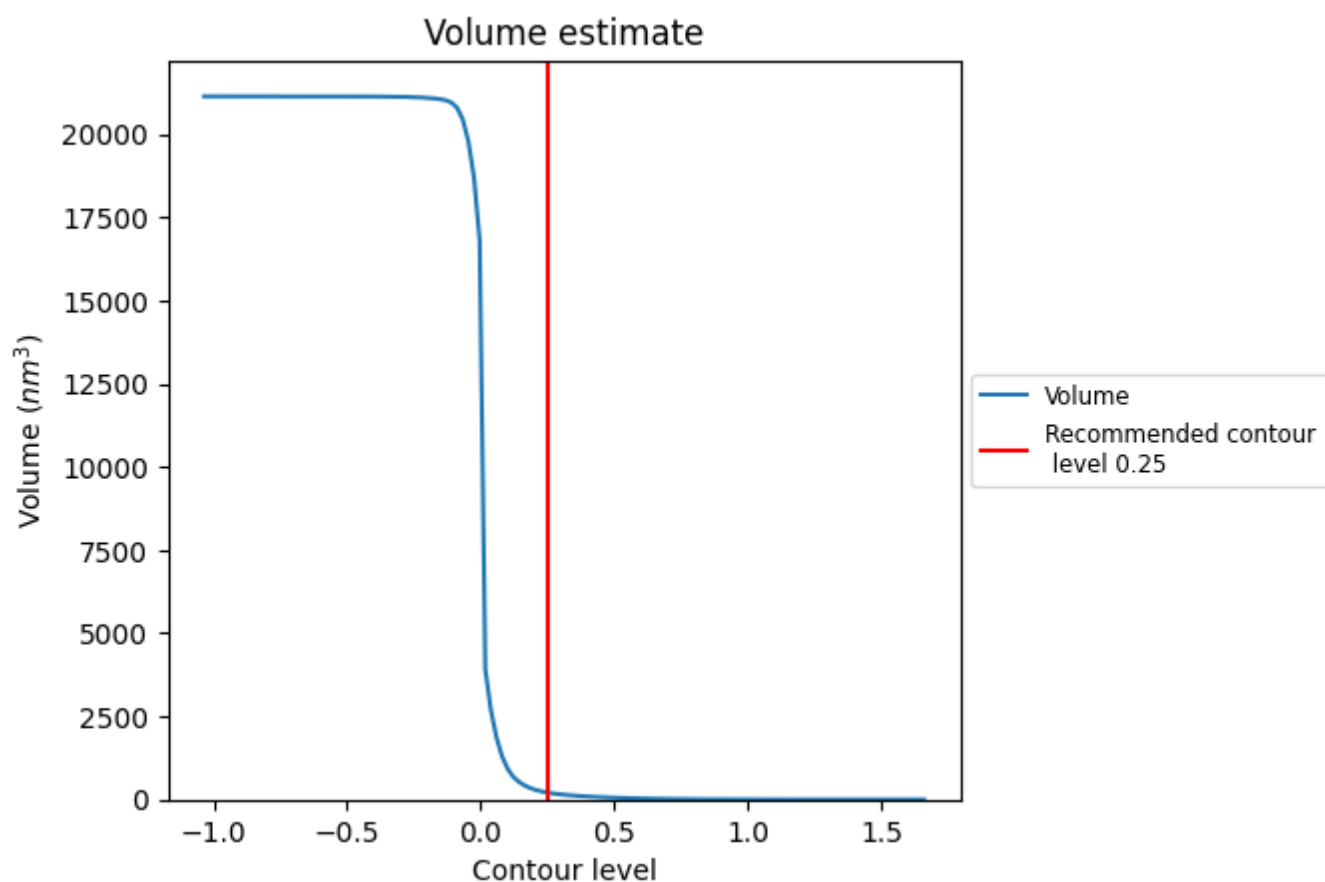
This section contains the results of statistical analysis of the map.

### 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](#)

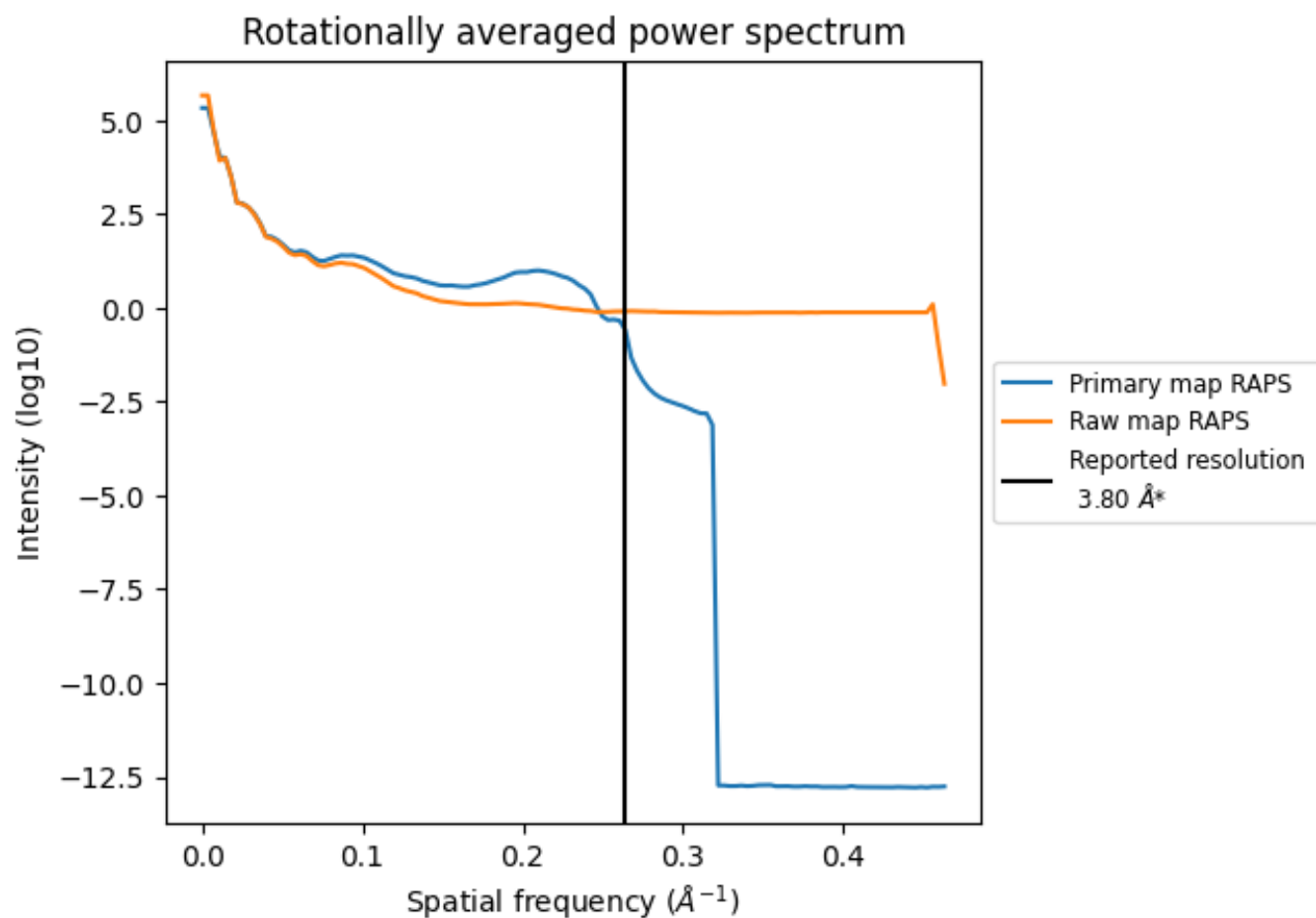


The volume at the recommended contour level is 209 nm<sup>3</sup>; this corresponds to an approximate mass of 189 kDa.

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 ⓘ

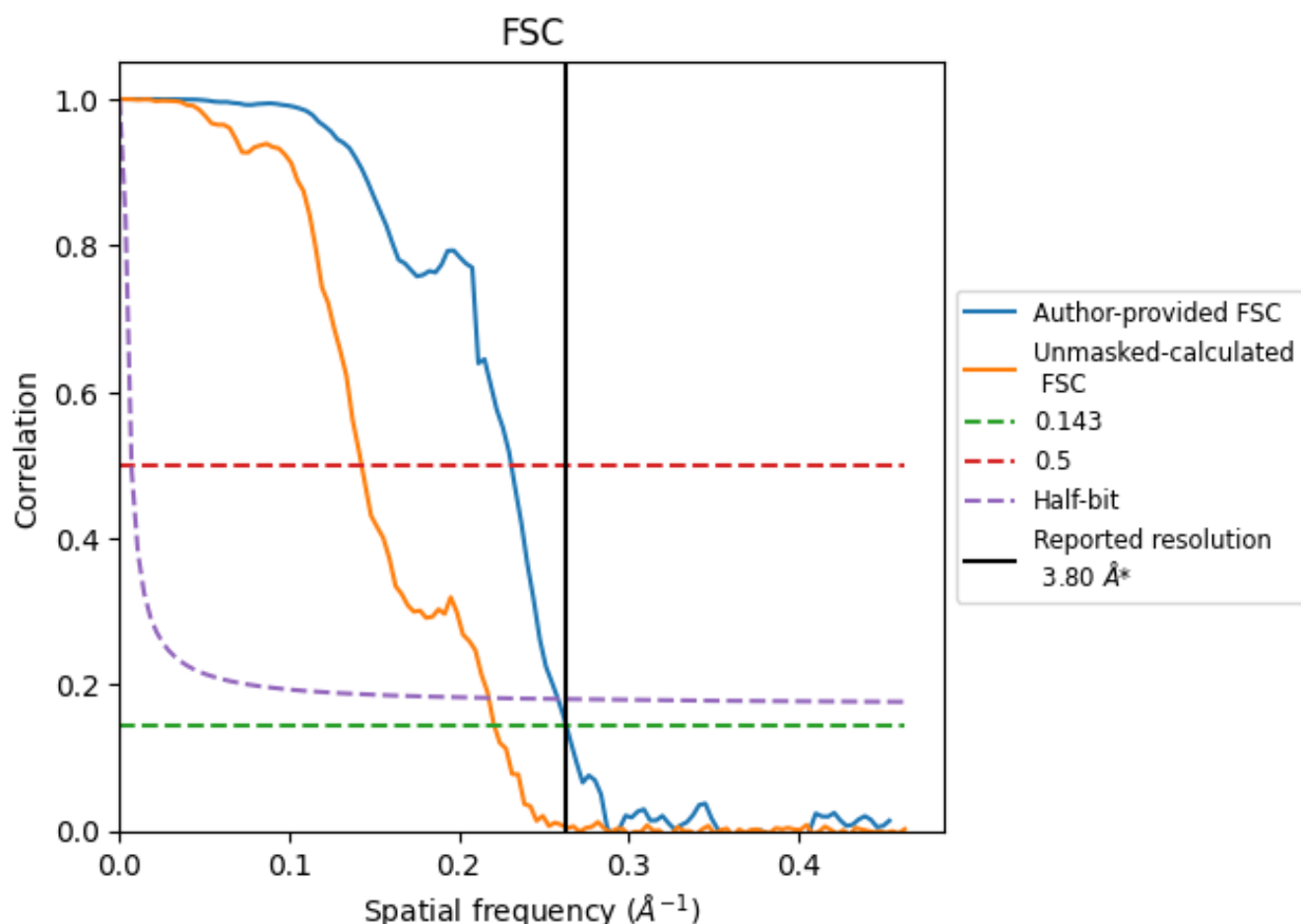


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

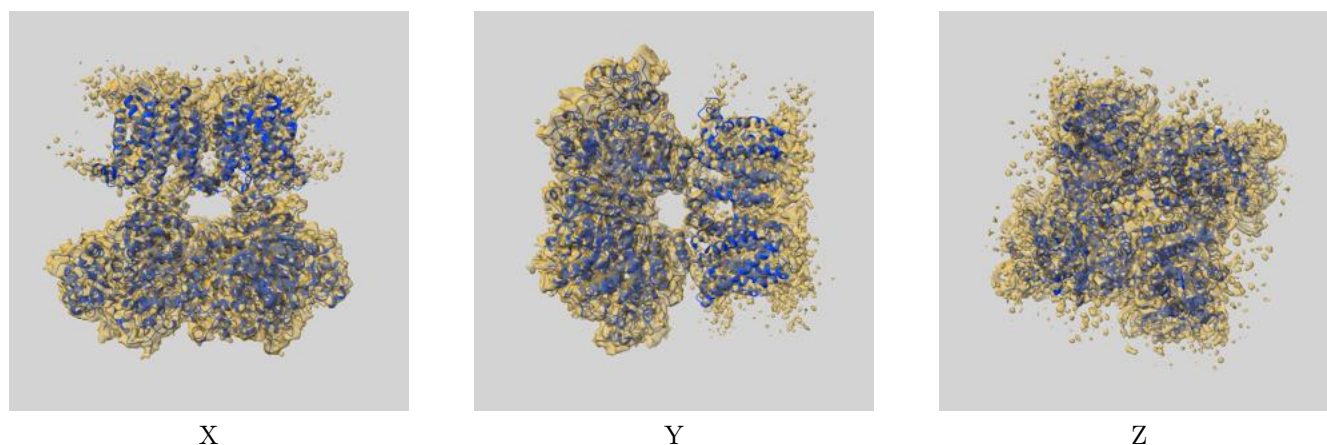
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.33	3.87
Unmasked-calculated*	4.52	7.01	4.59

\*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 4.52 differs from the reported value 3.8 by more than 10 %

## 9 Map-model fit [i](#)

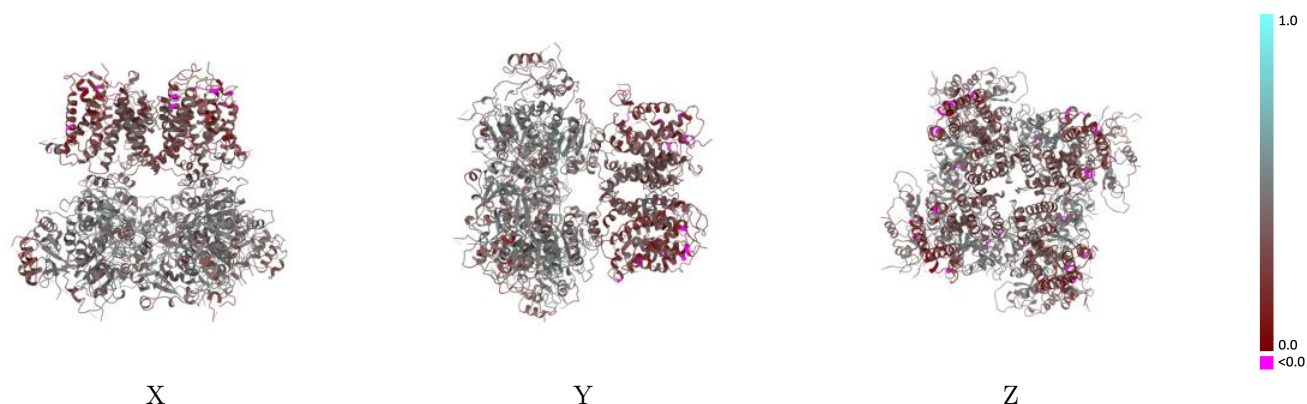
This section contains information regarding the fit between EMDB map EMD-40038 and PDB model 8GH9. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



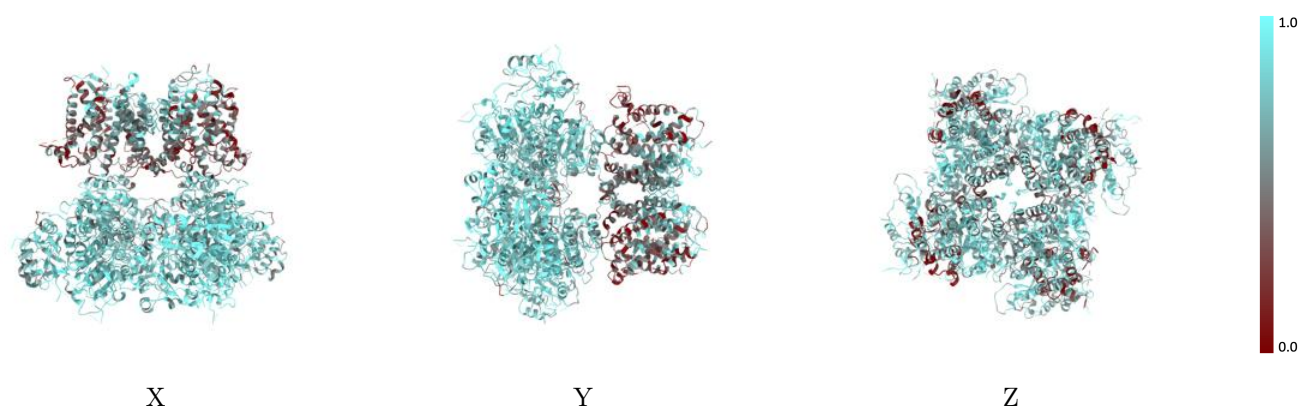
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



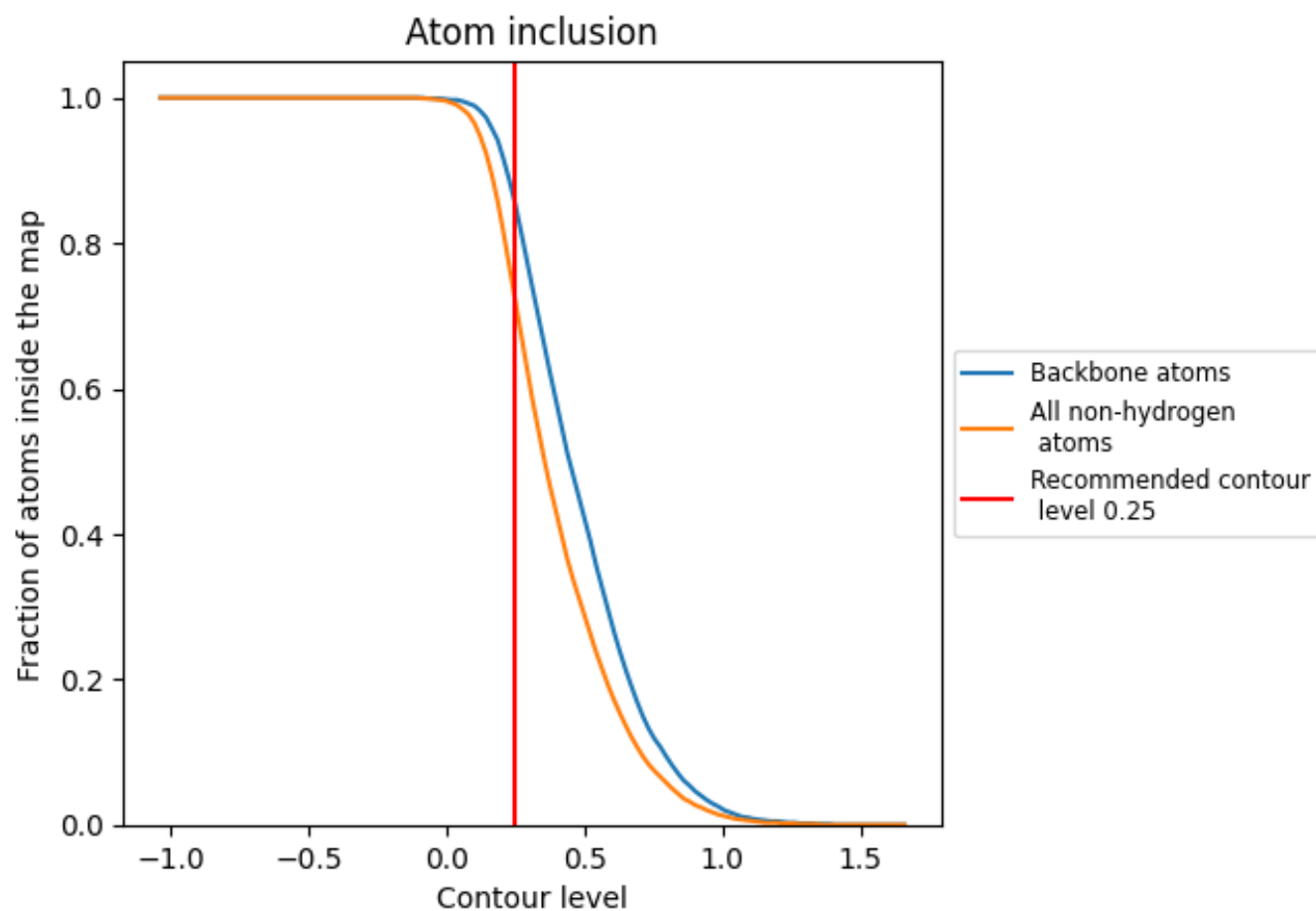
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7220	<div></div> 0.3970
A	<div></div> 0.7280	<div></div> 0.4000
B	<div></div> 0.7260	<div></div> 0.3970
C	<div></div> 0.7140	<div></div> 0.3910
D	<div></div> 0.7200	<div></div> 0.4000

