



Full wwPDB EM Validation Report ⓘ

Aug 28, 2025 – 01:25 pm BST

PDB ID : 9HN4 / pdb_00009hn4
EMDB ID : EMD-52306
Title : Cryo-EM structure of human separase bound to phosphorylated SCC1 (310-550 aa)
Authors : Yu, J.; Schmidt, S.; Botto, M.; Boland, A.
Deposited on : 2024-12-10
Resolution : 2.93 Å(reported)
Based on initial model : 7NJ1

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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

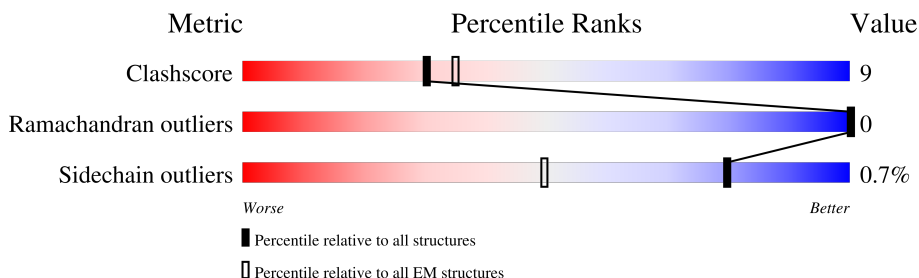
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	
2	B	2172	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10855 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 Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	35	Total	C	N	O	P	S	0	0
			283	172	45	63	1	2		

- Molecule 2 is a protein called Separin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1424	Total	C	N	O	S	0	0
			10571	6707	1863	1953	48		

There are 113 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-54	MET	-	initiating methionine	UNP Q14674
B	-53	ASP	-	expression tag	UNP Q14674
B	-52	TYR	-	expression tag	UNP Q14674
B	-51	LYS	-	expression tag	UNP Q14674
B	-50	ASP	-	expression tag	UNP Q14674
B	-49	HIS	-	expression tag	UNP Q14674
B	-48	ASP	-	expression tag	UNP Q14674
B	-47	GLY	-	expression tag	UNP Q14674
B	-46	ASP	-	expression tag	UNP Q14674
B	-45	TYR	-	expression tag	UNP Q14674
B	-44	LYS	-	expression tag	UNP Q14674
B	-43	ASP	-	expression tag	UNP Q14674
B	-42	HIS	-	expression tag	UNP Q14674
B	-41	ASP	-	expression tag	UNP Q14674
B	-40	ILE	-	expression tag	UNP Q14674
B	-39	ASP	-	expression tag	UNP Q14674
B	-38	TYR	-	expression tag	UNP Q14674
B	-37	LYS	-	expression tag	UNP Q14674
B	-36	ASP	-	expression tag	UNP Q14674
B	-35	ASP	-	expression tag	UNP Q14674
B	-34	ASP	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	ASP	-	expression tag	UNP Q14674
B	-32	LYS	-	expression tag	UNP Q14674
B	-31	SER	-	expression tag	UNP Q14674
B	-30	GLY	-	expression tag	UNP Q14674
B	-29	PRO	-	expression tag	UNP Q14674
B	-28	GLY	-	expression tag	UNP Q14674
B	-27	GLY	-	expression tag	UNP Q14674
B	-26	SER	-	expression tag	UNP Q14674
B	-25	GLY	-	expression tag	UNP Q14674
B	-24	GLY	-	expression tag	UNP Q14674
B	-23	SER	-	expression tag	UNP Q14674
B	-22	GLY	-	expression tag	UNP Q14674
B	-21	GLY	-	expression tag	UNP Q14674
B	-20	GLY	-	expression tag	UNP Q14674
B	-19	SER	-	expression tag	UNP Q14674
B	-18	GLY	-	expression tag	UNP Q14674
B	-17	GLY	-	expression tag	UNP Q14674
B	-16	GLY	-	expression tag	UNP Q14674
B	-15	SER	-	expression tag	UNP Q14674
B	-14	GLY	-	expression tag	UNP Q14674
B	-13	GLU	-	expression tag	UNP Q14674
B	-12	ASN	-	expression tag	UNP Q14674
B	-11	LEU	-	expression tag	UNP Q14674
B	-10	TYR	-	expression tag	UNP Q14674
B	-9	PHE	-	expression tag	UNP Q14674
B	-8	GLN	-	expression tag	UNP Q14674
B	-7	GLY	-	expression tag	UNP Q14674
B	-6	GLY	-	expression tag	UNP Q14674
B	-5	GLY	-	expression tag	UNP Q14674
B	-4	SER	-	expression tag	UNP Q14674
B	-3	GLY	-	expression tag	UNP Q14674
B	-2	GLY	-	expression tag	UNP Q14674
B	-1	SER	-	expression tag	UNP Q14674
B	0	GLY	-	expression tag	UNP Q14674
B	25	ASP	ALA	conflict	UNP Q14674
B	116	VAL	ALA	conflict	UNP Q14674
B	1372	SER	ARG	conflict	UNP Q14674
B	1525	GLY	-	linker	UNP Q14674
B	1526	LEU	-	linker	UNP Q14674
B	1527	GLU	-	linker	UNP Q14674
B	1528	VAL	-	linker	UNP Q14674
B	1529	LEU	-	linker	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1530	PHE	-	linker	UNP Q14674
B	1531	GLN	-	linker	UNP Q14674
B	1532	GLY	-	linker	UNP Q14674
B	1533	PRO	-	linker	UNP Q14674
B	1534	GLY	-	linker	UNP Q14674
B	1535	SER	-	linker	UNP Q14674
B	1536	GLY	-	linker	UNP Q14674
B	1561	GLN	ARG	conflict	UNP Q14674
B	2029	SER	CYS	conflict	UNP Q14674
B	2037	HIS	ARG	conflict	UNP Q14674
B	2121	SER	-	expression tag	UNP Q14674
B	2122	SER	-	expression tag	UNP Q14674
B	2123	LEU	-	expression tag	UNP Q14674
B	2124	ALA	-	expression tag	UNP Q14674
B	2125	GLU	-	expression tag	UNP Q14674
B	2126	GLU	-	expression tag	UNP Q14674
B	2127	ASN	-	expression tag	UNP Q14674
B	2128	LEU	-	expression tag	UNP Q14674
B	2129	TYR	-	expression tag	UNP Q14674
B	2130	PHE	-	expression tag	UNP Q14674
B	2131	GLN	-	expression tag	UNP Q14674
B	2132	SER	-	expression tag	UNP Q14674
B	2133	TRP	-	expression tag	UNP Q14674
B	2134	SER	-	expression tag	UNP Q14674
B	2135	HIS	-	expression tag	UNP Q14674
B	2136	PRO	-	expression tag	UNP Q14674
B	2137	GLN	-	expression tag	UNP Q14674
B	2138	PHE	-	expression tag	UNP Q14674
B	2139	GLU	-	expression tag	UNP Q14674
B	2140	LYS	-	expression tag	UNP Q14674
B	2141	GLY	-	expression tag	UNP Q14674
B	2142	GLY	-	expression tag	UNP Q14674
B	2143	GLY	-	expression tag	UNP Q14674
B	2144	SER	-	expression tag	UNP Q14674
B	2145	GLY	-	expression tag	UNP Q14674
B	2146	GLY	-	expression tag	UNP Q14674
B	2147	GLY	-	expression tag	UNP Q14674
B	2148	SER	-	expression tag	UNP Q14674
B	2149	GLY	-	expression tag	UNP Q14674
B	2150	GLY	-	expression tag	UNP Q14674
B	2151	GLY	-	expression tag	UNP Q14674
B	2152	SER	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2153	TRP	-	expression tag	UNP Q14674
B	2154	SER	-	expression tag	UNP Q14674
B	2155	HIS	-	expression tag	UNP Q14674
B	2156	PRO	-	expression tag	UNP Q14674
B	2157	GLN	-	expression tag	UNP Q14674
B	2158	PHE	-	expression tag	UNP Q14674
B	2159	GLU	-	expression tag	UNP Q14674
B	2160	LYS	-	expression tag	UNP Q14674

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	



GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298574	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	20.078	Depositor
Minimum map value	-0.249	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	0.338	Depositor
Recommended contour level	3	Depositor
Map size (Å)	360.96002, 360.96002, 360.96002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9024001, 0.9024001, 0.9024001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.72	0/277	0.76	0/372
2	B	0.49	0/10768	0.65	2/14667 (0.0%)
All	All	0.49	0/11045	0.65	2/15039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1688	PRO	N-CD-CG	-5.85	96.78	103.80
2	B	1803	LYS	N-CA-C	-5.72	106.28	113.72

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	283	0	257	25	0
2	B	10571	0	10310	188	0
3	B	1	0	0	0	0
All	All	10855	0	10567	189	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 (189) 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:471:PRO:HA	2:B:505:ARG:NH1	1.77	0.98
1:A:471:PRO:HG3	2:B:462:ASN:HA	1.46	0.94
1:A:471:PRO:CG	2:B:462:ASN:HA	1.98	0.92
2:B:1765:LYS:HE2	2:B:2063:ASP:OD2	1.75	0.87
1:A:444:ILE:HD13	2:B:2017:ARG:HH21	1.51	0.76
1:A:471:PRO:HA	2:B:505:ARG:CZ	2.18	0.72
2:B:1689:GLN:HB2	2:B:1690:PRO:HD3	1.72	0.71
1:A:444:ILE:HG23	2:B:2013:GLN:HG3	1.73	0.70
2:B:735:PHE:CZ	2:B:1019:THR:HA	2.29	0.68
1:A:443:PRO:HB3	2:B:1006:GLU:HG3	1.77	0.66
2:B:504:HIS:HD1	2:B:530:TRP:HZ2	1.49	0.61
2:B:504:HIS:O	2:B:508:ARG:HG3	2.01	0.60
2:B:1807:LEU:HD13	2:B:1913:LEU:HD11	1.82	0.59
2:B:1897:LYS:O	2:B:1900:GLN:NE2	2.35	0.59
2:B:569:LEU:HD23	2:B:585:LEU:HG	1.83	0.59
2:B:1277:LEU:HD11	2:B:1288:PHE:HZ	1.68	0.59
2:B:1220:ASP:HB3	2:B:1261:LEU:HD11	1.85	0.59
2:B:1629:ARG:HG3	2:B:1677:PHE:HD2	1.67	0.59
2:B:1723:ASN:HD21	2:B:1751:ARG:HB2	1.67	0.58
2:B:1191:CYS:HB2	2:B:1223:LEU:HD13	1.85	0.58
2:B:855:LEU:HD21	2:B:896:ALA:HB1	1.86	0.58
2:B:617:GLU:OE2	2:B:617:GLU:N	2.20	0.58
2:B:534:LEU:HB3	2:B:537:CYS:HB2	1.86	0.57
2:B:946:LEU:HB3	2:B:987:VAL:HG22	1.87	0.57
2:B:1248:GLN:O	2:B:1252:LYS:HG3	2.04	0.57
1:A:471:PRO:HD3	2:B:465:TYR:CG	2.39	0.57
2:B:492:PRO:HG3	2:B:535:GLN:HG2	1.86	0.57
2:B:1966:ARG:HH11	2:B:1966:ARG:HG2	1.70	0.56
2:B:528:ILE:HA	2:B:531:LEU:HD12	1.87	0.56
2:B:539:PRO:HA	2:B:542:MET:HB3	1.86	0.56
2:B:729:LEU:HG	2:B:1053:GLN:HE22	1.70	0.56
1:A:427:ARG:NH2	2:B:2027:PHE:O	2.39	0.56
2:B:530:TRP:CE2	2:B:545:PRO:HG3	2.41	0.56
2:B:618:THR:HG22	2:B:621:GLY:H	1.71	0.55
2:B:1242:SER:O	2:B:1246:VAL:HG23	2.05	0.55
2:B:1162:ARG:HH11	2:B:1162:ARG:HG2	1.72	0.55
2:B:556:ALA:HB2	2:B:564:LEU:HD12	1.87	0.55
1:A:471:PRO:HD3	2:B:465:TYR:CB	2.36	0.55
2:B:603:ARG:O	2:B:607:ILE:HG13	2.06	0.54
2:B:1820:SER:HA	2:B:1836:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:LEU:HD13	2:B:795:VAL:HG22	1.90	0.54
2:B:1168:ALA:HB2	2:B:1183:LEU:HB2	1.89	0.54
2:B:554:MET:HE3	2:B:554:MET:HA	1.90	0.54
2:B:633:ALA:O	2:B:637:CYS:HB2	2.08	0.54
2:B:1676:LEU:HD21	2:B:1925:LEU:HB2	1.89	0.54
2:B:521:ALA:HA	2:B:564:LEU:HD21	1.88	0.53
2:B:934:THR:HG22	2:B:936:GLU:H	1.73	0.53
2:B:1203:GLN:HE21	2:B:1211:PRO:HA	1.73	0.53
2:B:1244:GLN:HE22	2:B:1275:THR:HG21	1.72	0.53
2:B:1699:LEU:HD21	2:B:1730:LEU:HD22	1.90	0.53
2:B:1181:LEU:O	2:B:1185:GLN:HG2	2.09	0.53
1:A:454:SEP:O1P	2:B:895:LYS:HB2	2.09	0.53
1:A:471:PRO:HD3	2:B:465:TYR:CD2	2.44	0.53
2:B:665:PRO:HG3	2:B:670:ARG:HD3	1.91	0.53
2:B:1953:ASN:HD21	2:B:1956:ASN:HA	1.74	0.53
2:B:682:LEU:HD13	2:B:779:LEU:HD13	1.91	0.53
2:B:2107:GLY:O	2:B:2110:PRO:HD2	2.10	0.52
2:B:1004:VAL:HG13	2:B:1037:LEU:HD22	1.91	0.52
2:B:1586:ARG:HH22	2:B:1690:PRO:HG2	1.75	0.51
2:B:2016:LEU:HD11	2:B:2051:MET:HE2	1.92	0.51
1:A:471:PRO:HD3	2:B:465:TYR:HB3	1.92	0.51
2:B:2028:GLY:O	2:B:2060:ASN:ND2	2.43	0.51
2:B:1930:ILE:HG23	2:B:1935:ALA:HB3	1.93	0.51
2:B:582:ALA:HB2	2:B:613:LEU:HD13	1.92	0.50
2:B:757:LEU:HD11	2:B:764:PRO:HB3	1.93	0.50
2:B:797:LEU:HD11	2:B:1206:LEU:HD23	1.92	0.50
2:B:862:LEU:HD13	2:B:884:VAL:HG11	1.93	0.50
2:B:470:HIS:C	2:B:472:LEU:H	2.20	0.49
2:B:986:GLU:HA	2:B:986:GLU:OE1	2.13	0.49
2:B:2064:VAL:HB	2:B:2069:ILE:HG13	1.93	0.49
2:B:820:THR:HG22	2:B:863:LEU:HD22	1.93	0.49
2:B:831:TYR:OH	2:B:1203:GLN:NE2	2.45	0.49
2:B:914:LEU:HD22	2:B:1259:PRO:HG2	1.94	0.49
2:B:581:LEU:CD1	2:B:613:LEU:HD11	2.43	0.49
2:B:549:TRP:HZ3	2:B:569:LEU:HD13	1.78	0.49
2:B:1794:LEU:HD11	2:B:1902:LEU:HD13	1.95	0.48
2:B:527:VAL:O	2:B:531:LEU:HG	2.14	0.48
2:B:589:LEU:HD12	2:B:603:ARG:HG2	1.95	0.48
2:B:971:LEU:O	2:B:976:ASN:ND2	2.40	0.48
2:B:793:LEU:HD11	2:B:819:ILE:HG23	1.96	0.48
2:B:735:PHE:HE2	2:B:1018:THR:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:PHE:CE2	2:B:1027:CYS:HB2	2.49	0.48
1:A:468:MET:SD	2:B:509:LEU:HD23	2.54	0.47
2:B:1986:GLU:H	2:B:1986:GLU:CD	2.22	0.47
2:B:1203:GLN:NE2	2:B:1211:PRO:HA	2.28	0.47
2:B:830:SER:O	2:B:834:LEU:HG	2.14	0.47
1:A:454:SEP:HA	2:B:893:SER:O	2.15	0.47
2:B:1875:GLU:CD	2:B:1879:ARG:HH22	2.23	0.47
2:B:1165:LEU:HD21	2:B:1225:GLN:HG2	1.97	0.47
2:B:1890:HIS:CE1	2:B:2116:PRO:HD3	2.50	0.47
2:B:843:LEU:HA	2:B:846:LEU:HD13	1.98	0.47
2:B:553:LYS:HD2	2:B:564:LEU:HB3	1.96	0.46
2:B:553:LYS:HE2	2:B:564:LEU:HD22	1.96	0.46
2:B:1953:ASN:ND2	2:B:1956:ASN:HA	2.30	0.46
1:A:446:GLU:O	2:B:947:ARG:NH2	2.48	0.46
2:B:919:LEU:HG	2:B:923:LEU:HB2	1.96	0.46
2:B:1899:LEU:HD22	2:B:1904:TRP:HZ2	1.80	0.46
2:B:549:TRP:CD1	2:B:553:LYS:HG2	2.51	0.46
2:B:781:ALA:HB1	2:B:981:TRP:HB2	1.97	0.46
2:B:972:ASP:OD1	2:B:972:ASP:N	2.44	0.46
2:B:542:MET:C	2:B:545:PRO:HD2	2.41	0.46
2:B:1018:THR:HG21	2:B:1027:CYS:N	2.30	0.46
2:B:1162:ARG:HG2	2:B:1162:ARG:NH1	2.29	0.46
2:B:1288:PHE:CD2	2:B:1606:LEU:HD22	2.51	0.46
2:B:1745:GLN:HG2	2:B:1746:ASN:N	2.30	0.46
2:B:915:PRO:HB2	2:B:917:ASN:OD1	2.17	0.45
2:B:1276:LYS:HE2	2:B:1573:THR:HG23	1.98	0.45
2:B:2026:LEU:HD22	2:B:2057:PHE:CE2	2.51	0.45
2:B:540:GLU:N	2:B:540:GLU:OE1	2.46	0.45
2:B:732:ASN:HA	2:B:735:PHE:CE1	2.51	0.45
2:B:1831:TRP:NE1	2:B:1861:LEU:HD22	2.31	0.45
2:B:590:GLN:HE22	2:B:771:GLN:HE21	1.64	0.45
2:B:1004:VAL:HG11	2:B:1041:ARG:HG3	1.97	0.45
2:B:1597:TYR:HB3	2:B:1626:ILE:HD13	1.99	0.45
2:B:627:THR:O	2:B:631:GLU:HG2	2.16	0.45
2:B:1780:ARG:HB3	2:B:2102:LEU:HD21	1.99	0.45
2:B:1787:MET:HE3	2:B:2062:TRP:CH2	2.52	0.45
1:A:429:ASP:HA	2:B:2003:HIS:HB3	1.99	0.44
1:A:471:PRO:HG2	2:B:462:ASN:HA	1.93	0.44
2:B:1846:ALA:HA	2:B:1849:LEU:HD12	1.99	0.44
2:B:1223:LEU:HD23	2:B:1253:PHE:CE1	2.53	0.44
2:B:1592:PRO:HB2	2:B:1597:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:813:ALA:HB3	2:B:856:LEU:HD13	1.99	0.44
2:B:1232:LEU:HD11	2:B:1718:PRO:HG2	1.99	0.44
2:B:768:CYS:SG	2:B:770:GLN:HB2	2.57	0.44
2:B:1891:LEU:HD23	2:B:1915:VAL:HG22	2.00	0.44
1:A:455:VAL:HG23	2:B:893:SER:HB2	1.99	0.44
2:B:1727:LEU:HB3	2:B:1739:VAL:HG12	2.00	0.44
2:B:2056:LEU:HD11	2:B:2112:ALA:HB1	1.99	0.44
2:B:1687:PHE:HA	2:B:1688:PRO:HA	1.77	0.44
2:B:2072:TYR:CZ	2:B:2110:PRO:HG2	2.52	0.44
1:A:471:PRO:HB3	2:B:505:ARG:NH2	2.32	0.44
2:B:1991:ALA:O	2:B:1995:HIS:HB2	2.18	0.44
1:A:470:PRO:O	1:A:471:PRO:C	2.62	0.43
2:B:1270:LEU:HD13	2:B:1600:LEU:HD23	2.01	0.43
2:B:670:ARG:HH11	2:B:673:LEU:HD23	1.83	0.43
1:A:424:GLU:HB3	2:B:2066:ASP:OD1	2.18	0.43
2:B:511:VAL:O	2:B:515:LYS:N	2.49	0.43
2:B:1588:ILE:HD11	2:B:1600:LEU:HD12	2.00	0.43
2:B:1675:ARG:CZ	2:B:1675:ARG:HB3	2.48	0.43
2:B:1984:ARG:HB3	2:B:1986:GLU:OE2	2.18	0.43
1:A:446:GLU:HB2	2:B:944:LYS:HD2	2.00	0.43
2:B:1710:VAL:HG22	2:B:1894:VAL:HB	2.01	0.43
2:B:1574:LEU:HD23	2:B:1611:ARG:HH12	1.83	0.42
2:B:1813:PRO:O	2:B:1817:GLN:HG2	2.19	0.42
2:B:634:GLN:HG2	2:B:683:TRP:CE2	2.54	0.42
2:B:549:TRP:HE1	2:B:553:LYS:NZ	2.17	0.42
2:B:900:LEU:O	2:B:904:VAL:HG23	2.19	0.42
2:B:1730:LEU:HD23	2:B:1736:PRO:HB3	2.02	0.42
2:B:2072:TYR:CE2	2:B:2110:PRO:HG2	2.54	0.42
2:B:943:HIS:CE1	2:B:947:ARG:HD2	2.55	0.42
1:A:443:PRO:HG2	2:B:1005:SER:C	2.45	0.42
2:B:878:VAL:HG21	2:B:919:LEU:HD22	2.02	0.42
2:B:1294:TRP:CG	2:B:1802:TRP:HZ2	2.38	0.42
2:B:556:ALA:HB1	2:B:561:ASP:HB3	2.02	0.42
2:B:2072:TYR:C	2:B:2072:TYR:CD1	2.97	0.42
2:B:1008:LYS:HE2	2:B:1008:LYS:HB3	1.76	0.42
2:B:1743:THR:O	2:B:1749:HIS:HB3	2.20	0.42
2:B:589:LEU:HB2	2:B:606:ILE:HG21	2.01	0.42
2:B:1148:CYS:O	2:B:1149:SER:C	2.63	0.42
2:B:1868:ARG:O	2:B:1872:LEU:HD13	2.20	0.42
2:B:2031:SER:OG	2:B:2059:GLY:CA	2.68	0.42
2:B:550:VAL:HG21	2:B:591:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:GLN:O	2:B:983:VAL:HG23	2.20	0.41
2:B:510:GLN:O	2:B:514:LEU:HG	2.20	0.41
2:B:544:GLU:HB2	2:B:545:PRO:HD3	2.02	0.41
2:B:653:ILE:HD12	2:B:653:ILE:HA	1.91	0.41
2:B:764:PRO:HD2	2:B:805:ARG:CD	2.51	0.41
2:B:733:ILE:HD11	2:B:1056:PHE:CD2	2.55	0.41
2:B:650:LEU:O	2:B:654:ARG:HG3	2.20	0.41
2:B:685:TYR:CE1	2:B:782:LEU:HD13	2.55	0.41
2:B:729:LEU:HG	2:B:1053:GLN:NE2	2.36	0.41
2:B:1586:ARG:HH22	2:B:1690:PRO:CG	2.33	0.41
2:B:2004:GLY:O	2:B:2028:GLY:HA3	2.20	0.41
2:B:1826:LEU:HD22	2:B:1862:CYS:SG	2.61	0.41
2:B:2029:SER:HB3	2:B:2063:ASP:HA	2.03	0.41
2:B:764:PRO:HB2	2:B:766:VAL:HG13	2.03	0.41
2:B:1000:ARG:HH11	2:B:1000:ARG:HG3	1.85	0.41
2:B:1586:ARG:NH2	2:B:1690:PRO:HD2	2.36	0.41
2:B:549:TRP:CD1	2:B:549:TRP:C	2.96	0.41
2:B:1177:GLN:C	2:B:1179:GLN:H	2.29	0.41
2:B:762:GLN:H	2:B:762:GLN:HG3	1.74	0.40
1:A:471:PRO:HB3	2:B:505:ARG:HH22	1.86	0.40
2:B:483:LEU:H	2:B:483:LEU:HG	1.69	0.40
2:B:874:VAL:O	2:B:875:THR:C	2.64	0.40
2:B:1837:THR:O	2:B:1841:ILE:HG12	2.21	0.40
2:B:514:LEU:HD13	2:B:523:GLY:HA2	2.03	0.40
2:B:892:LYS:HB2	2:B:897:TRP:CD1	2.56	0.40
2:B:1823:GLN:HG3	2:B:1834:PRO:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	28/241 (12%)	27 (96%)	1 (4%)	0	100	100
2	B	1412/2172 (65%)	1366 (97%)	46 (3%)	0	100	100
All	All	1440/2413 (60%)	1393 (97%)	47 (3%)	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	32/223 (14%)	31 (97%)	1 (3%)	35	59
2	B	1059/1814 (58%)	1052 (99%)	7 (1%)	81	89
All	All	1091/2037 (54%)	1083 (99%)	8 (1%)	80	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	MET
2	B	490	VAL
2	B	843	LEU
2	B	1196	GLU
2	B	1765	LYS
2	B	1982	VAL
2	B	2061	LEU
2	B	2078	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	590	GLN
2	B	749	GLN
2	B	777	GLN
2	B	818	HIS
2	B	835	HIS

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Mol	Chain	Res	Type
2	B	845	HIS
2	B	871	HIS
2	B	891	GLN
2	B	982	GLN
2	B	1022	GLN
2	B	1048	GLN
2	B	1244	GLN
2	B	1248	GLN
2	B	1637	HIS
2	B	1674	GLN
2	B	1717	GLN
2	B	1723	ASN
2	B	1957	ASN
2	B	2060	ASN
2	B	2095	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	SEP	A	454	1	8,9,10	0.62	0	8,12,14	0.84	0

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
1	SEP	A	454	1	-	0/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	454	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

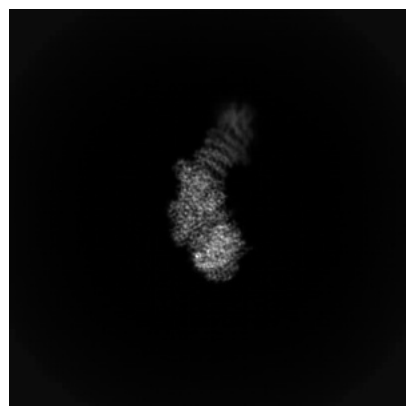
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52306. These allow visual inspection of the internal detail of the map and identification of artifacts.

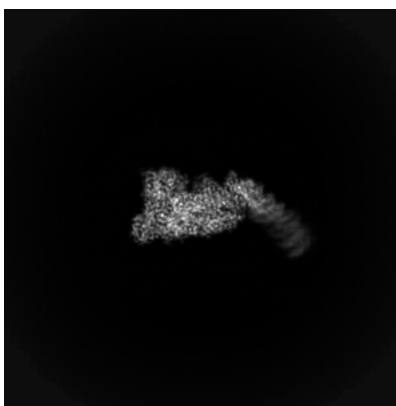
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

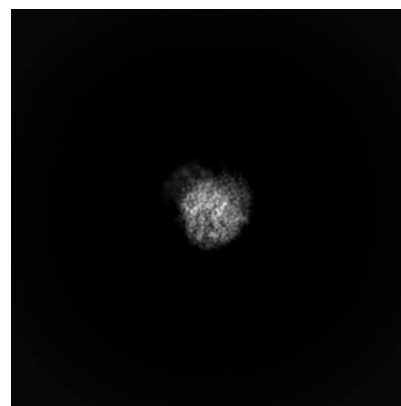
6.1.1 Primary map



X

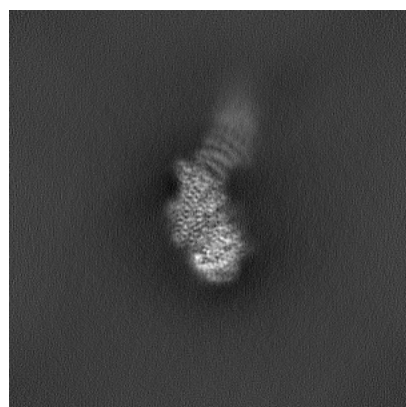


Y

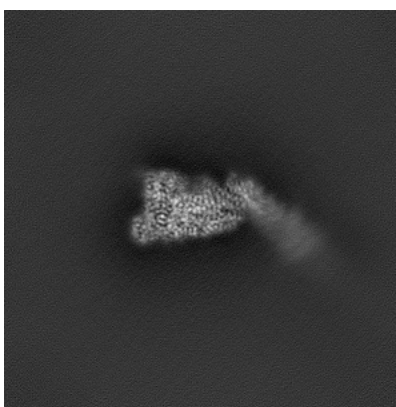


Z

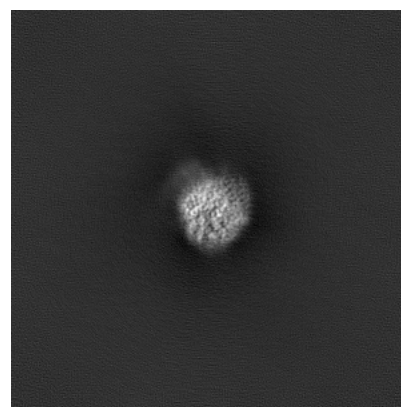
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

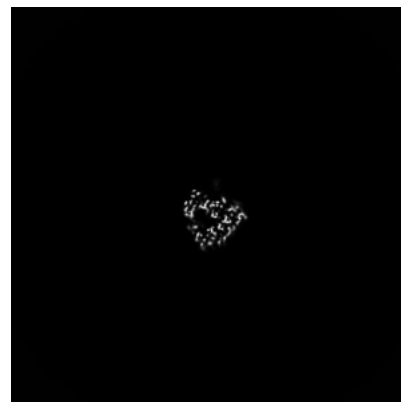
6.2.1 Primary map



X Index: 200



Y Index: 200

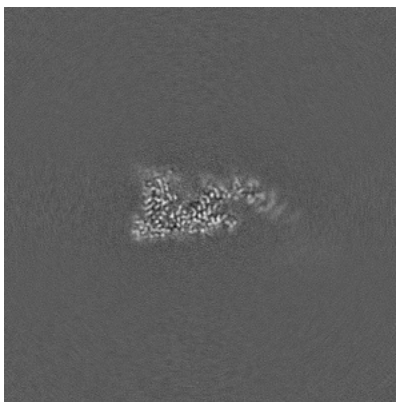


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

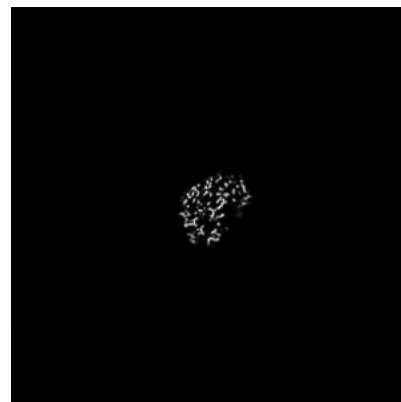
6.3.1 Primary map



X Index: 189



Y Index: 204

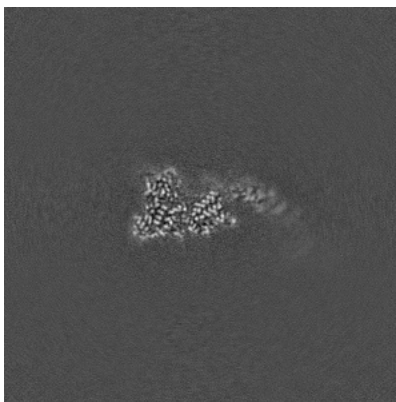


Z Index: 171

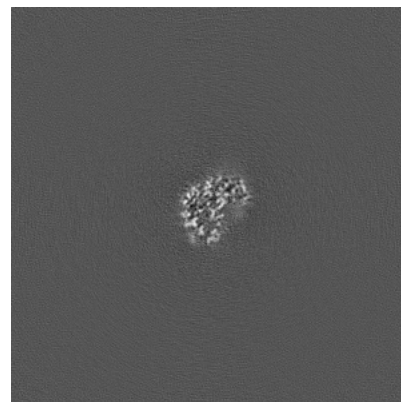
6.3.2 Raw map



X Index: 189



Y Index: 203



Z Index: 171

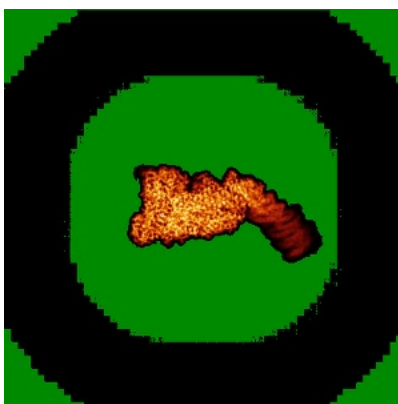
The images above show the largest variance slices of the map in three orthogonal directions.

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

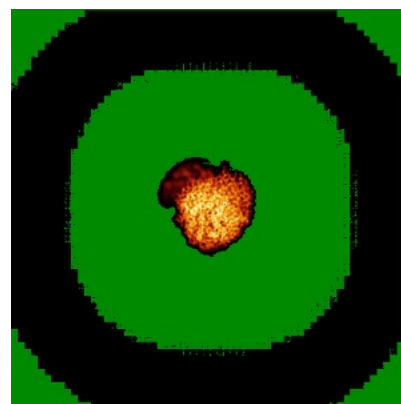
6.4.1 Primary map



X



Y

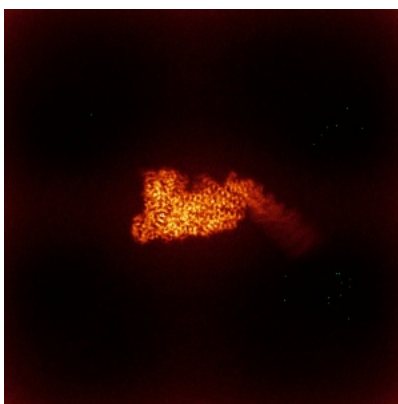


Z

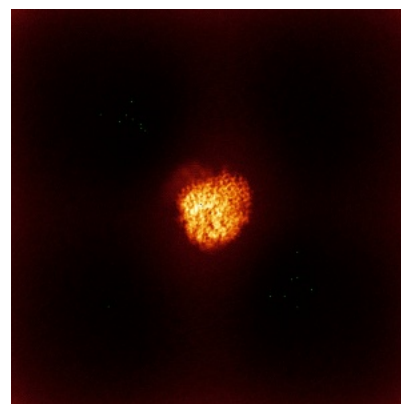
6.4.2 Raw map



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.

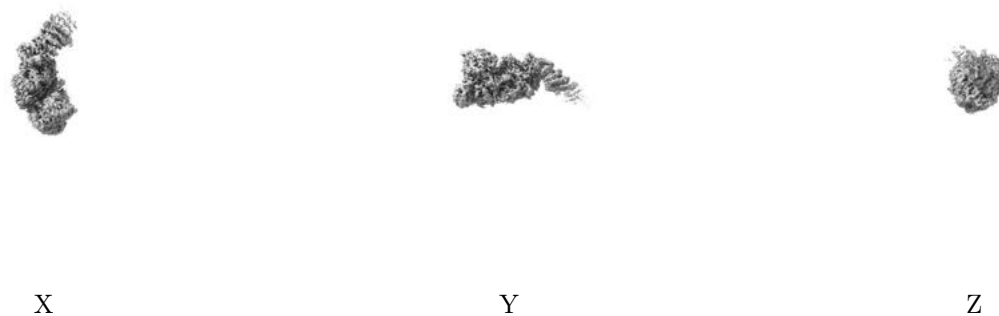
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

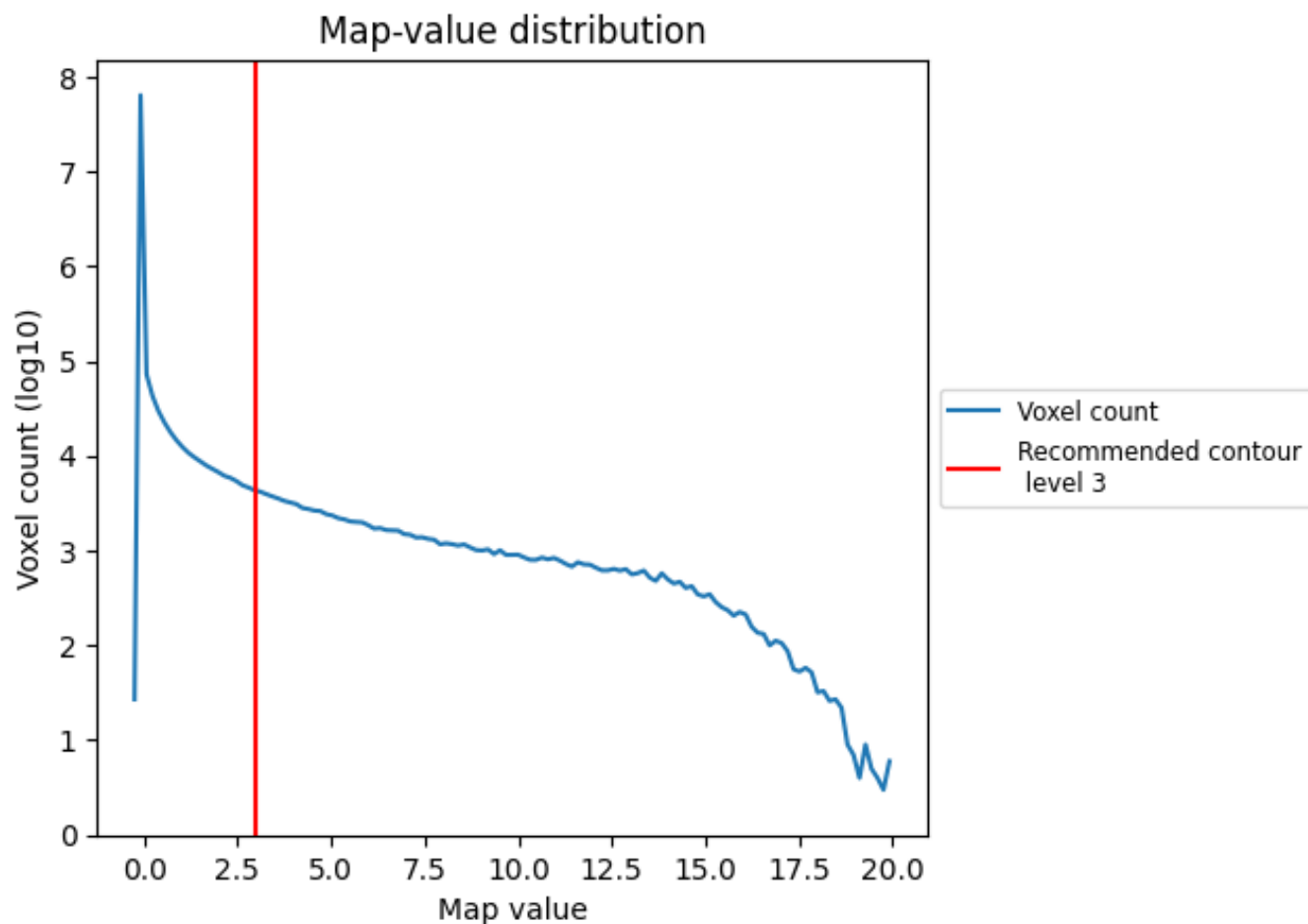
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

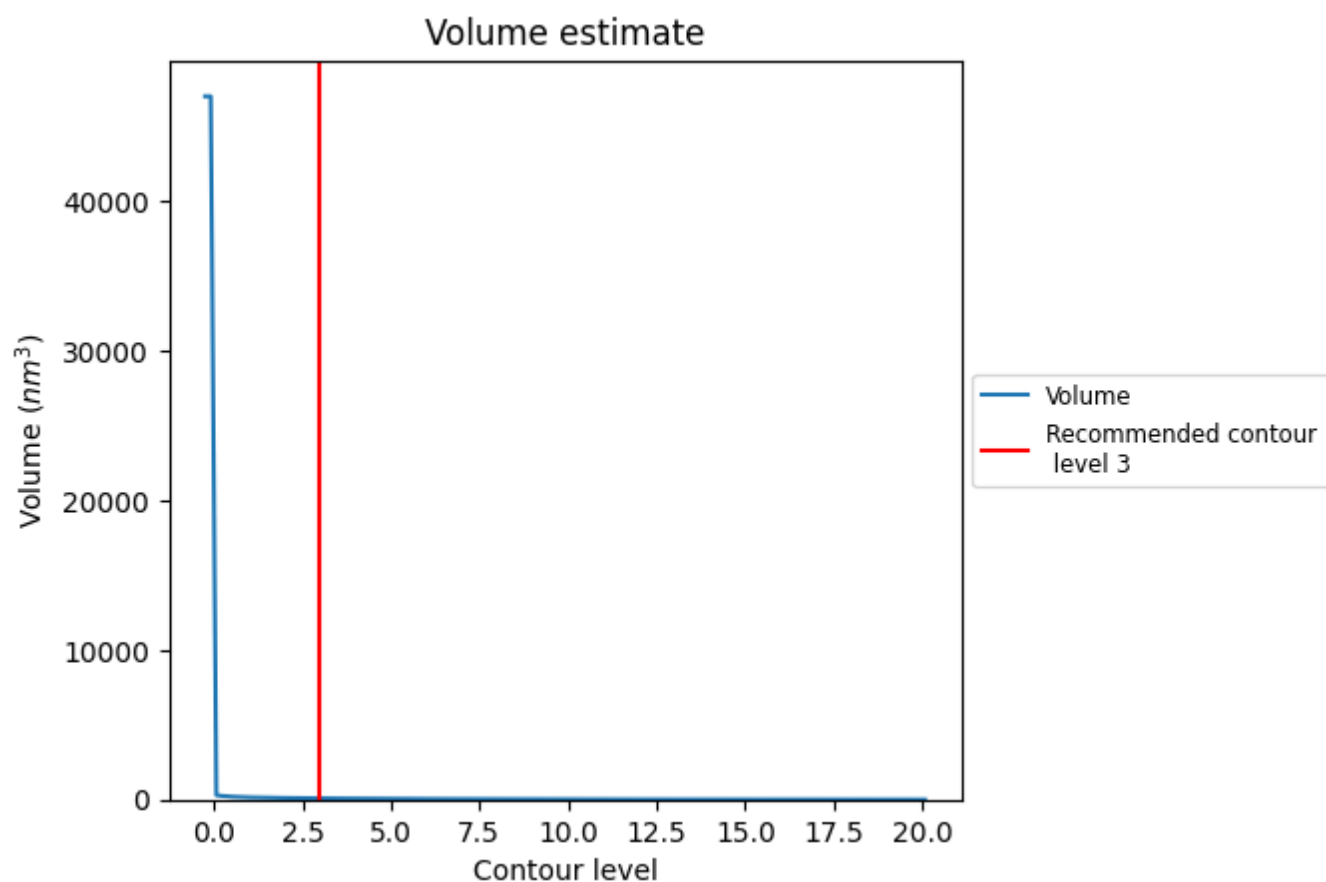
This section contains the results of statistical analysis of the map.

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.

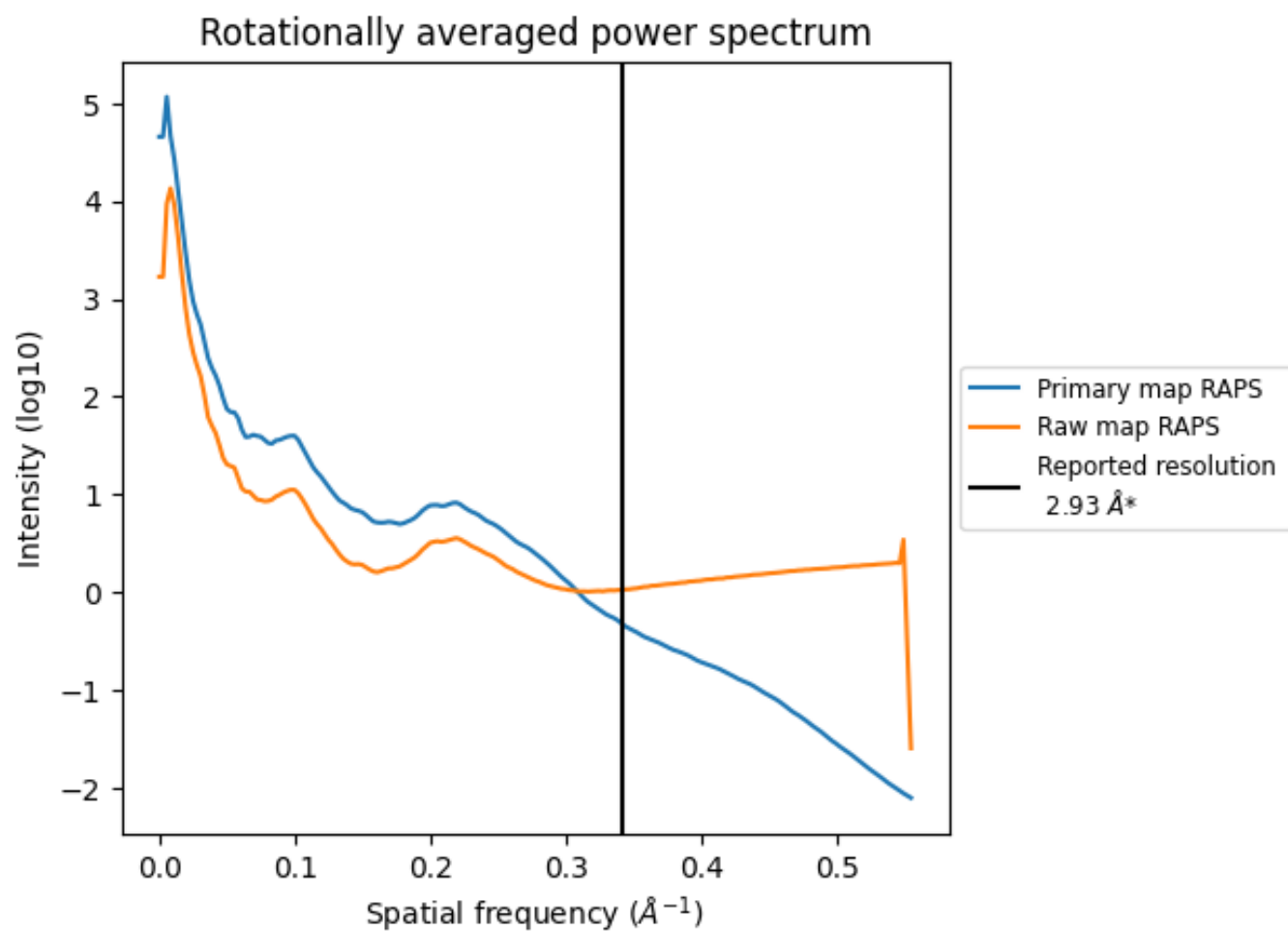
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 73 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

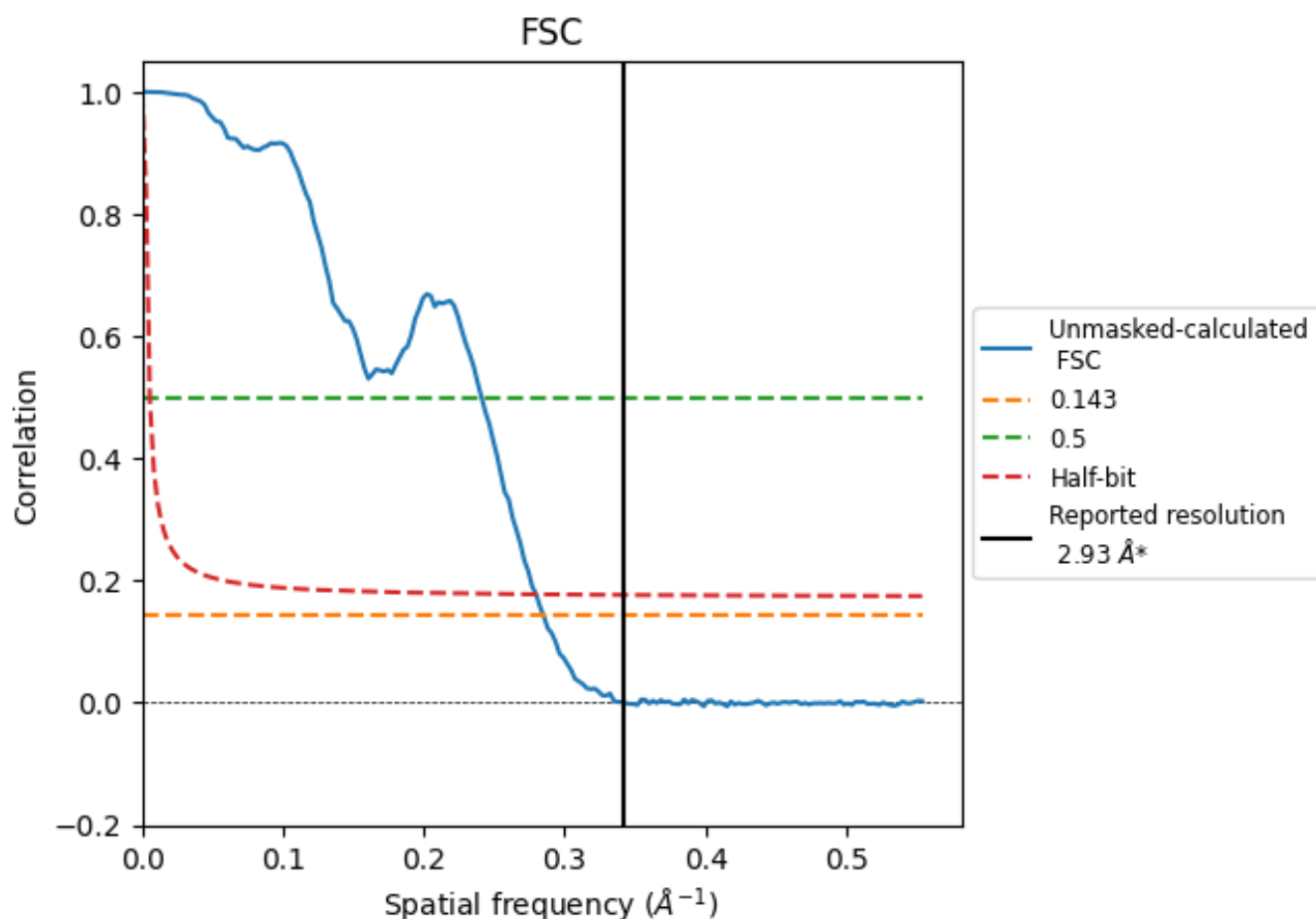


*Reported resolution corresponds to spatial frequency of 0.341 \AA^{-1}

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 0.341 \AA^{-1}

8.2 Resolution estimates [i](#)

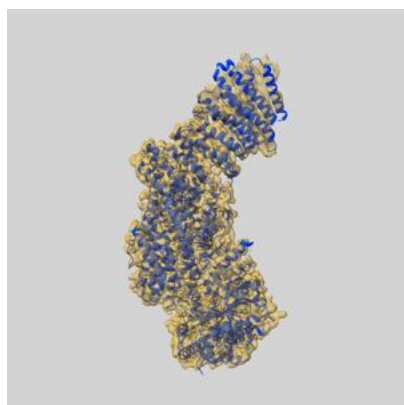
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.15	3.57

*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 3.51 differs from the reported value 2.93 by more than 10 %

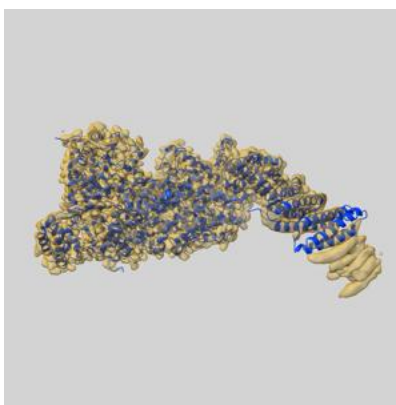
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52306 and PDB model 9HN4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

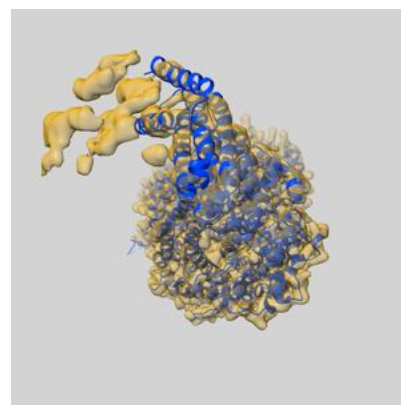
9.1 Map-model overlay [i](#)



X



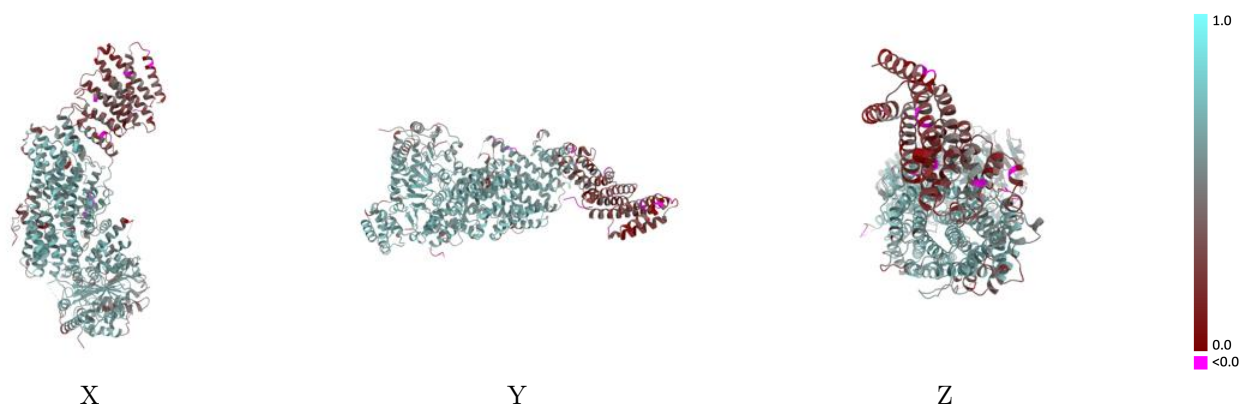
Y



Z

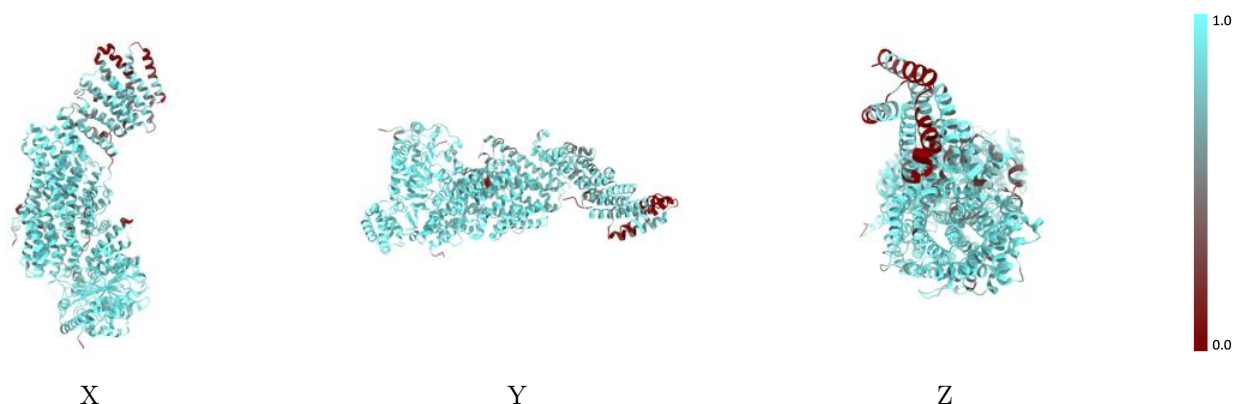
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



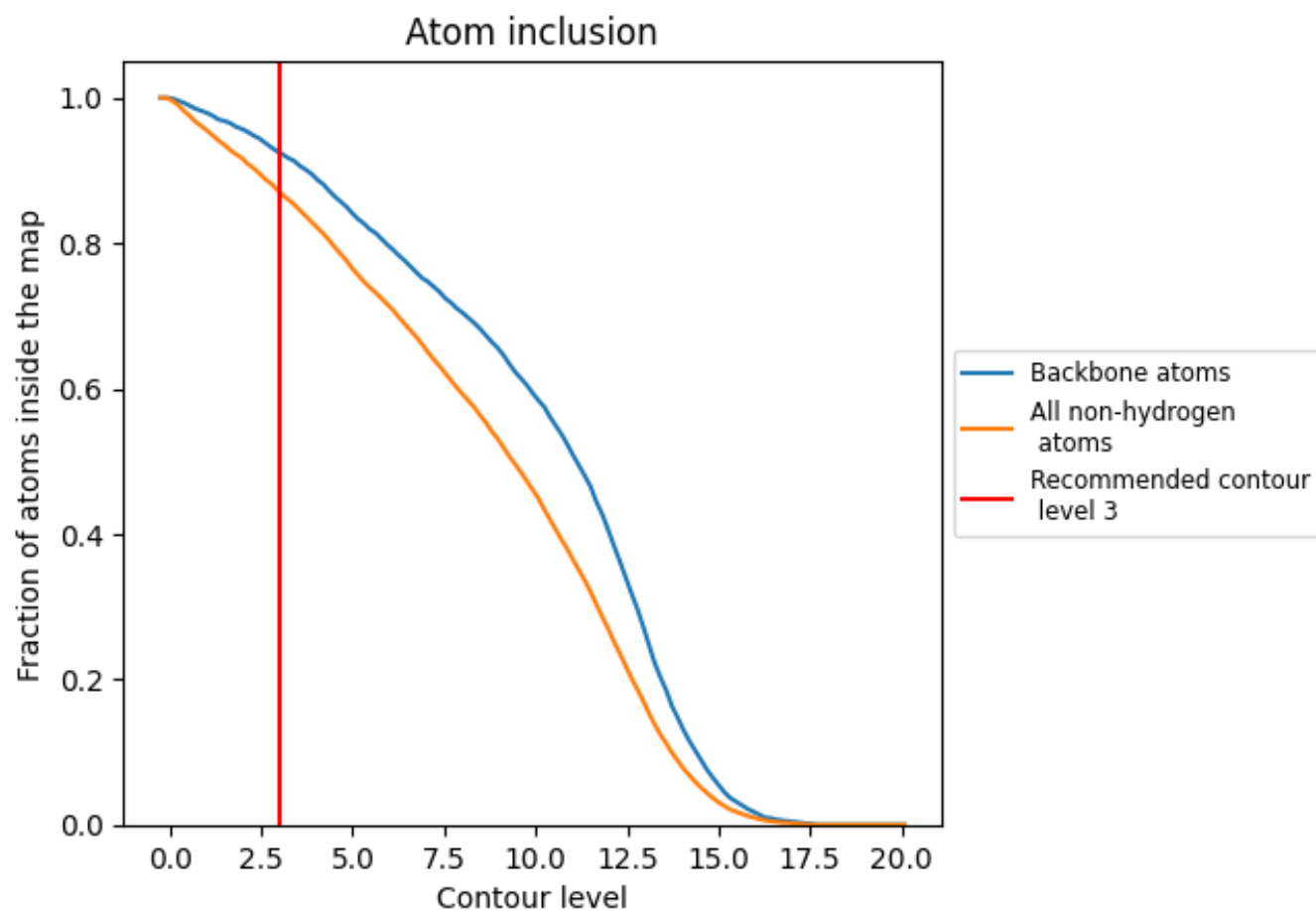
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8700	<div></div> 0.5490
A	<div></div> 0.5340	<div></div> 0.4040
B	<div></div> 0.8790	<div></div> 0.5530

