



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 08:03 AM UTC

PDB ID : 9G8R / pdb_00009g8r
EMDB ID : EMD-51137
Title : human SKI7-SKI238 complex in the open state
Authors : Koegel, A.; Keidel, A.; Loukeri, M.J.; Kuhn, C.C.; Langer, L.M.; Schaefer, I.B.; Conti, E.
Deposited on : 2024-07-23
Resolution : 3.40 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

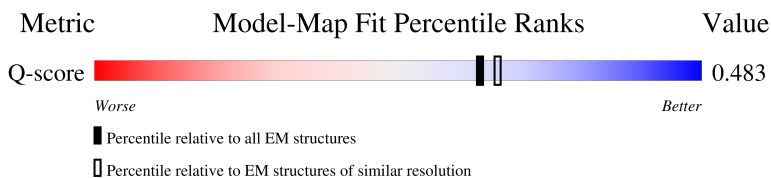
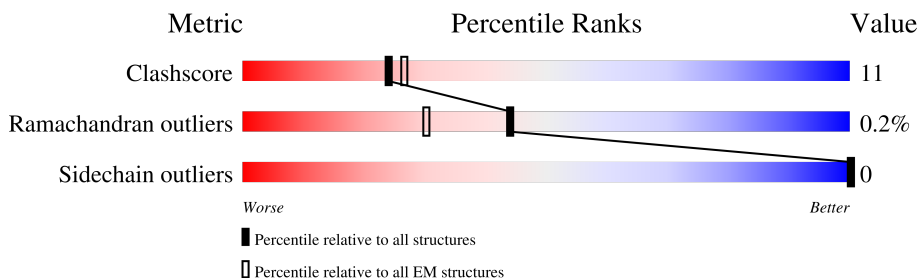
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	B	1568	11% 56% 15% 29%
2	C	305	73% 27%
2	D	305	6% 69% 31%
3	E	179	7% 7% 92%

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Mol	Chain	Length	Quality of chain
4	A	976	 A horizontal bar chart showing the quality of chain A. The bar is divided into three segments: a red segment on the left labeled '12%', a green segment in the middle labeled '5%', and a grey segment on the right labeled '83%'. The total length of the bar represents 100%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14837 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 Superkiller complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1113	Total	C	N	O	S	0	0
			8718	5537	1501	1629	51		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q6PGP7
B	-2	PRO	-	expression tag	UNP Q6PGP7
B	-1	ASP	-	expression tag	UNP Q6PGP7
B	0	SER	-	expression tag	UNP Q6PGP7

- Molecule 2 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	305	Total	C	N	O	S	0	0
			2373	1507	399	462	5		
2	D	305	Total	C	N	O	S	0	0
			2373	1507	399	462	5		

- Molecule 3 is a protein called Isoform 2 of HBS1-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	14	Total	C	N	O	0	0
			105	66	15	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	368	GLY	-	expression tag	UNP Q9Y450
E	369	PRO	-	expression tag	UNP Q9Y450
E	370	ASP	-	expression tag	UNP Q9Y450
E	371	SER	-	expression tag	UNP Q9Y450

- Molecule 4 is a protein called Superkiller complex protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	163	Total	C	N	O	S	0	0
			1268	809	210	243	6		

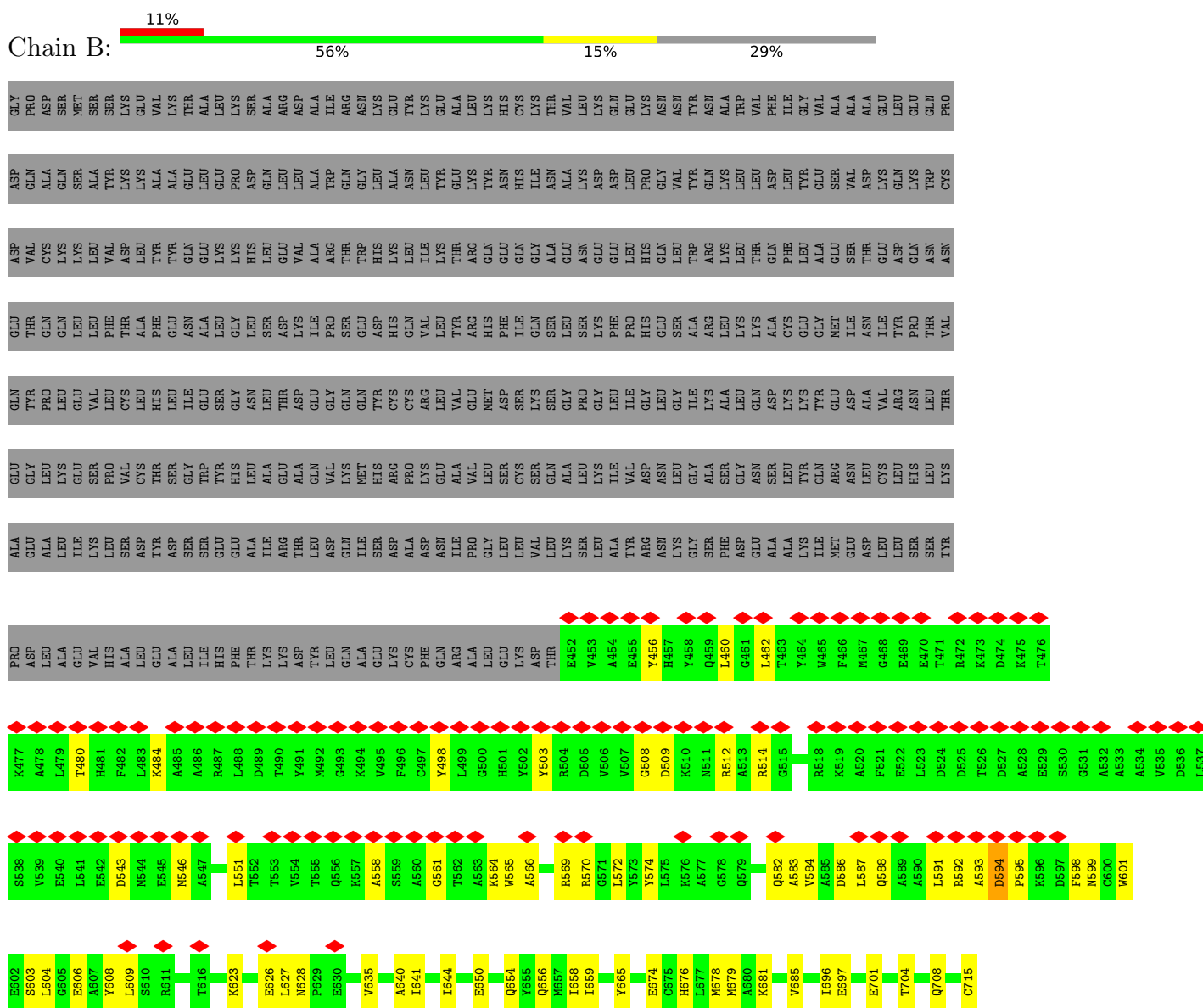
There are 4 discrepancies between the modelled and reference sequences:

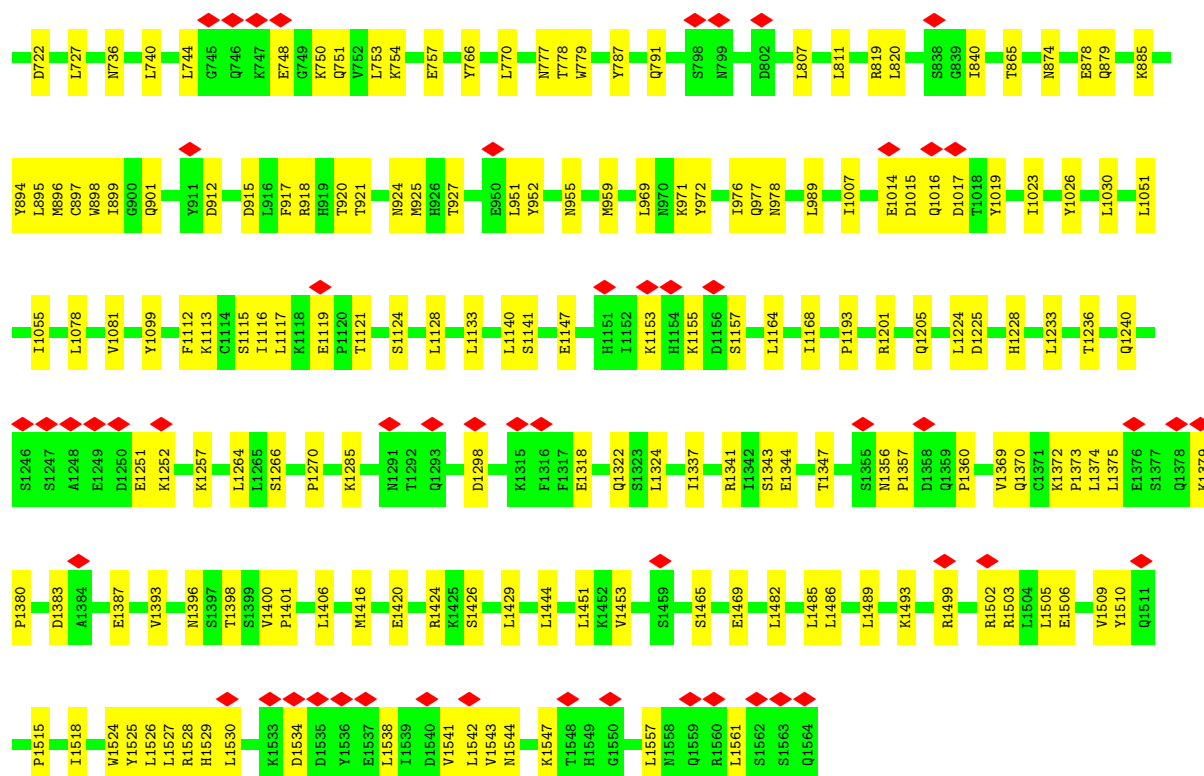
Chain	Residue	Modelled	Actual	Comment	Reference
A	775	GLY	-	linker	UNP Q15477
A	776	SER	-	linker	UNP Q15477
A	777	ARG	-	linker	UNP Q15477
A	778	GLY	-	linker	UNP Q15477

3 Residue-property plots

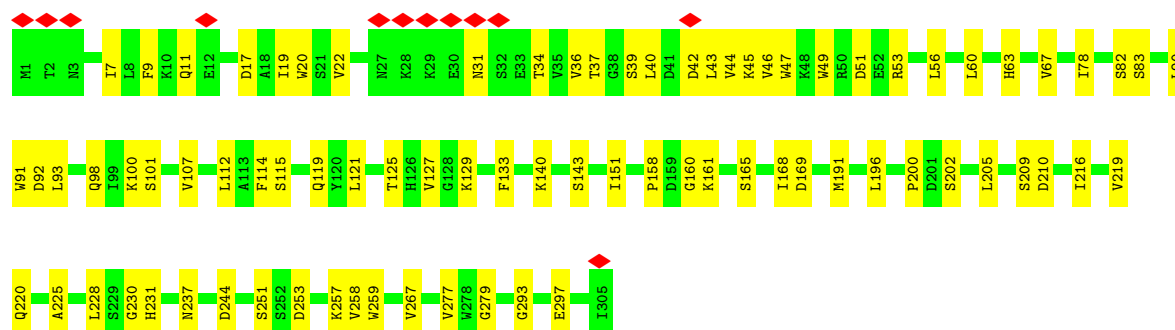
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Superkiller complex protein 3

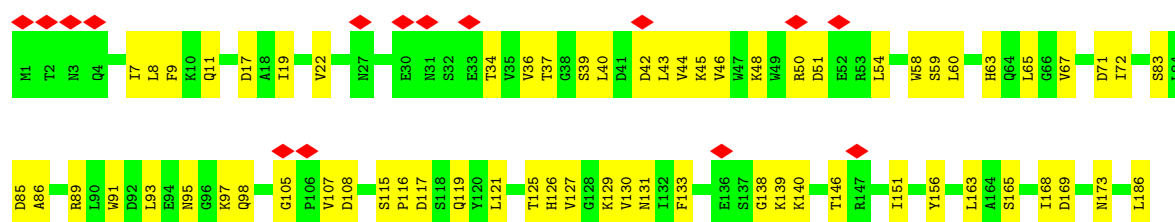


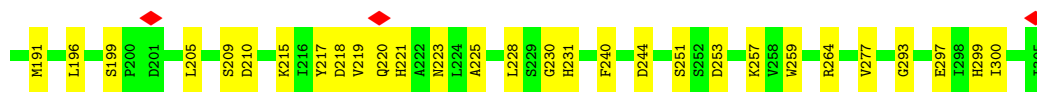


• Molecule 2: WD repeat-containing protein 61

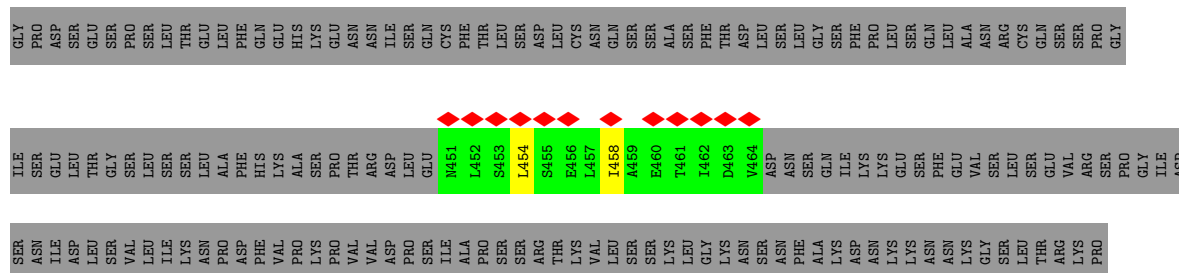


• Molecule 2: WD repeat-containing protein 61

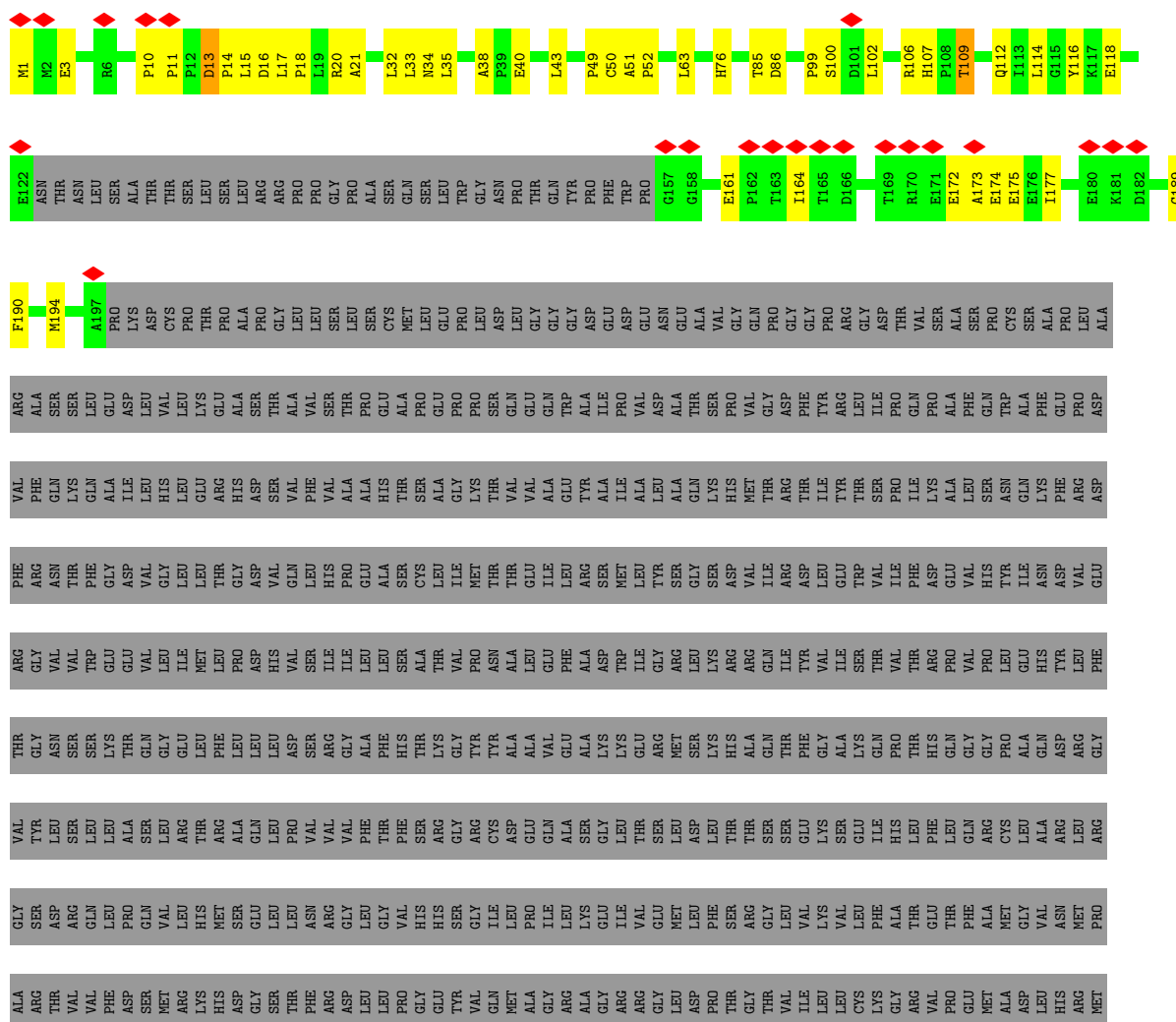




• Molecule 3: Isoform 2 of HBS1-like protein



• Molecule 4: Superkiller complex protein 2



LEU	TYR	THR	GLN	SER	GLU	ALA	ARG	THR	MET
				GLY	LEU	GLY	THR	LEU	MET
				ALA	ASP	GLN	GLY	TYR	LYS
				GLY	LEU	PRO	VAL	ASP	SER
				LEU	PRO	ASN	ASP	GLN	GLY
				SER	GLY	THR	GLY	ALA	LEU
				THR	LEU	LEU	ALA	GLN	GLN
				PRO	LYS	GLN	THR	GLN	SER
				GLY	GLY	ILE	VAL	PHE	ARG
				GLY	LEU	ILE	LYS	ARG	THR
				VAL	GLU	ARG	LEU	THR	LEU
				VAL	ARG	VAL	GLY	TYR	THR
				ARG	VAL	VAL	GLY	ARG	MET
				CYS	ARG	ALA	VAL	VAL	ILE
				ILE	ALA	VAL	ALA	VAL	THR
				GLN	ARG	ALA	CYS	GLY	LEU
				LEU	LYS	ALA	ALA	ASN	LEU
				ALA	ARG	LEU	MET	LEU	LEU
				GLY	ILE	SER	SER	ARG	LEU
				MET	GLY	GLU	HIS	VAL	ARG
				CYS	ARG	VAL	GLY	ASP	VAL
				ARG	VAL	GLN	LEU	LEU	ASP
				SER	LEU	VAL	LEU	LEU	ALA
				LEU	VAL	ALA	THR	ARG	VAL
				GLY	CYS	GLY	GLY	VAL	VAL
				ALA	ALA	LEU	LEU	ASP	GLY
				ARG	ASN	GLN	PHE	MET	LYS
				LEU	THR	THR	THR	GLY	ARG
				VAL	VAL	GLY	LEU	PHE	GLY
				GLY	ALA	GLU	ARG	PRO	THR
				ALA	LEU	LEU	PRO	GLY	GLY
				LYS	ASN	GLY	SER	SER	ARG
				MET	GLY	PHE	GLY	GLY	LEU
				GLY	THR	GLY	ILE	ALA	LEU
				ALA	LEU	VAL	ALA	LEU	LEU
				THR	GLU	VAL	LEU	LEU	LEU
				LEU	VAL	VAL	SER	PRO	GLY
				ARG	TYR	GLY	GLY	TYR	HIS
				ARG	ASP	TRP	VAL	VAL	GLN
				ILE	ALA	ALA	CYS	ARG	ARG
				VAL	ARG	GLY	GLN	VAL	GLY
				PHE	GLY	MET	SER	PRO	GLY
				ALA	ALA	ARG	GLY	GLY	VAL
				SER	PHE	PRO	ARG	VAL	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151860	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 ($e^-/\text{\AA}^2$)	67.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	708.19836, 708.19836, 708.19836	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	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	B	0.15	0/8880	0.44	0/12019
2	C	0.15	0/2432	0.49	0/3311
2	D	0.17	0/2432	0.54	0/3311
3	E	0.14	0/104	0.36	0/141
4	A	0.19	0/1304	0.64	0/1782
All	All	0.15	0/15152	0.48	0/20564

There are no bond length outliers.

There are no bond angle outliers.

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	B	8718	0	8799	172	0
2	C	2373	0	2290	51	0
2	D	2373	0	2290	73	0
3	E	105	0	107	5	0
4	A	1268	0	1246	42	0
All	All	14837	0	14732	318	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 (318) 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:B:1379:LYS:HD2	1:B:1380:PRO:HD2	1.58	0.85
2:D:95:ASN:HB3	2:D:97:LYS:HZ1	1.42	0.84
1:B:509:ASP:HB3	1:B:512:ARG:HH21	1.46	0.80
4:A:10:PRO:HG2	4:A:11:PRO:HD3	1.65	0.79
1:B:740:LEU:HB3	1:B:750:LYS:HE3	1.67	0.76
1:B:1499:ARG:O	1:B:1502:ARG:HG3	1.86	0.73
1:B:1201:ARG:NH2	4:A:52:PRO:O	2.22	0.72
2:C:67:VAL:HA	2:C:83:SER:HB3	1.71	0.72
1:B:715:CYS:SG	4:A:100:SER:OG	2.46	0.72
1:B:1499:ARG:HE	1:B:1502:ARG:HH21	1.36	0.71
1:B:1420:GLU:OE2	1:B:1424:ARG:NE	2.25	0.70
1:B:820:LEU:HA	4:A:174:GLU:HB3	1.74	0.70
1:B:1530:LEU:HD13	1:B:1538:LEU:HB3	1.73	0.69
2:D:115:SER:HB3	2:D:119:GLN:H	1.58	0.69
1:B:543:ASP:HB3	1:B:546:MET:HE2	1.74	0.68
1:B:503:TYR:HB3	1:B:512:ARG:NH2	2.08	0.68
4:A:20:ARG:NH1	4:A:35:LEU:O	2.26	0.68
1:B:1444:LEU:HD13	1:B:1482:LEU:HD23	1.75	0.68
2:C:191:MET:HB3	2:C:210:ASP:HB3	1.74	0.67
1:B:1205:GLN:NE2	4:A:51:ALA:O	2.26	0.67
2:D:191:MET:HB3	2:D:210:ASP:HB3	1.76	0.66
4:A:13:ASP:HB3	4:A:16:ASP:OD1	1.95	0.66
2:D:42:ASP:HA	2:D:63:HIS:HB2	1.76	0.66
1:B:895:LEU:HD22	1:B:924:ASN:HB3	1.76	0.66
2:C:251:SER:OG	2:C:253:ASP:OD1	2.14	0.66
1:B:874:ASN:HB3	4:A:194:MET:HE1	1.77	0.66
1:B:1524:TRP:HH2	4:A:16:ASP:HA	1.60	0.66
1:B:722:ASP:OD1	1:B:766:TYR:OH	2.13	0.66
1:B:514:ARG:NH1	1:B:543:ASP:OD2	2.26	0.65
2:D:277:VAL:HA	2:D:293:GLY:HA2	1.78	0.65
1:B:1528:ARG:HH12	4:A:15:LEU:HD21	1.61	0.65
3:E:454:LEU:O	3:E:458:ILE:HG13	1.97	0.65
1:B:918:ARG:HH12	1:B:959:MET:HE3	1.61	0.64
2:D:43:LEU:HD13	2:D:45:LYS:HE3	1.78	0.64
2:D:251:SER:OG	2:D:253:ASP:OD1	2.16	0.64
1:B:1398:THR:HA	1:B:1429:LEU:HD21	1.79	0.64
4:A:102:LEU:HA	4:A:118:GLU:HA	1.80	0.63
2:D:17:ASP:HB3	2:D:40:LEU:HD23	1.80	0.63
1:B:915:ASP:OD1	1:B:918:ARG:NH2	2.32	0.63
2:C:43:LEU:HD13	2:C:45:LYS:HE3	1.81	0.63
1:B:1078:LEU:O	1:B:1081:VAL:HG12	1.99	0.62
1:B:1526:LEU:HD22	1:B:1542:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:VAL:O	2:C:125:THR:OG1	2.17	0.62
2:D:67:VAL:HA	2:D:83:SER:HB3	1.81	0.62
2:D:225:ALA:HB1	2:D:264:ARG:HH21	1.63	0.62
2:D:297:GLU:HG2	2:D:299:HIS:CD2	2.35	0.62
1:B:1324:LEU:HA	4:A:49:PRO:HG2	1.81	0.62
1:B:1360:PRO:HB2	1:B:1396:ASN:HB3	1.81	0.61
1:B:606:GLU:OE1	4:A:106:ARG:NH2	2.33	0.61
1:B:811:LEU:HD11	1:B:840:ILE:HD13	1.83	0.61
2:C:34:THR:HG21	2:C:93:LEU:HD11	1.82	0.61
1:B:609:LEU:HD12	1:B:641:ILE:HD11	1.82	0.61
2:C:17:ASP:HB3	2:C:40:LEU:HD23	1.81	0.61
2:C:133:PHE:HD1	2:C:140:LYS:H	1.47	0.61
1:B:565:TRP:O	1:B:569:ARG:HG2	2.01	0.61
1:B:1374:LEU:O	1:B:1375:LEU:HG	2.00	0.60
2:D:107:VAL:O	2:D:125:THR:OG1	2.18	0.60
4:A:20:ARG:HB3	4:A:33:LEU:O	2.01	0.60
3:E:454:LEU:HG	3:E:458:ILE:HD11	1.83	0.60
2:C:36:VAL:HG22	2:C:46:VAL:HG22	1.83	0.59
1:B:899:ILE:HG12	1:B:920:THR:HG21	1.83	0.59
1:B:1193:PRO:HG3	1:B:1224:LEU:HB3	1.83	0.59
4:A:13:ASP:OD1	4:A:14:PRO:HD2	2.02	0.59
1:B:584:VAL:HG13	1:B:588:GLN:HE22	1.66	0.59
1:B:1524:TRP:HE1	1:B:1557:LEU:HD22	1.68	0.59
2:D:71:ASP:OD1	2:D:72:ILE:N	2.35	0.59
1:B:1499:ARG:NE	1:B:1502:ARG:HE	2.00	0.59
1:B:665:TYR:HH	4:A:116:TYR:HH	1.50	0.58
2:C:42:ASP:HA	2:C:63:HIS:HB2	1.84	0.58
1:B:598:PHE:HD1	1:B:628:ASN:HD22	1.50	0.58
1:B:819:ARG:HA	4:A:177:ILE:HD12	1.83	0.58
2:C:98:GLN:NE2	2:C:100:LYS:O	2.37	0.58
2:D:7:ILE:O	2:D:8:LEU:HG	2.04	0.58
1:B:1416:MET:HE3	1:B:1453:VAL:HG22	1.85	0.58
1:B:1113:LYS:O	1:B:1116:ILE:HG22	2.04	0.58
1:B:480:THR:O	1:B:484:LYS:HG2	2.03	0.58
1:B:1528:ARG:HH12	4:A:15:LEU:CD2	2.17	0.58
1:B:503:TYR:HB3	1:B:512:ARG:HH22	1.68	0.57
1:B:635:VAL:HG12	1:B:658:ILE:HD11	1.86	0.57
1:B:1270:PRO:HB2	1:B:1324:LEU:HD21	1.85	0.57
2:D:36:VAL:HG22	2:D:46:VAL:HG22	1.85	0.57
1:B:787:TYR:CZ	1:B:791:GLN:NE2	2.72	0.57
1:B:588:GLN:NE2	1:B:608:TYR:OH	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:VAL:HA	2:C:293:GLY:HA2	1.85	0.57
1:B:462:LEU:HD21	1:B:498:TYR:CE2	2.40	0.56
1:B:1524:TRP:CH2	4:A:16:ASP:HA	2.39	0.56
2:D:65:LEU:N	2:D:85:ASP:OD1	2.39	0.56
2:D:264:ARG:HG3	2:D:264:ARG:HH11	1.69	0.56
4:A:189:GLY:C	4:A:190:PHE:HD1	2.12	0.56
2:D:34:THR:HG21	2:D:93:LEU:HD11	1.86	0.56
2:C:258:VAL:HG13	2:C:267:VAL:HG23	1.88	0.56
2:D:95:ASN:HB3	2:D:97:LYS:NZ	2.19	0.56
2:D:218:ASP:HB3	2:D:223:ASN:OD1	2.06	0.56
1:B:599:ASN:OD1	4:A:112:GLN:NE2	2.38	0.55
1:B:1117:LEU:HD23	1:B:1119:GLU:H	1.71	0.55
1:B:1285:LYS:NZ	4:A:40:GLU:OE1	2.40	0.55
1:B:1383:ASP:O	1:B:1387:GLU:HG2	2.06	0.55
1:B:1400:VAL:HG23	1:B:1426:SER:HB2	1.88	0.55
1:B:1257:LYS:NZ	2:C:17:ASP:OD2	2.38	0.55
2:D:127:VAL:HG23	2:D:129:LYS:HG3	1.89	0.55
2:D:133:PHE:HD1	2:D:140:LYS:H	1.54	0.55
2:D:156:TYR:CE1	2:D:163:LEU:HD13	2.42	0.54
1:B:736:ASN:OD1	1:B:754:LYS:NZ	2.29	0.54
1:B:1236:THR:O	1:B:1240:GLN:HG3	2.07	0.54
1:B:1016:GLN:HG2	1:B:1017:ASP:N	2.21	0.54
2:D:219:VAL:O	2:D:220:GLN:HG2	2.06	0.54
2:C:151:ILE:HD11	2:C:165:SER:HB2	1.90	0.53
2:C:219:VAL:O	2:C:220:GLN:HG2	2.08	0.53
1:B:1485:LEU:HD22	1:B:1518:ILE:HG12	1.89	0.53
2:D:196:LEU:HD22	2:D:205:LEU:HD11	1.91	0.53
1:B:1356:ASN:OD1	1:B:1357:PRO:HD2	2.08	0.53
1:B:1530:LEU:O	1:B:1534:ASP:N	2.41	0.53
1:B:1155:LYS:NZ	1:B:1157:SER:O	2.42	0.52
2:C:115:SER:HB3	2:C:119:GLN:H	1.74	0.52
1:B:1541:VAL:HA	1:B:1544:ASN:HD21	1.75	0.52
2:D:22:VAL:HG23	2:D:37:THR:HG22	1.91	0.52
1:B:665:TYR:OH	4:A:116:TYR:OH	2.22	0.52
1:B:1225:ASP:OD2	1:B:1228:HIS:ND1	2.37	0.52
1:B:594:ASP:N	1:B:595:PRO:HD2	2.25	0.51
2:D:86:ALA:CB	2:D:105:GLY:HA2	2.40	0.51
2:D:65:LEU:H	2:D:85:ASP:CG	2.18	0.51
2:D:199:SER:HB2	2:D:240:PHE:CE2	2.45	0.51
1:B:1400:VAL:CG1	1:B:1401:PRO:HD3	2.41	0.51
4:A:20:ARG:HH21	4:A:40:GLU:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LYS:CD	1:B:595:PRO:HG3	2.40	0.51
2:D:130:VAL:HG11	2:D:163:LEU:HD21	1.92	0.51
2:C:19:ILE:HA	2:C:39:SER:CB	2.40	0.51
1:B:1224:LEU:HD23	2:D:126:HIS:CE1	2.46	0.51
1:B:1493:LYS:O	1:B:1493:LYS:HD3	2.11	0.51
1:B:917:PHE:O	1:B:921:THR:HG23	2.11	0.51
1:B:1502:ARG:HB3	1:B:1529:HIS:CE1	2.46	0.51
1:B:1112:PHE:CD1	3:E:458:ILE:HG12	2.46	0.51
1:B:1318:GLU:O	1:B:1322:GLN:HG2	2.11	0.51
1:B:918:ARG:NH1	1:B:959:MET:HE3	2.26	0.50
1:B:969:LEU:HD12	1:B:989:LEU:HD12	1.93	0.50
1:B:1014:GLU:O	1:B:1015:ASP:OD1	2.28	0.50
2:C:168:ILE:O	2:C:169:ASP:OD1	2.30	0.50
2:D:19:ILE:HA	2:D:39:SER:CB	2.41	0.50
4:A:107:HIS:HB2	4:A:114:LEU:HD21	1.94	0.50
1:B:1524:TRP:CZ3	1:B:1525:TYR:HE1	2.30	0.49
2:D:168:ILE:O	2:D:169:ASP:OD1	2.30	0.49
1:B:1515:PRO:HG2	1:B:1518:ILE:HD12	1.94	0.49
2:D:11:GLN:O	2:D:297:GLU:HG3	2.13	0.49
4:A:1:MET:HG3	4:A:3:GLU:OE2	2.12	0.49
2:C:22:VAL:HG23	2:C:37:THR:HG22	1.94	0.49
2:D:156:TYR:HE1	2:D:163:LEU:HD13	1.77	0.49
2:C:127:VAL:HG23	2:C:129:LYS:HG3	1.93	0.49
2:C:7:ILE:HG22	2:C:9:PHE:H	1.78	0.49
2:D:215:LYS:HB3	2:D:217:TYR:HE1	1.77	0.49
4:A:175:GLU:HB3	4:A:177:ILE:HG13	1.94	0.49
1:B:572:LEU:HD12	4:A:109:THR:H	1.77	0.49
1:B:1007:ILE:HD13	1:B:1023:ILE:HD13	1.94	0.48
2:D:146:THR:OG1	2:D:173:ASN:ND2	2.46	0.48
1:B:676:HIS:HA	1:B:679:MET:HE3	1.94	0.48
2:D:151:ILE:HD11	2:D:165:SER:HB2	1.94	0.48
1:B:593:ALA:HB3	1:B:595:PRO:HD2	1.95	0.48
2:D:228:LEU:HD23	2:D:259:TRP:CE3	2.49	0.48
1:B:588:GLN:O	1:B:592:ARG:HG2	2.13	0.48
1:B:1016:GLN:HG2	1:B:1017:ASP:H	1.78	0.48
1:B:1147:GLU:HG3	3:E:454:LEU:HD22	1.95	0.48
1:B:1264:LEU:HD22	2:C:20:TRP:CE2	2.48	0.48
2:C:98:GLN:NE2	2:C:101:SER:HB2	2.29	0.48
1:B:480:THR:HG22	1:B:484:LYS:HZ3	1.78	0.47
1:B:587:LEU:HD11	1:B:603:SER:HB2	1.95	0.47
1:B:623:LYS:O	1:B:626:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLN:O	1:B:659:ILE:HG22	2.14	0.47
1:B:1400:VAL:HG13	1:B:1401:PRO:HD3	1.96	0.47
2:C:237:ASN:HD22	2:C:279:GLY:HA2	1.79	0.47
2:D:7:ILE:HG22	2:D:9:PHE:H	1.79	0.47
2:D:89:ARG:HD3	2:D:98:GLN:HE22	1.78	0.47
1:B:865:THR:HG21	1:B:896:MET:HB2	1.96	0.47
1:B:1451:LEU:HD13	1:B:1486:LEU:HD22	1.96	0.47
2:D:215:LYS:HB3	2:D:217:TYR:CE1	2.50	0.47
2:D:297:GLU:HG2	2:D:299:HIS:HD2	1.78	0.47
1:B:591:LEU:HD21	1:B:601:TRP:CZ3	2.50	0.47
1:B:1524:TRP:NE1	1:B:1557:LEU:HD22	2.29	0.47
4:A:20:ARG:NE	4:A:38:ALA:O	2.34	0.47
1:B:570:ARG:HD2	1:B:586:ASP:OD2	2.15	0.47
2:C:228:LEU:HD23	2:C:259:TRP:CE3	2.50	0.47
2:D:86:ALA:HB1	2:D:105:GLY:HA2	1.97	0.47
1:B:748:GLU:OE2	1:B:751:GLN:NE2	2.48	0.46
1:B:951:LEU:HD12	1:B:952:TYR:N	2.30	0.46
1:B:1133:LEU:HD21	1:B:1168:ILE:HD13	1.97	0.46
1:B:503:TYR:O	1:B:508:GLY:N	2.47	0.46
1:B:512:ARG:HD2	1:B:512:ARG:C	2.41	0.46
1:B:1233:LEU:HA	1:B:1236:THR:HG22	1.97	0.46
1:B:1503:ARG:O	1:B:1506:GLU:HG2	2.15	0.46
1:B:1506:GLU:HA	1:B:1509:VAL:HG12	1.97	0.46
2:C:51:ASP:OD1	2:C:51:ASP:N	2.47	0.46
1:B:456:TYR:O	1:B:460:LEU:HG	2.16	0.46
1:B:598:PHE:HB3	1:B:627:LEU:HD11	1.97	0.46
1:B:753:LEU:HD22	1:B:757:GLU:HB3	1.97	0.46
2:D:264:ARG:HG3	2:D:264:ARG:NH1	2.30	0.46
1:B:925:MET:HE2	1:B:971:LYS:HB3	1.97	0.46
1:B:951:LEU:O	1:B:955:ASN:HB2	2.16	0.46
2:D:230:GLY:HA3	2:D:259:TRP:HH2	1.80	0.46
2:D:240:PHE:CZ	2:D:244:ASP:HA	2.51	0.46
1:B:1019:TYR:O	1:B:1023:ILE:HG12	2.16	0.46
2:C:209:SER:OG	2:C:210:ASP:N	2.49	0.46
1:B:1121:THR:HG23	1:B:1124:SER:H	1.81	0.45
1:B:1485:LEU:O	1:B:1489:LEU:HD23	2.16	0.45
2:C:121:LEU:O	2:C:121:LEU:HD23	2.16	0.45
4:A:18:PRO:HG2	4:A:34:ASN:O	2.16	0.45
2:D:231:HIS:CE1	2:D:257:LYS:HD3	2.52	0.45
2:D:115:SER:OG	2:D:117:ASP:OD1	2.20	0.45
1:B:894:TYR:O	1:B:898:TRP:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:CYS:O	1:B:901:GLN:HG2	2.17	0.45
2:D:297:GLU:CD	2:D:299:HIS:HE2	2.24	0.45
2:D:44:VAL:HB	2:D:60:LEU:HD11	1.99	0.45
2:D:51:ASP:OD1	2:D:51:ASP:N	2.47	0.45
1:B:564:LYS:HD2	1:B:595:PRO:HG3	1.99	0.45
2:C:60:LEU:HD13	2:C:91:TRP:CD2	2.52	0.45
2:C:158:PRO:HG3	2:C:200:PRO:HA	1.99	0.45
1:B:551:LEU:HD22	1:B:566:ALA:HA	1.99	0.45
1:B:640:ALA:O	1:B:644:ILE:HG13	2.17	0.45
1:B:1128:LEU:HD11	1:B:1140:LEU:HD21	1.99	0.45
2:C:49:TRP:HA	2:C:53:ARG:O	2.16	0.45
1:B:1115:SER:HB2	3:E:454:LEU:HD21	1.99	0.45
2:C:231:HIS:CE1	2:C:257:LYS:HD3	2.52	0.44
2:D:9:PHE:HB3	2:D:300:ILE:HB	1.99	0.44
2:C:200:PRO:HD2	2:C:244:ASP:OD1	2.18	0.44
2:D:116:PRO:HD3	2:D:156:TYR:CD2	2.53	0.44
2:D:121:LEU:HD23	2:D:121:LEU:O	2.17	0.44
1:B:1527:LEU:HD21	1:B:1561:LEU:HD21	1.99	0.44
2:C:47:TRP:CZ3	2:C:56:LEU:HB2	2.53	0.44
2:D:115:SER:HA	2:D:156:TYR:CE2	2.51	0.44
1:B:1153:LYS:HB2	1:B:1153:LYS:HE2	1.84	0.44
2:C:114:PHE:CE1	2:C:121:LEU:HD12	2.52	0.44
1:B:1465:SER:O	1:B:1469:GLU:HG2	2.18	0.44
2:D:220:GLN:O	2:D:221:HIS:ND1	2.50	0.44
1:B:584:VAL:O	1:B:588:GLN:OE1	2.35	0.44
1:B:583:ALA:O	1:B:587:LEU:HD23	2.18	0.44
2:C:78:ILE:HD11	2:C:90:LEU:HD13	1.99	0.44
4:A:161:GLU:HA	4:A:164:ILE:HD11	2.00	0.44
1:B:1543:VAL:HG12	1:B:1547:LYS:NZ	2.33	0.43
2:D:9:PHE:HE2	2:D:54:LEU:HD12	1.82	0.43
1:B:587:LEU:HB3	1:B:604:LEU:HD13	1.99	0.43
2:D:209:SER:OG	2:D:210:ASP:N	2.51	0.43
2:D:108:ASP:O	2:D:131:ASN:ND2	2.50	0.43
1:B:807:LEU:HD22	1:B:840:ILE:HD11	2.01	0.43
2:C:44:VAL:HG12	2:C:44:VAL:O	2.18	0.43
4:A:76:HIS:ND1	4:A:76:HIS:O	2.51	0.43
1:B:976:ILE:HG22	1:B:978:ASN:H	1.82	0.43
2:D:240:PHE:HZ	2:D:244:ASP:HA	1.83	0.43
1:B:976:ILE:O	1:B:977:GLN:HG2	2.18	0.43
1:B:1099:TYR:CE2	4:A:63:LEU:HD23	2.54	0.43
1:B:574:TYR:CD2	1:B:582:GLN:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1489:LEU:HD13	1:B:1525:TYR:CE2	2.53	0.43
2:C:216:ILE:O	2:C:225:ALA:N	2.43	0.43
1:B:650:GLU:O	1:B:654:GLN:HG3	2.19	0.43
1:B:770:LEU:HD11	1:B:779:TRP:NE1	2.34	0.43
2:D:42:ASP:OD1	2:D:42:ASP:N	2.51	0.43
2:C:158:PRO:HD2	2:C:202:SER:HB3	2.00	0.42
2:C:230:GLY:HA3	2:C:259:TRP:HH2	1.84	0.42
1:B:674:GLU:O	1:B:678:MET:HG2	2.19	0.42
1:B:1298:ASP:OD2	1:B:1341:ARG:NH2	2.53	0.42
1:B:1343:SER:O	1:B:1347:THR:HG23	2.20	0.42
1:B:591:LEU:HD11	1:B:601:TRP:CZ2	2.53	0.42
1:B:744:LEU:HD21	1:B:753:LEU:HD21	2.01	0.42
2:D:44:VAL:HG12	2:D:44:VAL:O	2.18	0.42
4:A:172:GLU:HG3	4:A:173:ALA:N	2.35	0.42
1:B:558:ALA:HB1	1:B:561:GLY:O	2.20	0.42
1:B:696:ILE:HG13	1:B:727:LEU:HG	2.01	0.42
1:B:704:THR:O	1:B:708:GLN:HG2	2.19	0.42
1:B:1505:LEU:HD21	1:B:1525:TYR:HB3	2.01	0.42
4:A:164:ILE:HG22	4:A:164:ILE:O	2.19	0.42
2:C:11:GLN:O	2:C:297:GLU:HG2	2.19	0.42
1:B:512:ARG:HE	1:B:512:ARG:HB3	1.41	0.42
1:B:1051:LEU:O	1:B:1055:ILE:HG12	2.19	0.42
4:A:85:THR:HG22	4:A:86:ASP:N	2.35	0.42
1:B:1266:SER:O	1:B:1266:SER:OG	2.34	0.42
1:B:1337:ILE:HD11	1:B:1369:VAL:HG22	2.02	0.42
2:C:82:SER:HB3	2:C:112:LEU:HD21	2.02	0.42
1:B:697:GLU:O	1:B:701:GLU:HG3	2.20	0.42
1:B:1393:VAL:HG21	1:B:1406:LEU:HB2	2.01	0.42
2:D:186:LEU:HD23	2:D:217:TYR:CD2	2.55	0.42
4:A:43:LEU:HD12	4:A:43:LEU:O	2.20	0.42
1:B:509:ASP:O	1:B:512:ARG:NH2	2.53	0.42
2:C:92:ASP:O	2:C:93:LEU:HB3	2.20	0.41
2:D:60:LEU:HD13	2:D:91:TRP:CD2	2.55	0.41
1:B:1026:TYR:CZ	1:B:1030:LEU:HD22	2.54	0.41
4:A:21:ALA:HA	4:A:32:LEU:HD23	2.02	0.41
4:A:50:CYS:SG	4:A:51:ALA:N	2.93	0.41
1:B:927:THR:HG23	1:B:972:TYR:CE2	2.55	0.41
1:B:1372:LYS:HB3	1:B:1373:PRO:HD3	2.02	0.41
2:D:44:VAL:HB	2:D:60:LEU:CD1	2.50	0.41
2:D:46:VAL:HB	2:D:58:TRP:HB2	2.02	0.41
2:D:138:GLY:C	2:D:139:LYS:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:SER:HB3	1:B:1168:ILE:HD11	2.02	0.41
1:B:1502:ARG:HD2	1:B:1503:ARG:N	2.35	0.41
2:C:196:LEU:HD22	2:C:205:LEU:HD11	2.01	0.41
1:B:895:LEU:O	1:B:899:ILE:HG13	2.20	0.41
2:C:140:LYS:HE3	2:C:143:SER:HB3	2.03	0.41
4:A:174:GLU:N	4:A:174:GLU:OE1	2.54	0.41
1:B:681:LYS:O	1:B:685:VAL:HG23	2.21	0.41
1:B:777:ASN:HD22	4:A:99:PRO:HG3	1.85	0.41
1:B:1506:GLU:O	1:B:1510:TYR:HB2	2.21	0.41
1:B:584:VAL:CG1	1:B:588:GLN:HE22	2.31	0.41
1:B:912:ASP:OD1	1:B:912:ASP:N	2.51	0.41
1:B:1164:LEU:O	1:B:1168:ILE:HG12	2.20	0.41
2:C:151:ILE:HD11	2:C:165:SER:CB	2.51	0.41
1:B:1344:GLU:OE1	1:B:1344:GLU:N	2.48	0.41
2:C:19:ILE:HA	2:C:39:SER:HB2	2.02	0.41
2:C:31:ASN:OD1	2:C:31:ASN:N	2.52	0.41
2:C:160:GLY:O	2:C:161:LYS:HG2	2.20	0.41
2:D:48:LYS:HB2	2:D:48:LYS:HE2	1.79	0.41
2:D:59:SER:O	2:D:59:SER:OG	2.38	0.41
1:B:878:GLU:HG2	1:B:879:GLN:H	1.85	0.40
2:C:107:VAL:C	2:C:125:THR:HG1	2.28	0.40
2:D:19:ILE:HA	2:D:39:SER:HB2	2.02	0.40
4:A:17:LEU:H	4:A:17:LEU:HD23	1.86	0.40
1:B:770:LEU:HD13	1:B:778:THR:OG1	2.21	0.40
1:B:1370:GLN:O	1:B:1373:PRO:HD2	2.20	0.40
1:B:885:LYS:HE2	1:B:901:GLN:HE22	1.86	0.40
1:B:1251:GLU:O	1:B:1252:LYS:HG2	2.20	0.40
1:B:1356:ASN:OD1	1:B:1357:PRO:CD	2.68	0.40
2:D:50:ARG:HB2	2:D:50:ARG:NH1	2.37	0.40
2:D:125:THR:O	2:D:151:ILE:HG22	2.22	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	B	1111/1568 (71%)	1087 (98%)	23 (2%)	1 (0%)	48	78
2	C	303/305 (99%)	288 (95%)	15 (5%)	0	100	100
2	D	303/305 (99%)	287 (95%)	16 (5%)	0	100	100
3	E	12/179 (7%)	12 (100%)	0	0	100	100
4	A	159/976 (16%)	148 (93%)	9 (6%)	2 (1%)	9	33
All	All	1888/3333 (57%)	1822 (96%)	63 (3%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	594	ASP
4	A	13	ASP
4	A	109	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	921/1316 (70%)	921 (100%)	0	100	100
2	C	260/260 (100%)	260 (100%)	0	100	100
2	D	260/260 (100%)	260 (100%)	0	100	100
3	E	13/165 (8%)	13 (100%)	0	100	100
4	A	140/824 (17%)	140 (100%)	0	100	100
All	All	1594/2825 (56%)	1594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	582	GLN
1	B	588	GLN
1	B	599	ASN
1	B	628	ASN
1	B	1187	HIS
1	B	1227	ASN
1	B	1281	HIS
1	B	1290	ASN
1	B	1564	GLN
2	C	98	GLN
2	D	57	GLN
2	D	126	HIS
4	A	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51137. These allow visual inspection of the internal detail of the map and identification of artifacts.

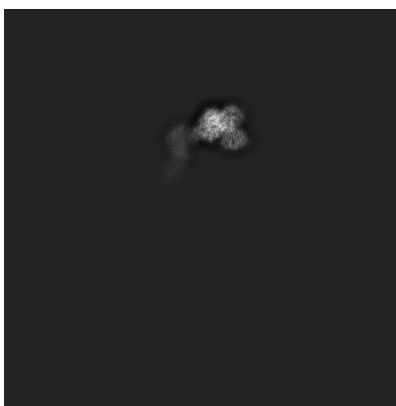
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

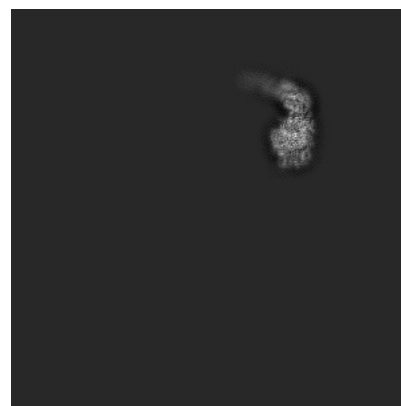
6.1.1 Primary map



X

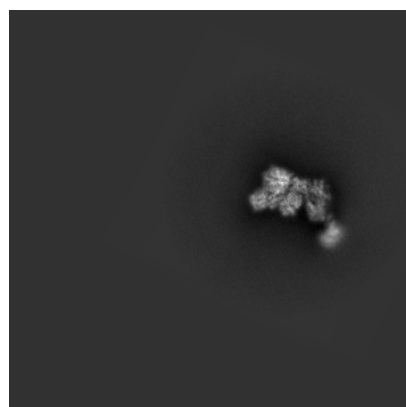


Y

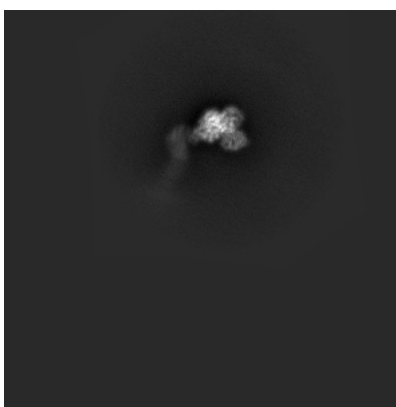


Z

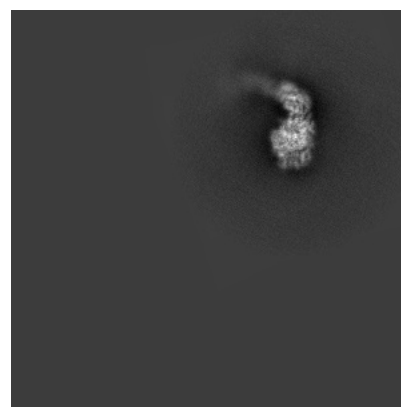
6.1.2 Raw map



X



Y

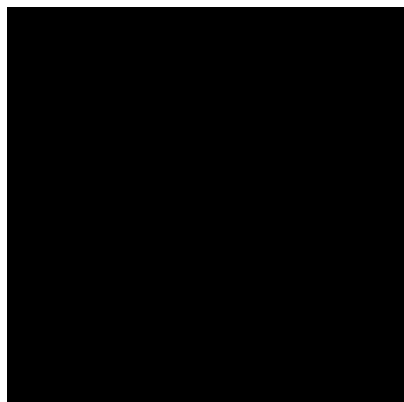


Z

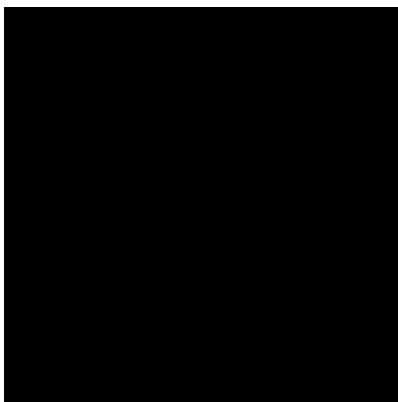
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

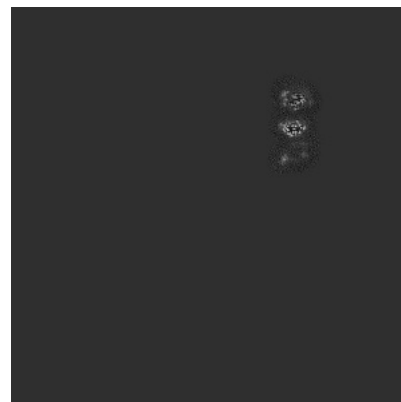
6.2.1 Primary map



X Index: 416

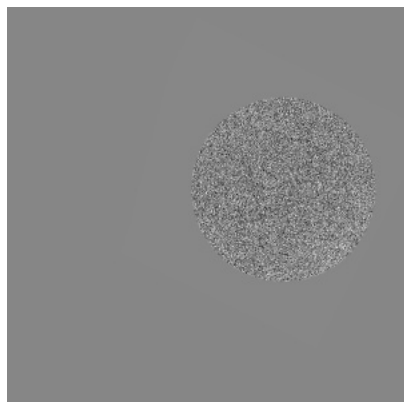


Y Index: 416

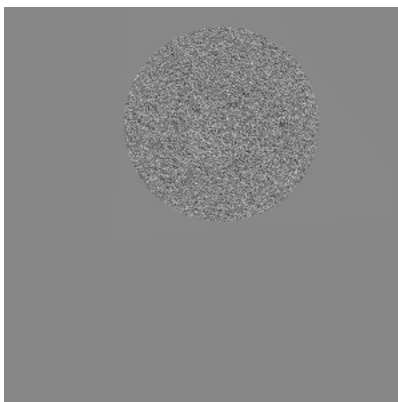


Z Index: 416

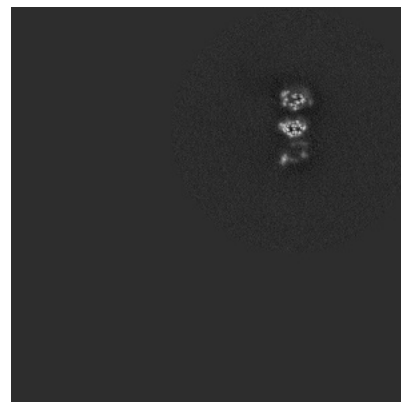
6.2.2 Raw map



X Index: 416



Y Index: 416



Z Index: 416

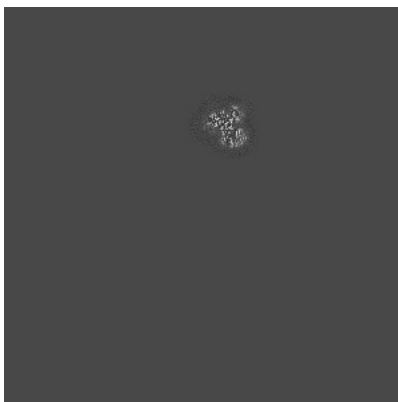
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

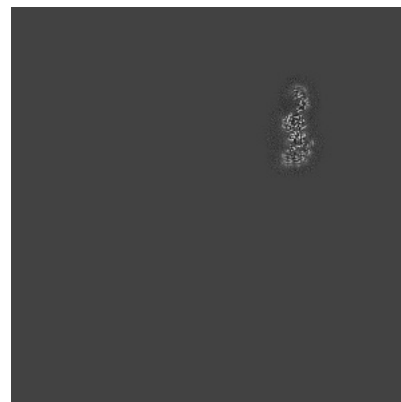
6.3.1 Primary map



X Index: 595

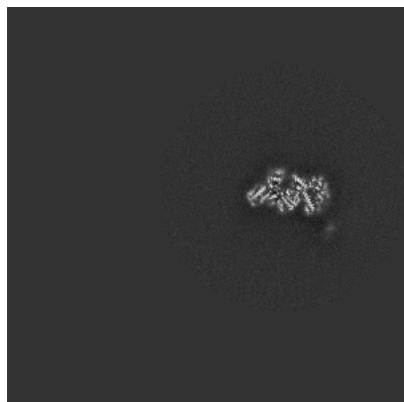


Y Index: 561

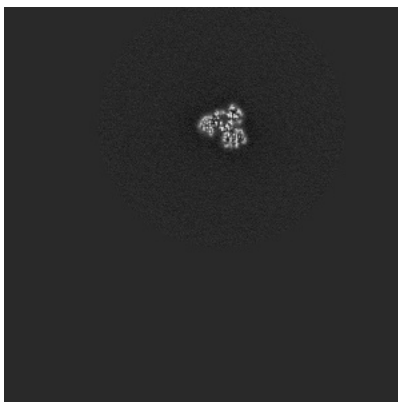


Z Index: 440

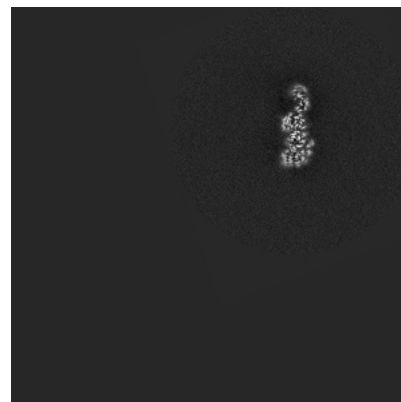
6.3.2 Raw map



X Index: 595



Y Index: 568

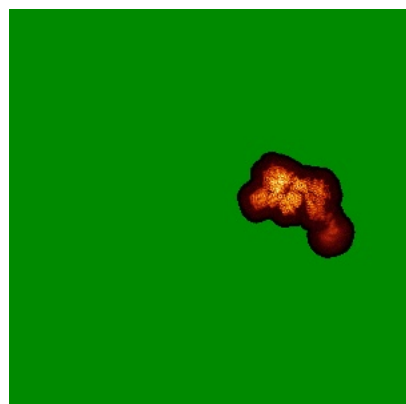


Z Index: 441

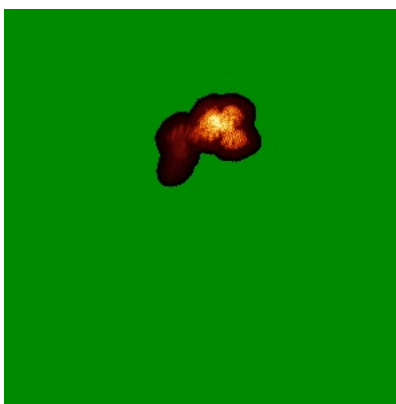
The images above show the largest variance slices of the map in three orthogonal directions.

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

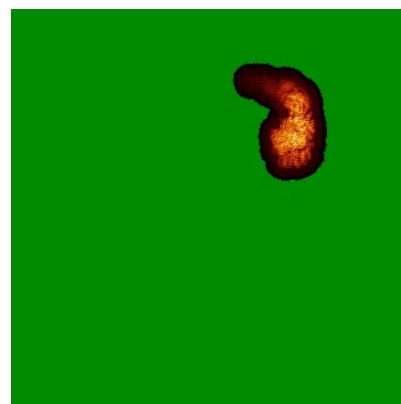
6.4.1 Primary map



X

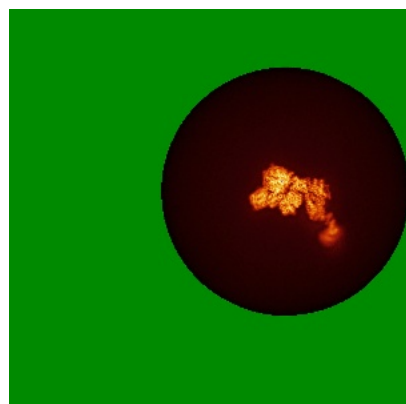


Y

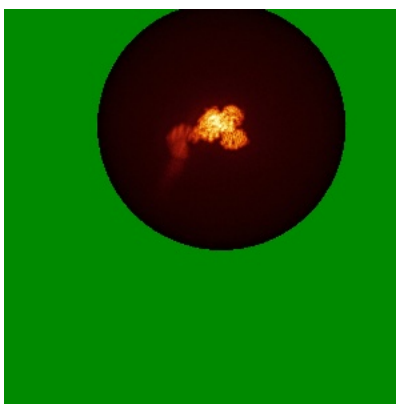


Z

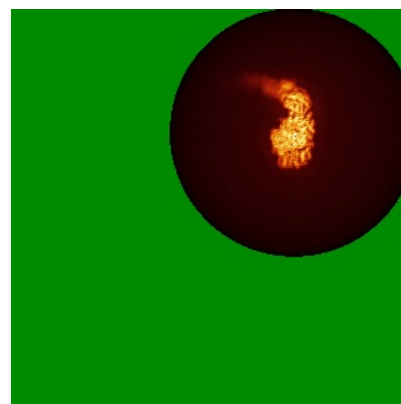
6.4.2 Raw map



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.

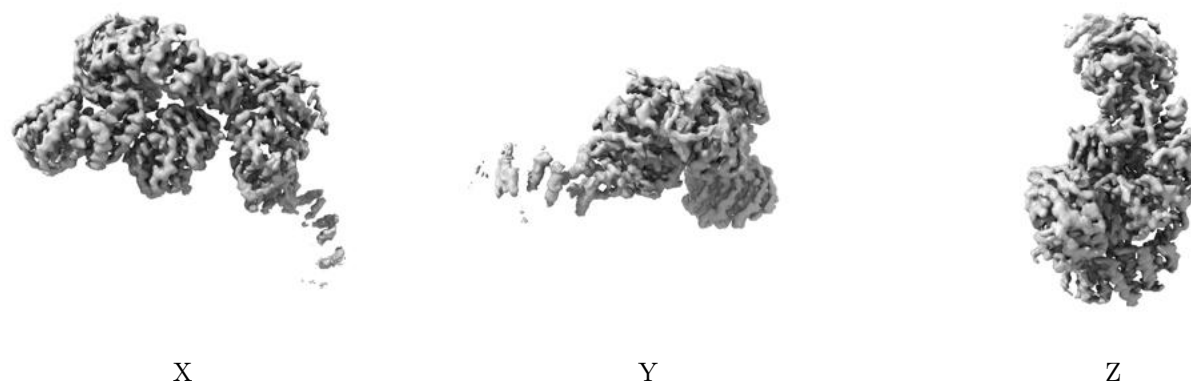
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

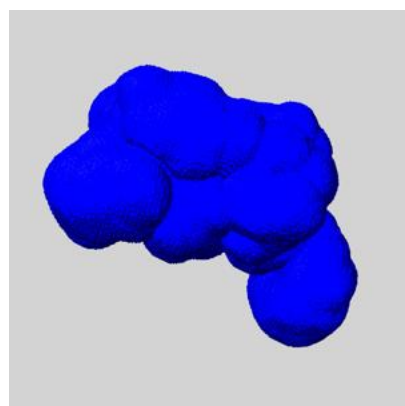
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

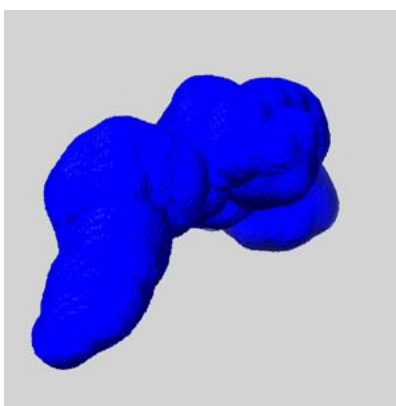
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

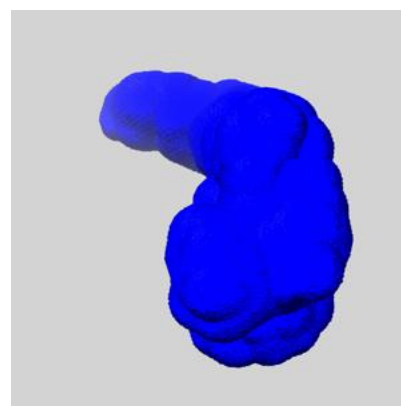
6.6.1 emd_51137_msk_1.map [i](#)



X



Y

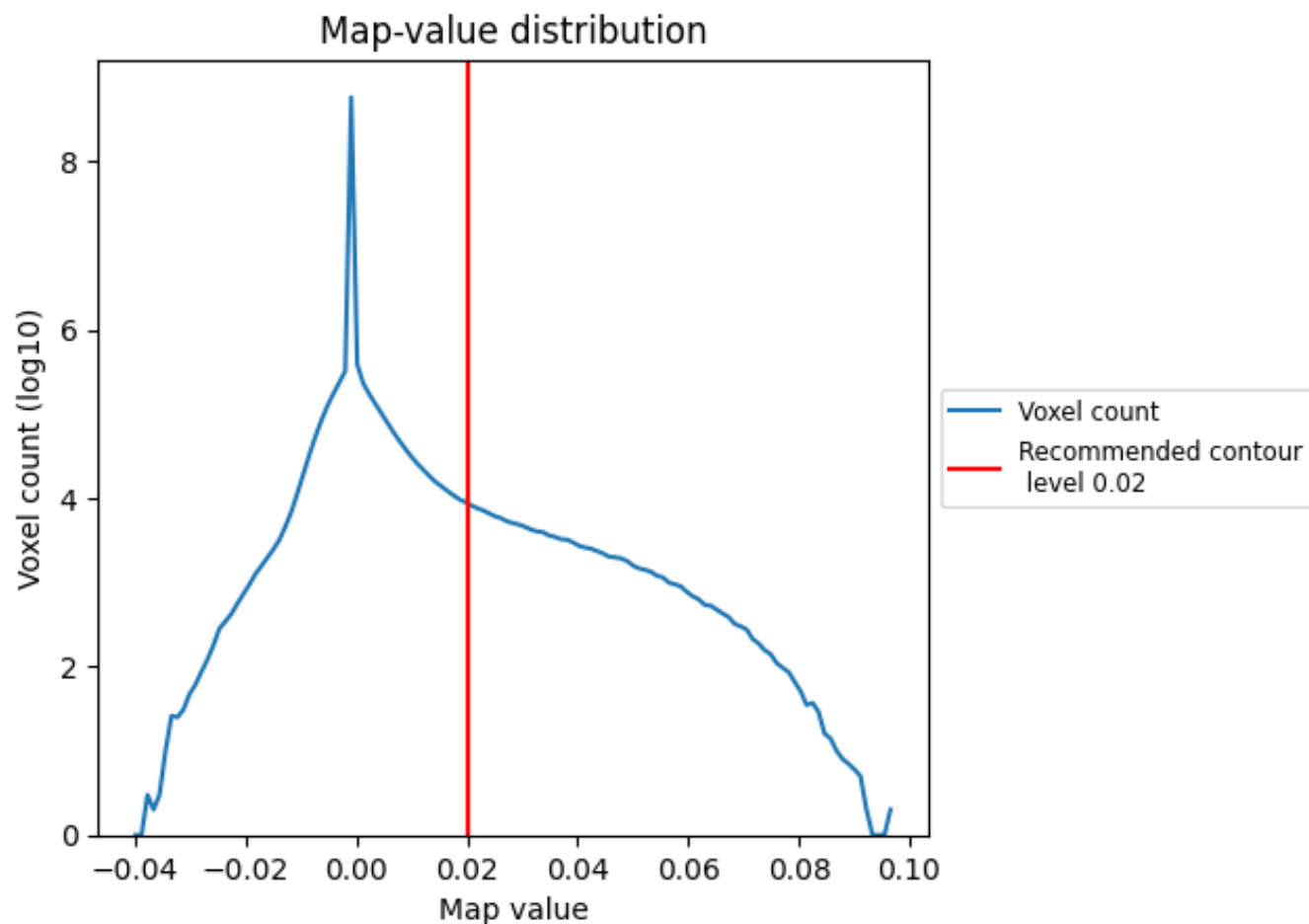


Z

7 Map analysis [i](#)

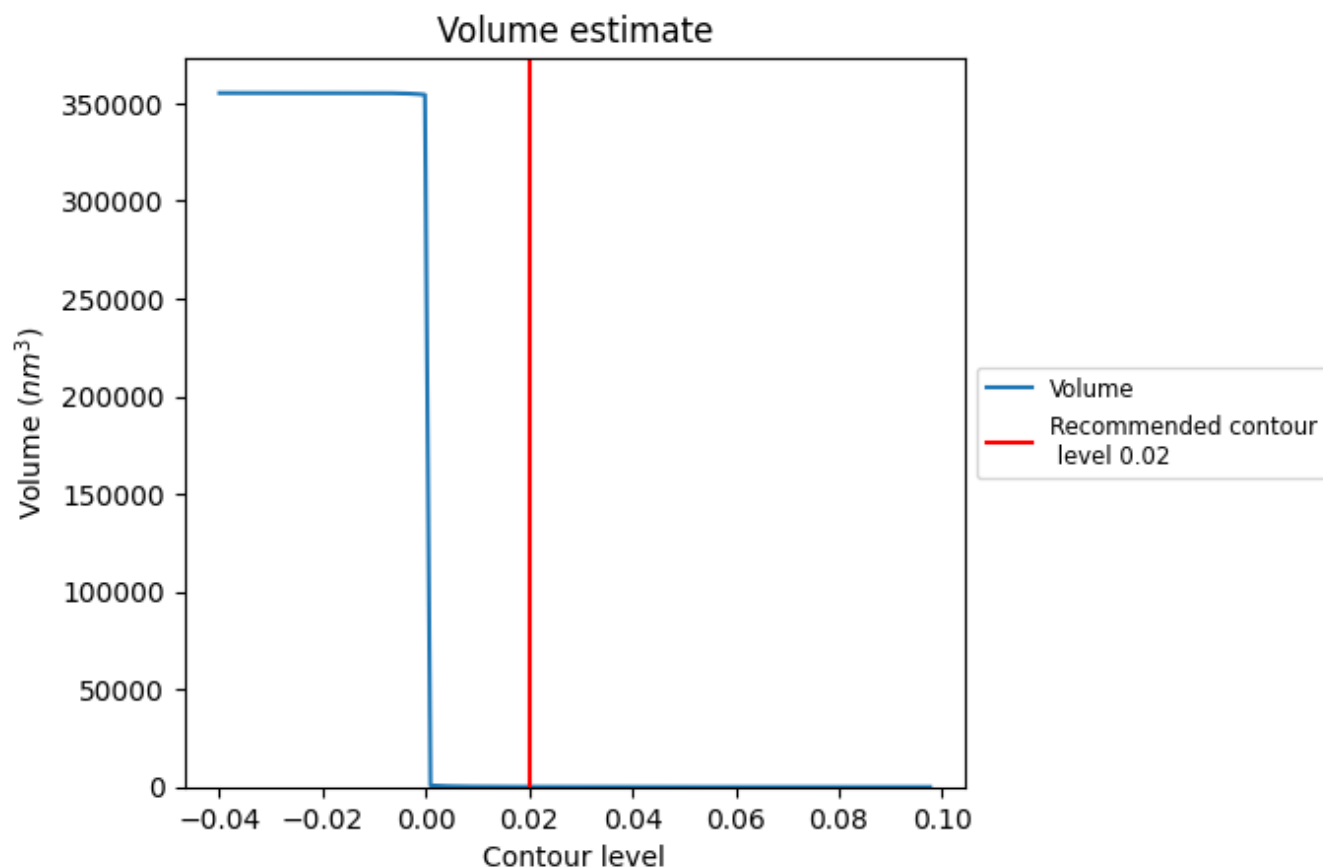
This section contains the results of statistical analysis of the map.

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.

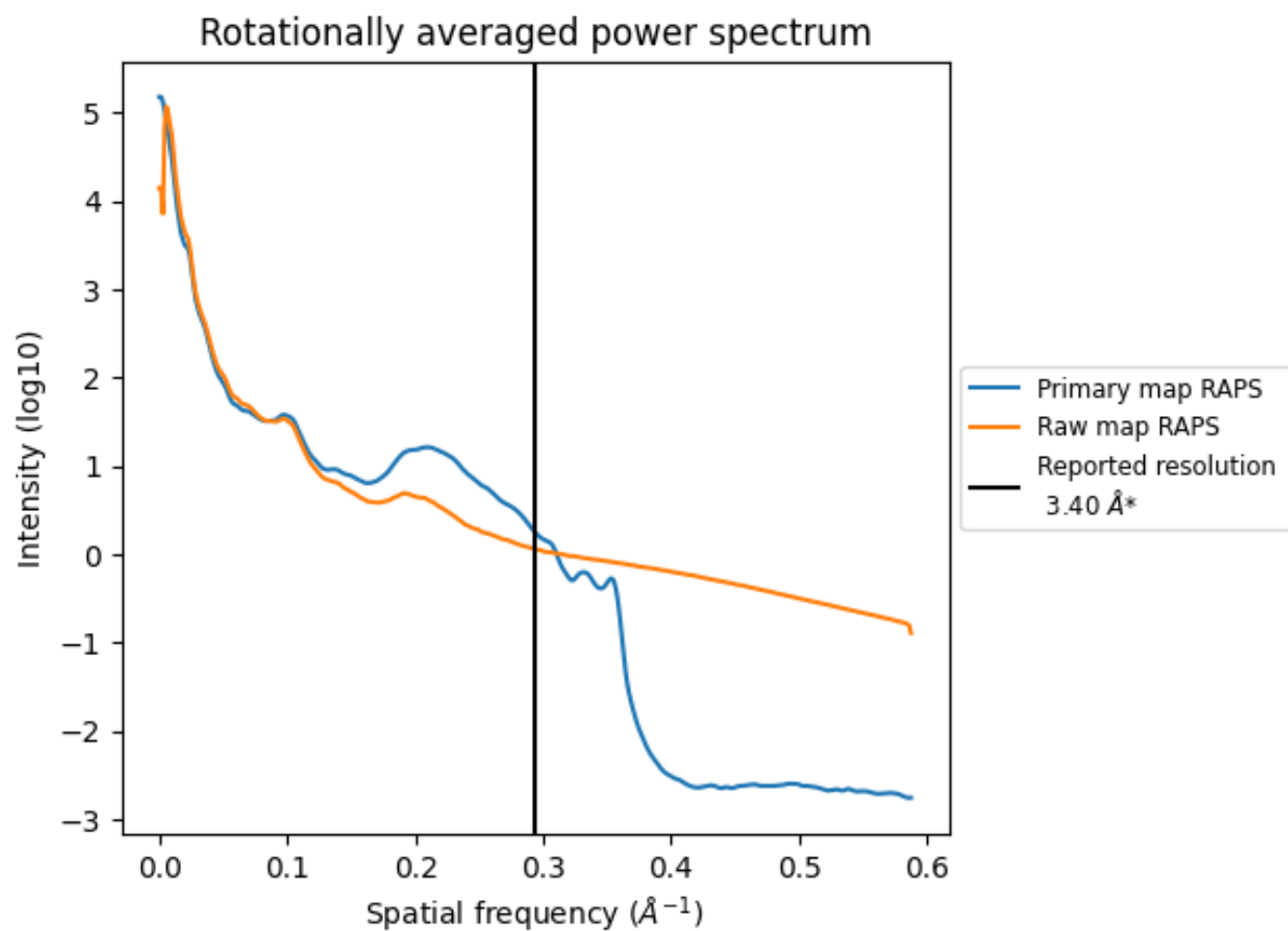
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 ⓘ

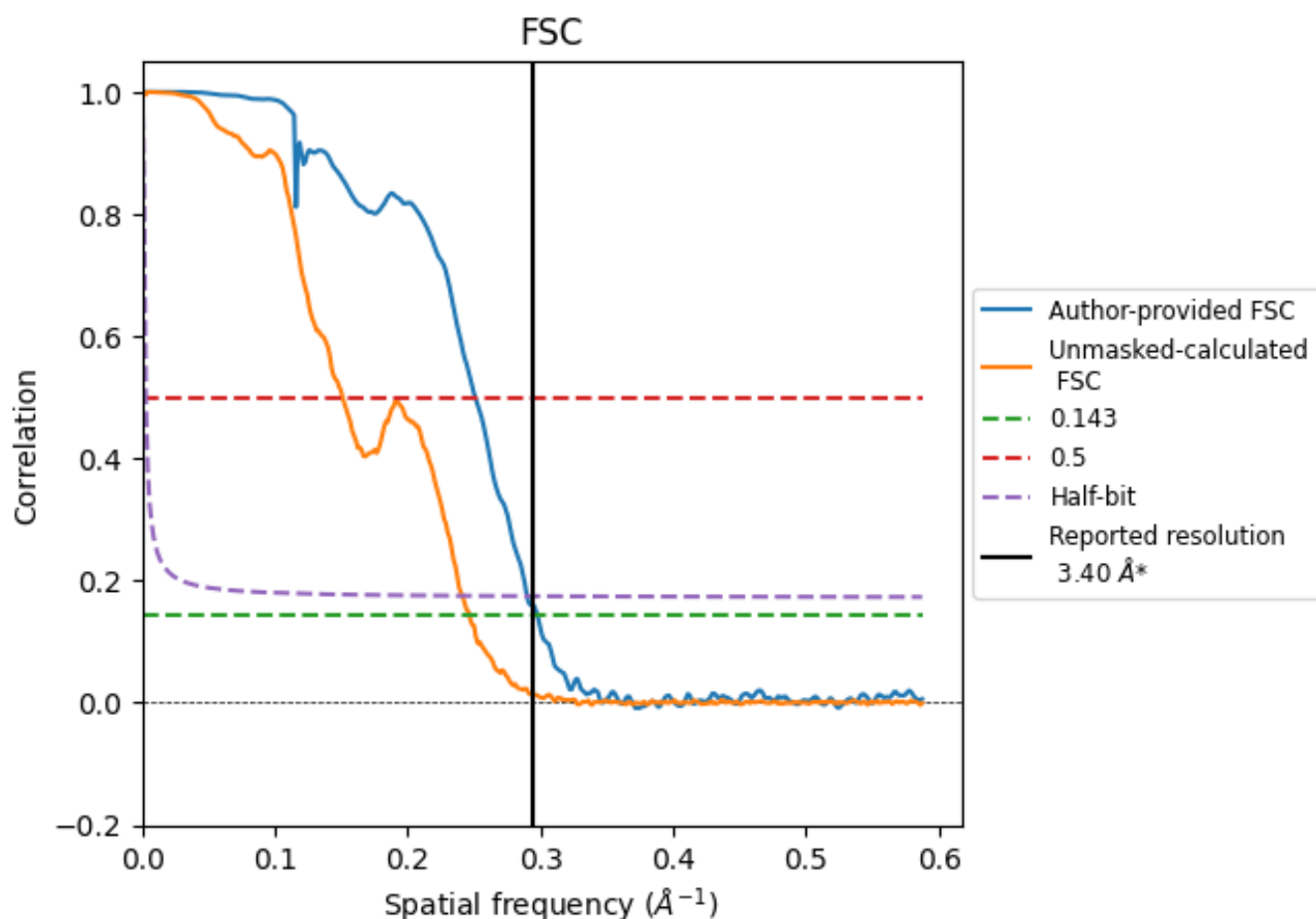


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

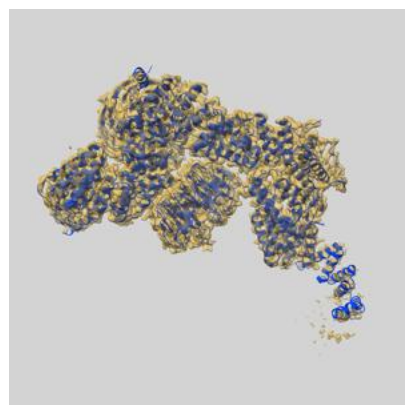
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.99	3.45
Unmasked-calculated*	4.06	6.63	4.15

*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 4.06 differs from the reported value 3.4 by more than 10 %

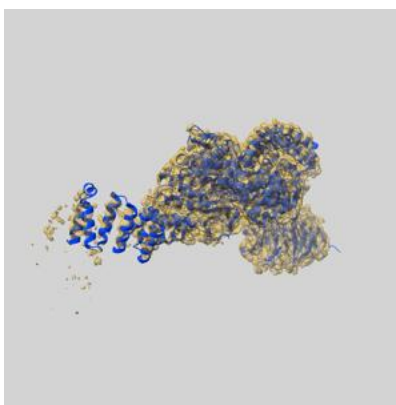
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51137 and PDB model 9G8R. Per-residue inclusion information can be found in section [3](#) on page [6](#).

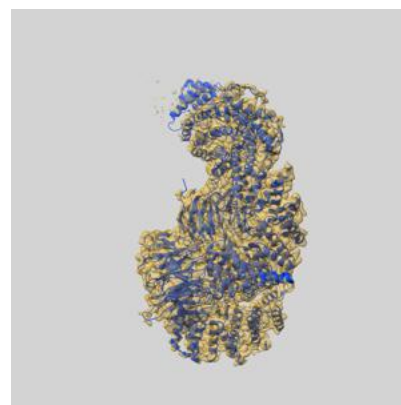
9.1 Map-model overlay [i](#)



X



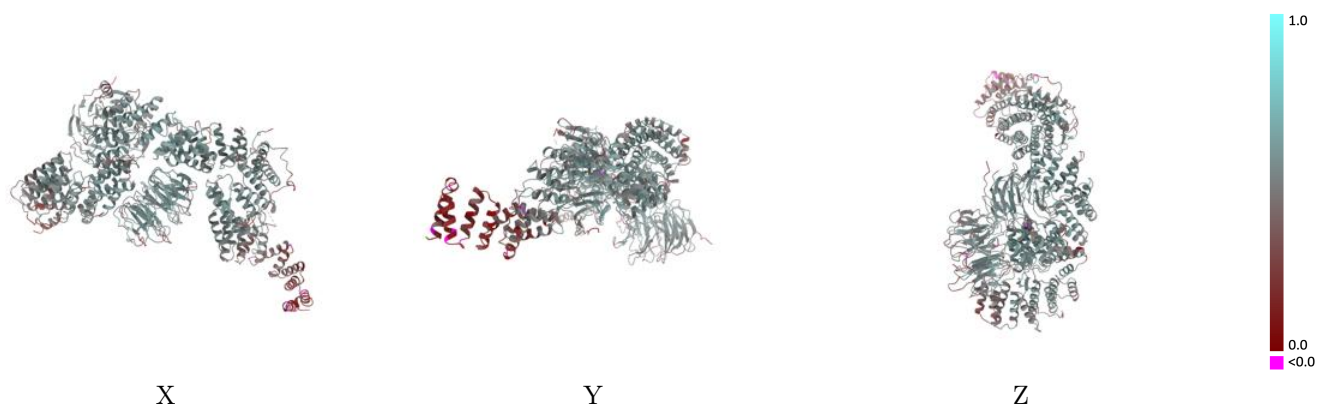
Y



Z

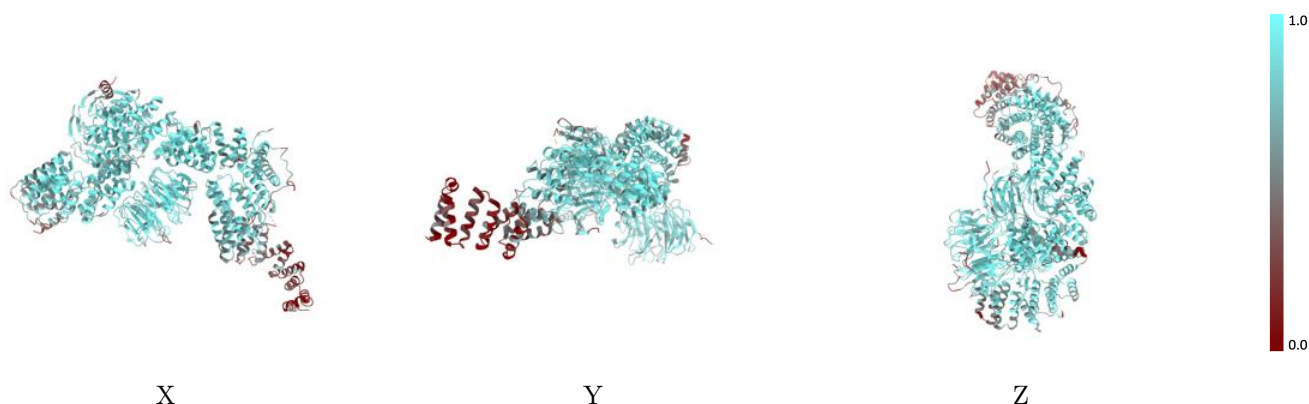
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



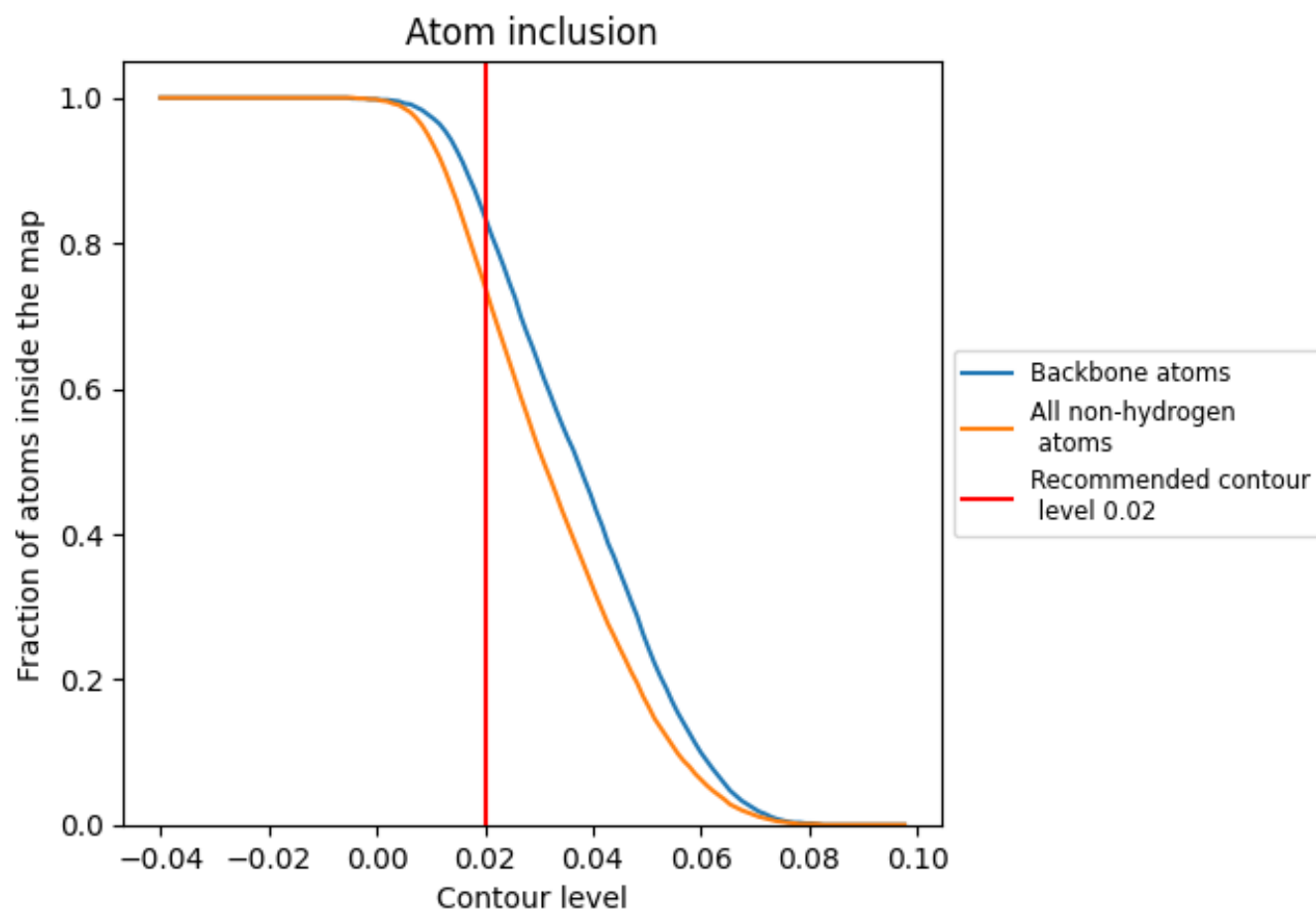
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.4830
A	0.7180	0.4890
B	0.7130	0.4750
C	0.8480	0.5230
D	0.7740	0.4770
E	0.2380	0.3840

