



## wwPDB EM Validation Summary Report ⓘ

Aug 28, 2025 – 01:22 pm BST

PDB ID : 9HN5 / pdb\_00009hn5  
EMDB ID : EMD-52307  
Title : Cryo-EM structure of human separase bound to phosphorylated SCC1 (100-320 aa)  
Authors : Yu, J.; Schmidt, S.; Botto, M.; Boland, A.  
Deposited on : 2024-12-10  
Resolution : 2.96 Å(reported)  
Based on initial model : 7NJ1

This is a wwPDB EM Validation Summary 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.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

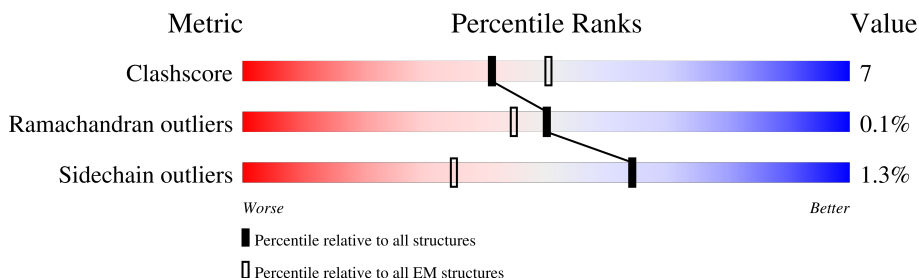
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.96 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  $\geq 3$ , 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	B	227	
2	A	2172	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11314 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	B	38	Total	C	N	O	P	S	0	0
			283	166	45	67	2	3		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	136	ILE	ASN	conflict	UNP O60216
B	245	GLU	-	insertion	UNP O60216
B	246	ILE	-	insertion	UNP O60216
B	247	MET	-	insertion	UNP O60216
B	248	ARG	-	insertion	UNP O60216
B	249	GLU	-	insertion	UNP O60216
B	250	GLY	-	insertion	UNP O60216

- Molecule 2 is a protein called Separin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1480	Total	C	N	O	S	0	0
			11030	7006	1927	2043	54		

There are 113 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-54	MET	-	initiating methionine	UNP Q14674
A	-53	ASP	-	expression tag	UNP Q14674
A	-52	TYR	-	expression tag	UNP Q14674
A	-51	LYS	-	expression tag	UNP Q14674
A	-50	ASP	-	expression tag	UNP Q14674
A	-49	HIS	-	expression tag	UNP Q14674
A	-48	ASP	-	expression tag	UNP Q14674
A	-47	GLY	-	expression tag	UNP Q14674
A	-46	ASP	-	expression tag	UNP Q14674
A	-45	TYR	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	LYS	-	expression tag	UNP Q14674
A	-43	ASP	-	expression tag	UNP Q14674
A	-42	HIS	-	expression tag	UNP Q14674
A	-41	ASP	-	expression tag	UNP Q14674
A	-40	ILE	-	expression tag	UNP Q14674
A	-39	ASP	-	expression tag	UNP Q14674
A	-38	TYR	-	expression tag	UNP Q14674
A	-37	LYS	-	expression tag	UNP Q14674
A	-36	ASP	-	expression tag	UNP Q14674
A	-35	ASP	-	expression tag	UNP Q14674
A	-34	ASP	-	expression tag	UNP Q14674
A	-33	ASP	-	expression tag	UNP Q14674
A	-32	LYS	-	expression tag	UNP Q14674
A	-31	SER	-	expression tag	UNP Q14674
A	-30	GLY	-	expression tag	UNP Q14674
A	-29	PRO	-	expression tag	UNP Q14674
A	-28	GLY	-	expression tag	UNP Q14674
A	-27	GLY	-	expression tag	UNP Q14674
A	-26	SER	-	expression tag	UNP Q14674
A	-25	GLY	-	expression tag	UNP Q14674
A	-24	GLY	-	expression tag	UNP Q14674
A	-23	SER	-	expression tag	UNP Q14674
A	-22	GLY	-	expression tag	UNP Q14674
A	-21	GLY	-	expression tag	UNP Q14674
A	-20	GLY	-	expression tag	UNP Q14674
A	-19	SER	-	expression tag	UNP Q14674
A	-18	GLY	-	expression tag	UNP Q14674
A	-17	GLY	-	expression tag	UNP Q14674
A	-16	GLY	-	expression tag	UNP Q14674
A	-15	SER	-	expression tag	UNP Q14674
A	-14	GLY	-	expression tag	UNP Q14674
A	-13	GLU	-	expression tag	UNP Q14674
A	-12	ASN	-	expression tag	UNP Q14674
A	-11	LEU	-	expression tag	UNP Q14674
A	-10	TYR	-	expression tag	UNP Q14674
A	-9	PHE	-	expression tag	UNP Q14674
A	-8	GLN	-	expression tag	UNP Q14674
A	-7	GLY	-	expression tag	UNP Q14674
A	-6	GLY	-	expression tag	UNP Q14674
A	-5	GLY	-	expression tag	UNP Q14674
A	-4	SER	-	expression tag	UNP Q14674
A	-3	GLY	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q14674
A	-1	SER	-	expression tag	UNP Q14674
A	0	GLY	-	expression tag	UNP Q14674
A	25	ASP	ALA	conflict	UNP Q14674
A	116	VAL	ALA	conflict	UNP Q14674
A	1372	SER	ARG	conflict	UNP Q14674
A	1525	GLY	-	linker	UNP Q14674
A	1526	LEU	-	linker	UNP Q14674
A	1527	GLU	-	linker	UNP Q14674
A	1528	VAL	-	linker	UNP Q14674
A	1529	LEU	-	linker	UNP Q14674
A	1530	PHE	-	linker	UNP Q14674
A	1531	GLN	-	linker	UNP Q14674
A	1532	GLY	-	linker	UNP Q14674
A	1533	PRO	-	linker	UNP Q14674
A	1534	GLY	-	linker	UNP Q14674
A	1535	SER	-	linker	UNP Q14674
A	1536	GLY	-	linker	UNP Q14674
A	1561	GLN	ARG	conflict	UNP Q14674
A	2029	SER	CYS	engineered mutation	UNP Q14674
A	2037	HIS	ARG	conflict	UNP Q14674
A	2121	SER	-	expression tag	UNP Q14674
A	2122	SER	-	expression tag	UNP Q14674
A	2123	LEU	-	expression tag	UNP Q14674
A	2124	ALA	-	expression tag	UNP Q14674
A	2125	GLU	-	expression tag	UNP Q14674
A	2126	GLU	-	expression tag	UNP Q14674
A	2127	ASN	-	expression tag	UNP Q14674
A	2128	LEU	-	expression tag	UNP Q14674
A	2129	TYR	-	expression tag	UNP Q14674
A	2130	PHE	-	expression tag	UNP Q14674
A	2131	GLN	-	expression tag	UNP Q14674
A	2132	SER	-	expression tag	UNP Q14674
A	2133	TRP	-	expression tag	UNP Q14674
A	2134	SER	-	expression tag	UNP Q14674
A	2135	HIS	-	expression tag	UNP Q14674
A	2136	PRO	-	expression tag	UNP Q14674
A	2137	GLN	-	expression tag	UNP Q14674
A	2138	PHE	-	expression tag	UNP Q14674
A	2139	GLU	-	expression tag	UNP Q14674
A	2140	LYS	-	expression tag	UNP Q14674
A	2141	GLY	-	expression tag	UNP Q14674

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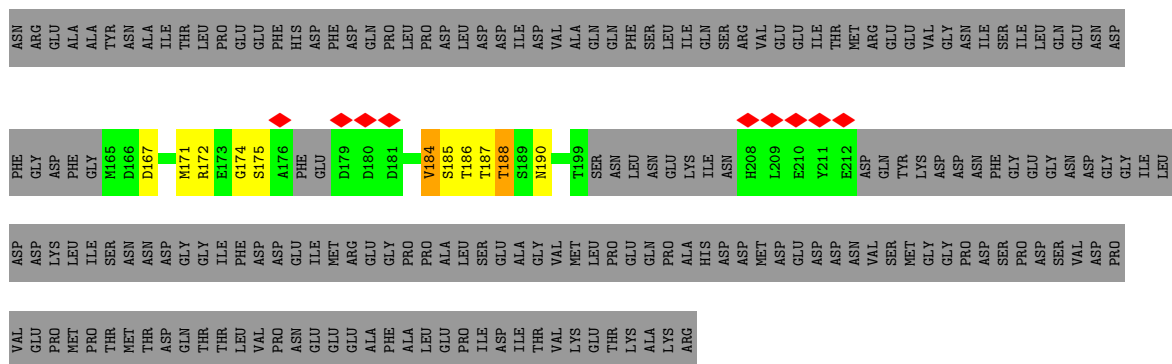
Chain	Residue	Modelled	Actual	Comment	Reference
A	2142	GLY	-	expression tag	UNP Q14674
A	2143	GLY	-	expression tag	UNP Q14674
A	2144	SER	-	expression tag	UNP Q14674
A	2145	GLY	-	expression tag	UNP Q14674
A	2146	GLY	-	expression tag	UNP Q14674
A	2147	GLY	-	expression tag	UNP Q14674
A	2148	SER	-	expression tag	UNP Q14674
A	2149	GLY	-	expression tag	UNP Q14674
A	2150	GLY	-	expression tag	UNP Q14674
A	2151	GLY	-	expression tag	UNP Q14674
A	2152	SER	-	expression tag	UNP Q14674
A	2153	TRP	-	expression tag	UNP Q14674
A	2154	SER	-	expression tag	UNP Q14674
A	2155	HIS	-	expression tag	UNP Q14674
A	2156	PRO	-	expression tag	UNP Q14674
A	2157	GLN	-	expression tag	UNP Q14674
A	2158	PHE	-	expression tag	UNP Q14674
A	2159	GLU	-	expression tag	UNP Q14674
A	2160	LYS	-	expression tag	UNP Q14674

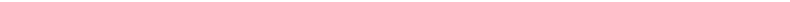
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

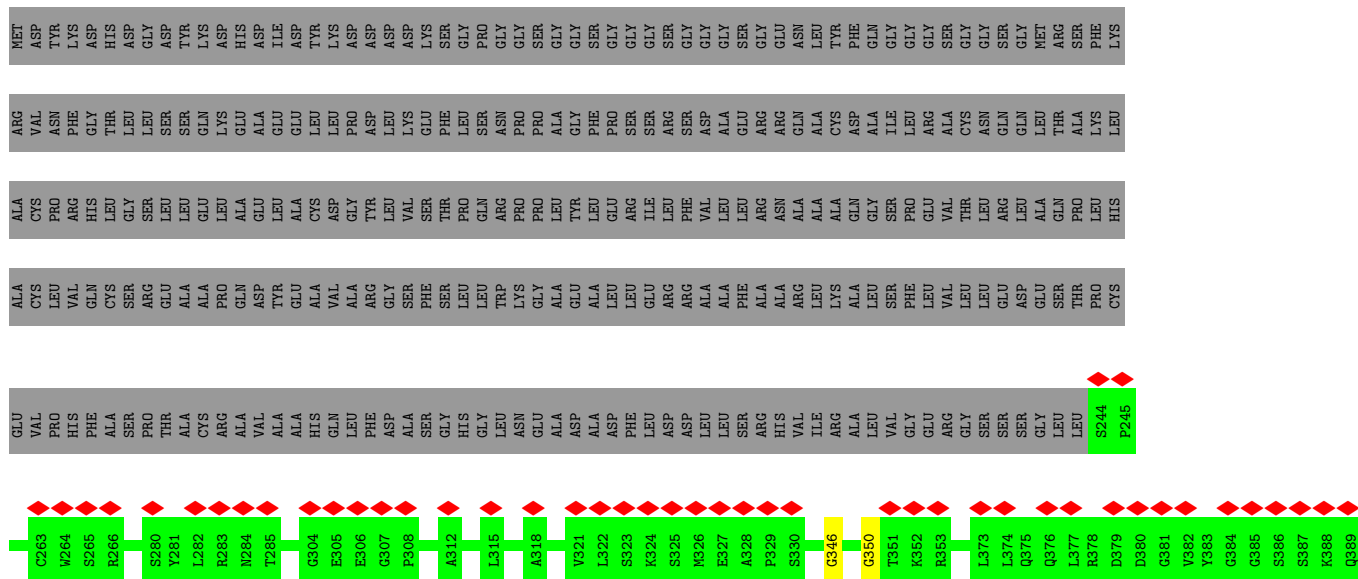
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0



- Molecule 1: Double-strand-break repair protein rad21 homolog



Chain A: 



LYS	V2046	E1867	SER	SER	LYS	THR	PRO	ARG	D1182	GLN	ALA	V802	Q644	L503	T405
	L2047	L1873	LEU	SER	LYS	ASP	GLY	SER	L1183	LEU	VAL	L806	T645	H604	T409
	M2051	V1877	GLN	LYS	VAL	VAL	GLN	GLY	V1186	PRO	T968	S816	L650	R505	Y409
	L2056	Q1881	PRO	LEU	PRO	ALA	ALA	ARG	C1191	GLY	Y978	T820	R664	R507	Q413
	D2068	V1885	ARG	SER	ARG	PRO	ARG	LYS	L1206	LEU	Q979	Q821	L882	L509	I417
	I2069	F1676	VAL	GLY	VAL	VAL	VAL	ALA	L1223	PHE	X960	L822	Y685	Q510	A421
	L2089	F1677	ALA	ALA	GLN	GLN	GLN	GLY	L1235	ARG	Y983	L823	I686	S513	D422
	I2106	L1699	ASN	GLY	VAL	VAL	VAL	ALA	L1236	PRO	E986	A832	Q704	L514	L423
	A2112	L1711	PRO	PRO	GLN	GLN	GLN	LEU	S1242	LEU	L994	L836	ALA	L426	T424
	P2116	A1712	THR	THR	THR	THR	THR	SER	V1246	GLY	L997	A839	PRO	L427	Q425
	V2117	A1713	LEU	LEU	LEU	LEU	LEU	LEU	V1250	VAL	H997	L843	ASN	V427	V427
	R2120	A1714	GLY	GLY	GLY	GLY	GLY	THR	G1250	ALA	K1008	L856	LEU	V434	V434
	SER	Q1717	ARG	ARG	ARG	ARG	ARG	VAL	V1254	THR	E1013	L861	GLY	M437	M437
	LEU	T1724	SER	SER	SER	SER	SER	VAL	L1261	ALA	E1028	L863	GLU	V527	V527
	ALA	L1730	PRO	PRO	PRO	PRO	PRO	GLN	G1271	GLY	A1032	L864	PHE	L528	L528
	GLU	T1743	LEU	LEU	LEU	LEU	LEU	LYS	G1278	PRO	V1032	R894	VAL	V530	V530
	ASN	L1748	GLY	GLY	GLY	GLY	GLY	ALA	GLY	ILE	L1033	K895	ASP	L534	L534
	LEU	H1749	ASP	ASP	ASP	ASP	ASP	ALA	GLY	SER	K1034	A896	LEU	E544	E544
	TYR	L1750	VAL	VAL	VAL	VAL	VAL	THR	GLY	THR	E1038	W897	TYR	P545	P545
	PHE	A1935	ALA	ALA	ALA	ALA	ALA	CYS	GLY	ASN	E1063	W898	GLN	V549	V549
	GLN	F1949	THR	THR	THR	THR	THR	THR	GLY	ASN	PHE	L899	LEU	V550	V550
	SER	P1954	GLY	GLY	GLY	GLY	GLY	CYS	ILE	SER	GLY	L914	GLY	K553	K553
	TRP	H1955	ARG	ARG	ARG	ARG	ARG	CYS	THR	SER	GLY	P915	GLU	L564	L564
	HIS	N1956	ALA	ALA	ALA	ALA	ALA	TYR	L1284	PRO	VAL	N918	ASP	L564	L564
	PRO	N1957	LYS	LYS	LYS	LYS	LYS	GLY	G1287	VAL	THR	Q903	ASP	T459	T459
	GLN	R1976	ARG	ARG	ARG	ARG	ARG	ASP	S1290	LYS	GLN	V904	ARG	T460	T460
	PHE	E1981	GLY	GLY	GLY	GLY	GLY	ILE	W1294	THR	HIS	L914	F728	L463	L463
	LYS	V1982	ALA	ALA	ALA	ALA	ALA	GLY	G1297	LYS	LEU	P915	L729	F467	F467
	GLY	A1991	ARG	ARG	ARG	ARG	ARG	GLY	LEU	PRO	LEU	N918	N732	H470	H470
	SER	H1995	GLY	GLY	GLY	GLY	GLY	THR	ILE	GLN	VAL	W932	L737	K471	K471
	GLY	H2003	GLY	GLY	GLY	GLY	GLY	THR	SER	GLN	SER	W932	A738	L472	L472
	GLY	A2014	GLY	GLY	GLY	GLY	GLY	THR	PRO	GLN	VAL	W932	Q743	A474	A474
	GLY	V2015	SER	SER	SER	SER	SER	THR	GLY	LYS	LYS	L946	E812	E475	E475
	GLY	L2016	LEU	LEU	LEU	LEU	LEU	PHE	ILE	VAL	VAL	R947	P815	S480	S480
	SER	R2017	ILE	ILE	ILE	ILE	ILE	GLY	C1146	HIS	HIS	L952	E812	C484	C484
	TRP	L2018	ALA	ALA	ALA	ALA	ALA	VAL	L1150	LEU	LEU	L939	P815	Q485	Q485
	SER	Q1817	ALA	ALA	ALA	ALA	ALA	CYS	C1151	GLN	GLN	L946	E812	L487	L487
	HIS	R1821	GLY	GLY	GLY	GLY	GLY	THR	L1156	LYS	LYS	L946	E812	G488	G488
	PRO	A2024	GLN	GLN	GLN	GLN	GLN	THR	V1159	VAL	VAL	L946	E812	L489	L489
	GLN	L2025	LEU	LEU	LEU	LEU	LEU	GLY	R1182	THR	THR	L946	E812	P499	P499
	PHE	L2026	GLY	GLY	GLY	GLY	GLY	THR	W1183	GLN	GLN	L946	E812	P500	P500
	GLU	S2031	GLY	GLY	GLY	GLY	GLY	LYS	V1164	GLY	CYS	L946	E812	T642	T642
			ASP	ASP	ASP	ASP	ASP	LYS	L1166	GLN	PRO	L946	E812	E501	E501
			LEU	LEU	LEU	LEU	LEU	LYS	V1166	GLN	PRO	L946	E812	K502	K502

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195231	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	21.826	Depositor
Minimum map value	-0.266	Depositor
Average map value	-0.019	Depositor
Map value standard deviation	0.354	Depositor
Recommended contour level	2.5	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

### 5.1 Standard geometry

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

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	0.84	0/259	1.08	0/343
2	A	0.40	0/11241	0.57	0/15311
All	All	0.42	0/11500	0.59	0/15654

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

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	283	0	243	9	0
2	A	11030	0	10738	143	0
3	A	1	0	0	0	0
All	All	11314	0	10981	149	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 7.

The worst 5 of 149 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:188:THR:HG23	1:B:190:ASN:H	1.37	0.89
1:B:167:ASP:HA	2:A:1773:LYS:HD2	1.57	0.86
2:A:1750:LEU:HD11	2:A:1798:VAL:HG13	1.62	0.79
2:A:427:VAL:HG21	2:A:475:GLU:HB3	1.64	0.79
2:A:894:SER:HB3	2:A:897:TRP:HD1	1.47	0.78

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	B	30/227 (13%)	26 (87%)	3 (10%)	1 (3%)	3	8
2	A	1466/2172 (68%)	1437 (98%)	29 (2%)	0	100	100
All	All	1496/2399 (62%)	1463 (98%)	32 (2%)	1 (0%)	50	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	VAL

### 5.3.2 Protein sidechains [i](#)

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	27/200 (14%)	26 (96%)	1 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	1113/1814 (61%)	1099 (99%)	14 (1%)	65	80
All	All	1140/2014 (57%)	1125 (99%)	15 (1%)	64	80

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1290	SER
2	A	2046	VAL
2	A	1881	GLN
2	A	2117	VAL
2	A	1982	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	918	ASN
2	A	1053	GLN
2	A	1957	ASN
2	A	1022	GLN
2	A	1203	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	B	185	1	8,9,10	0.64	0	8,12,14	0.61	0
1	SEP	B	175	1	8,9,10	0.65	0	8,12,14	0.62	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	B	185	1	-	0/5/8/10	-
1	SEP	B	175	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	185	SEP	1	0
1	B	175	SEP	1	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 ⓘ

There are no chain breaks in this entry.

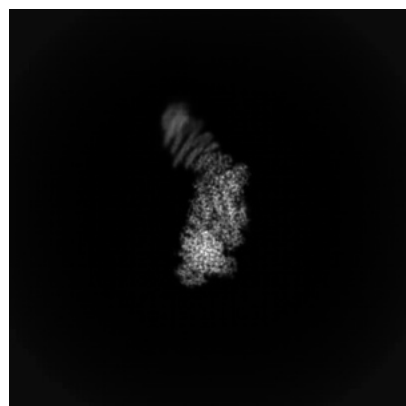
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52307. These allow visual inspection of the internal detail of the map and identification of artifacts.

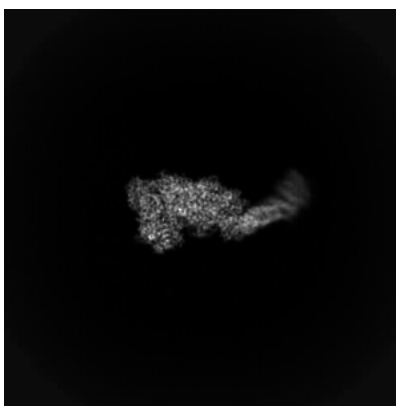
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

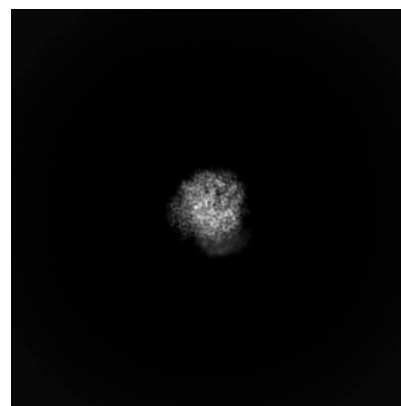
#### 6.1.1 Primary map



X

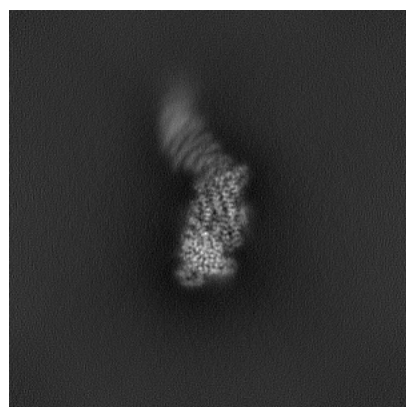


Y

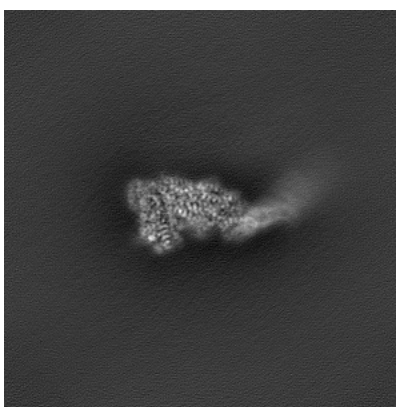


Z

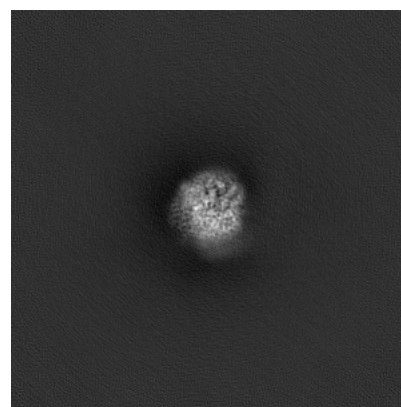
#### 6.1.2 Raw map



X



Y

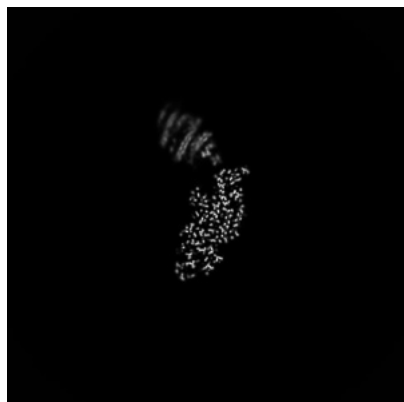


Z

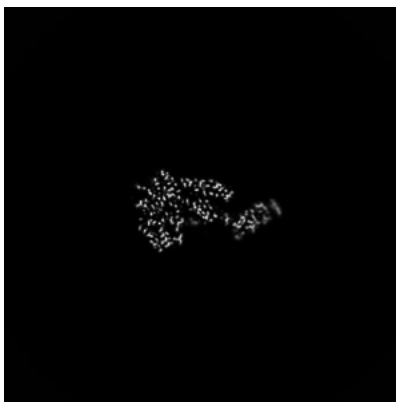
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

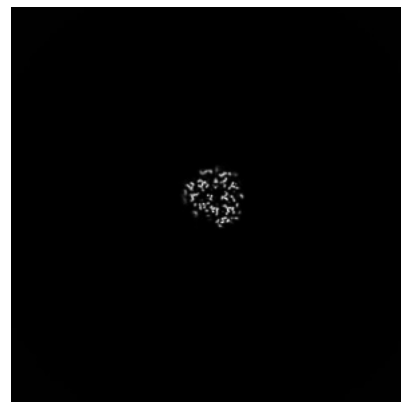
### 6.2.1 Primary map



X Index: 200

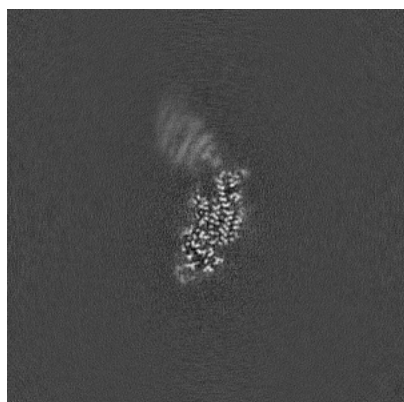


Y Index: 200

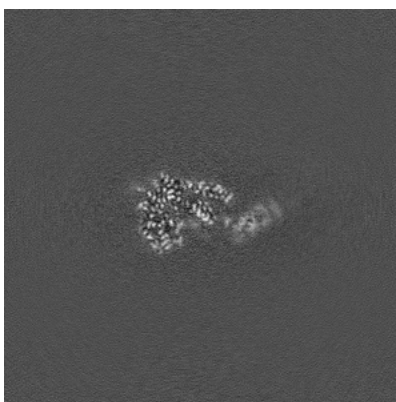


Z Index: 200

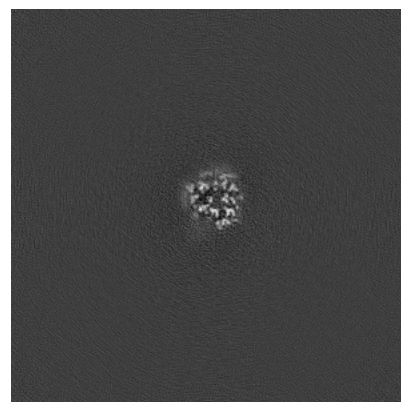
### 6.2.2 Raw map



X Index: 200



Y Index: 200

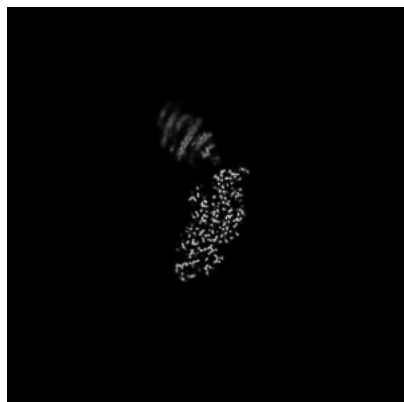


Z Index: 200

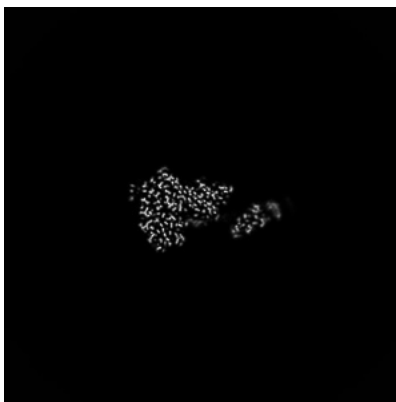
The images above show central slices of the map in three orthogonal directions.

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

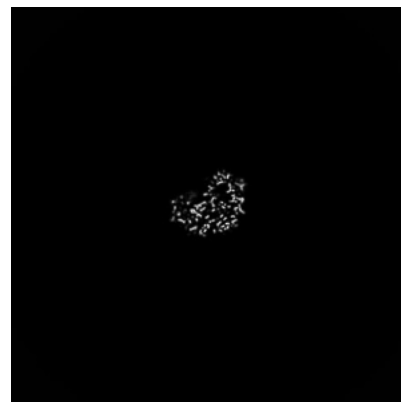
### 6.3.1 Primary map



X Index: 201

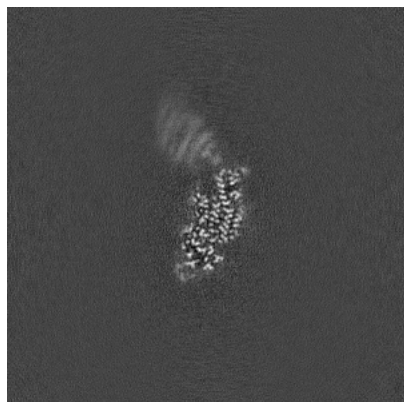


Y Index: 196

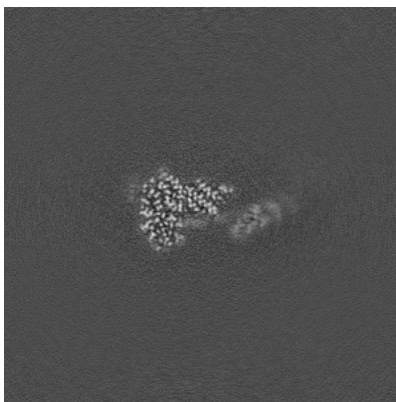


Z Index: 167

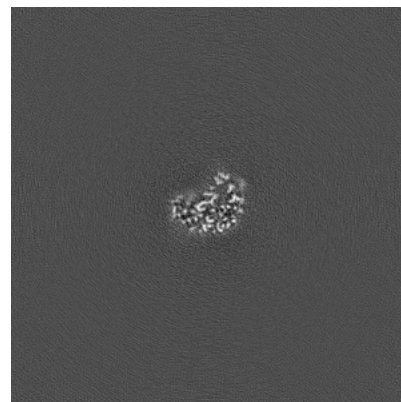
### 6.3.2 Raw map



X Index: 200



Y Index: 196

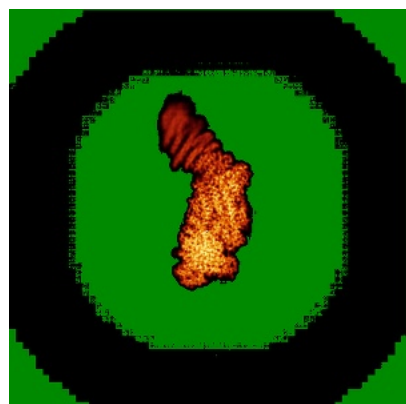


Z Index: 166

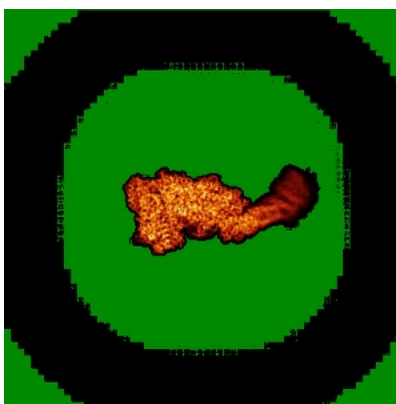
The images above show the largest variance slices of the map in three orthogonal directions.

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

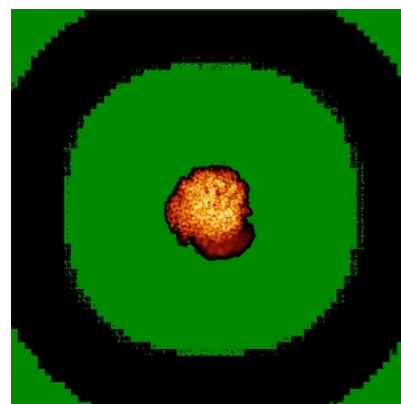
### 6.4.1 Primary map



X

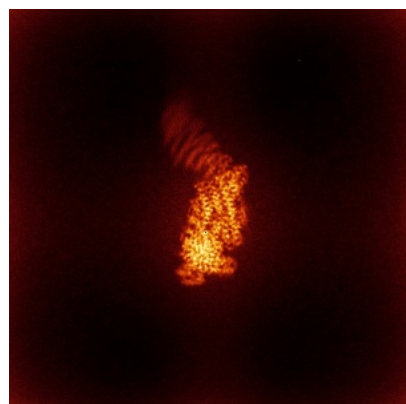


Y

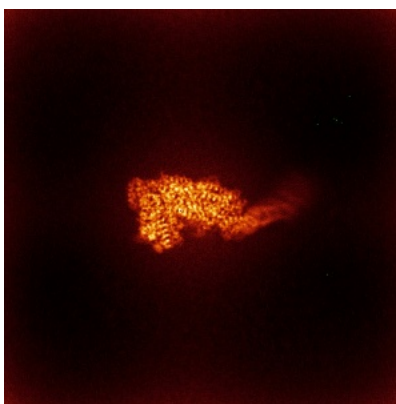


Z

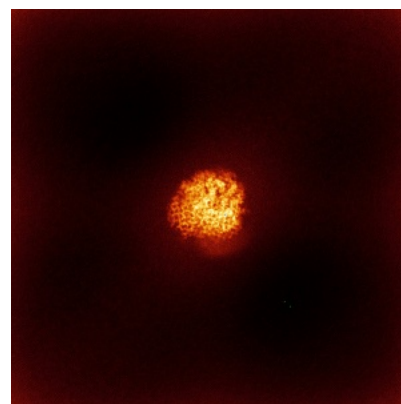
### 6.4.2 Raw map



X



Y

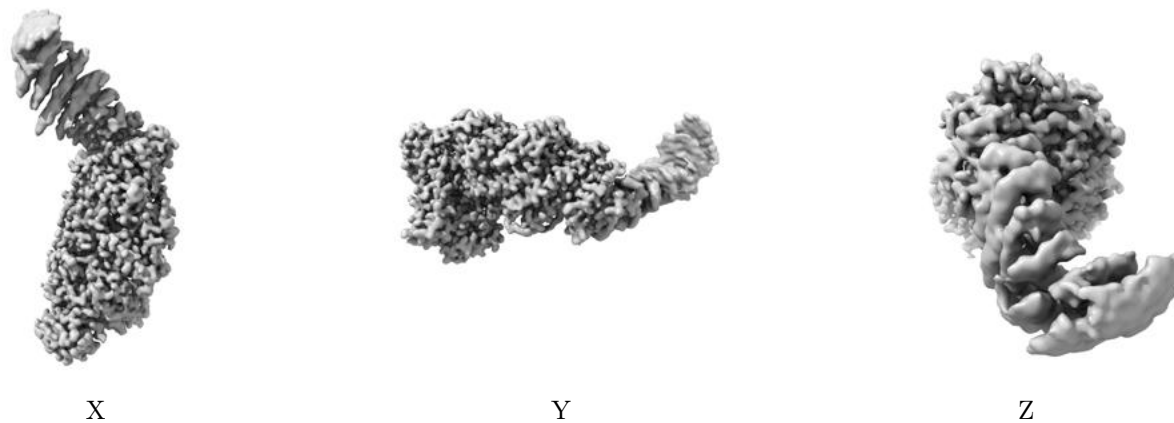


Z

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.

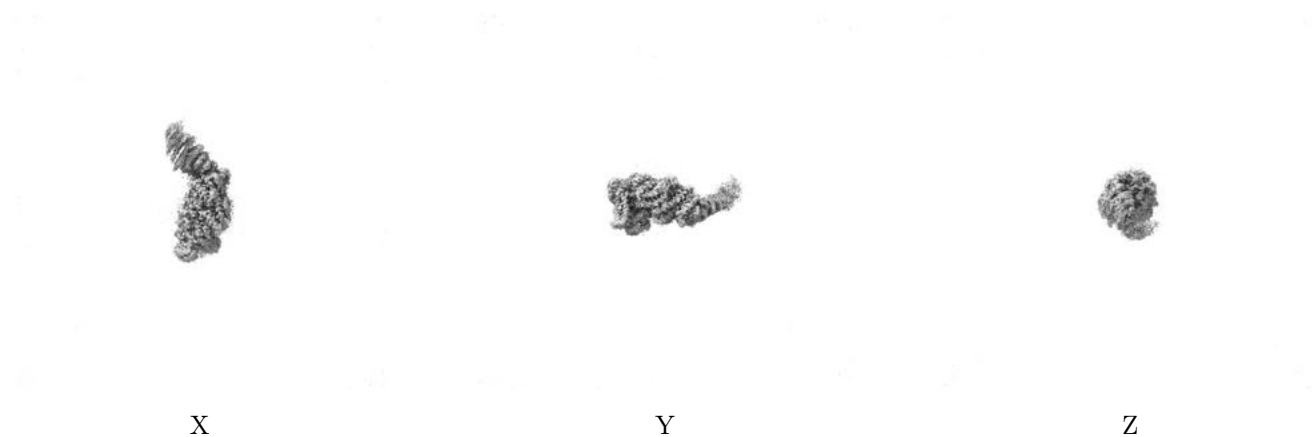
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

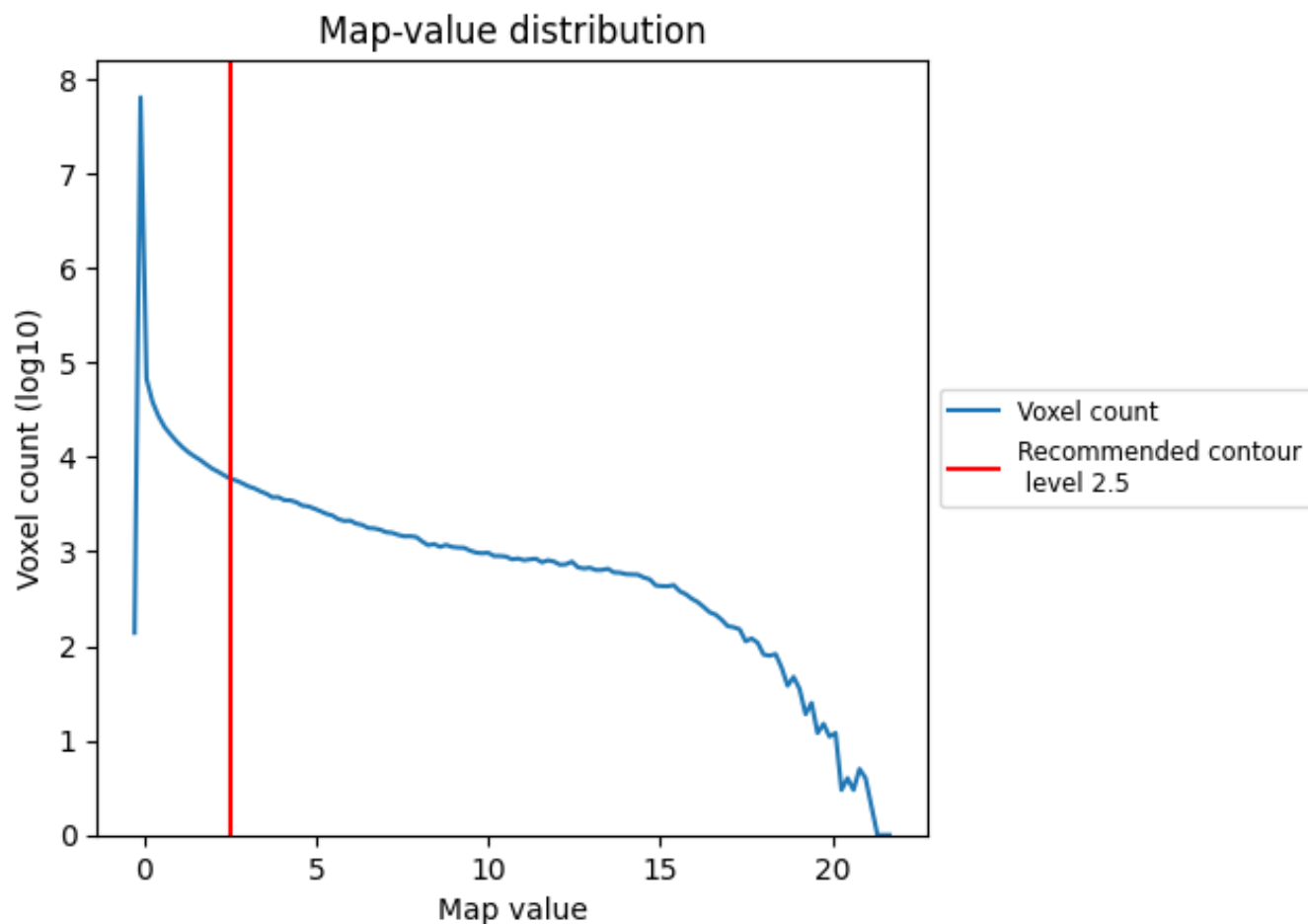
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

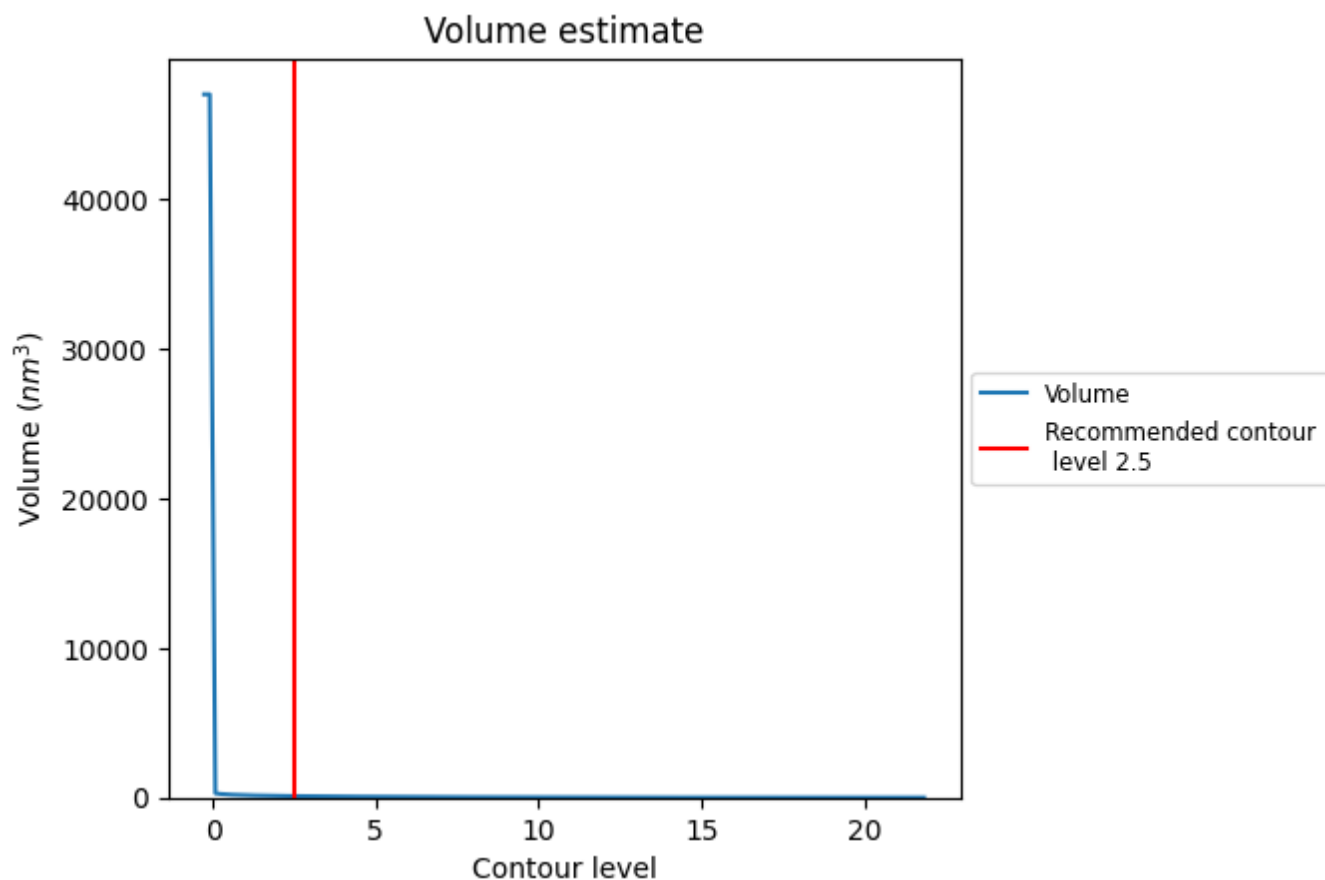
This section contains the results of statistical analysis of the map.

### 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.

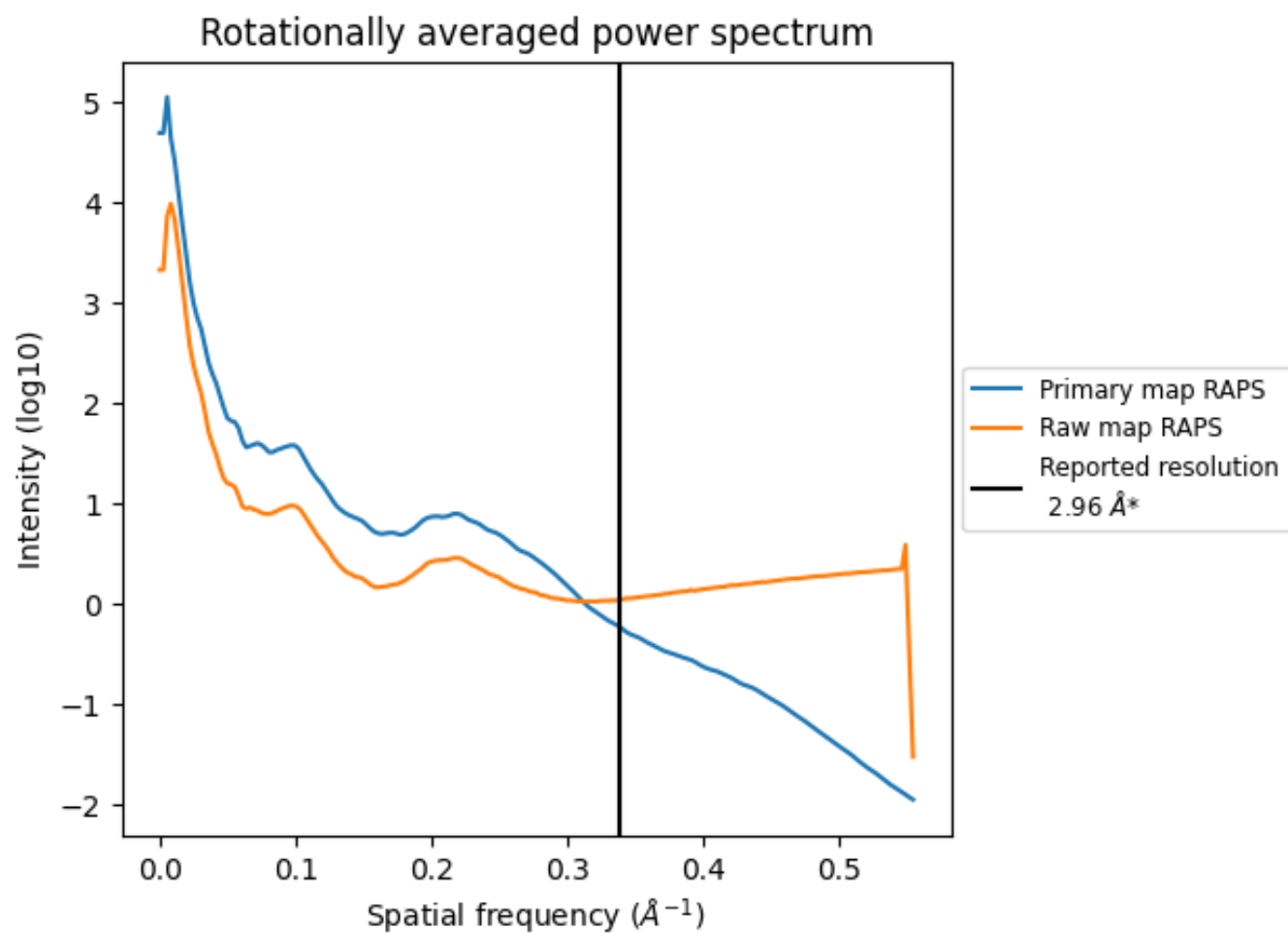
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm<sup>3</sup>; this corresponds to an approximate mass of 87 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](#)

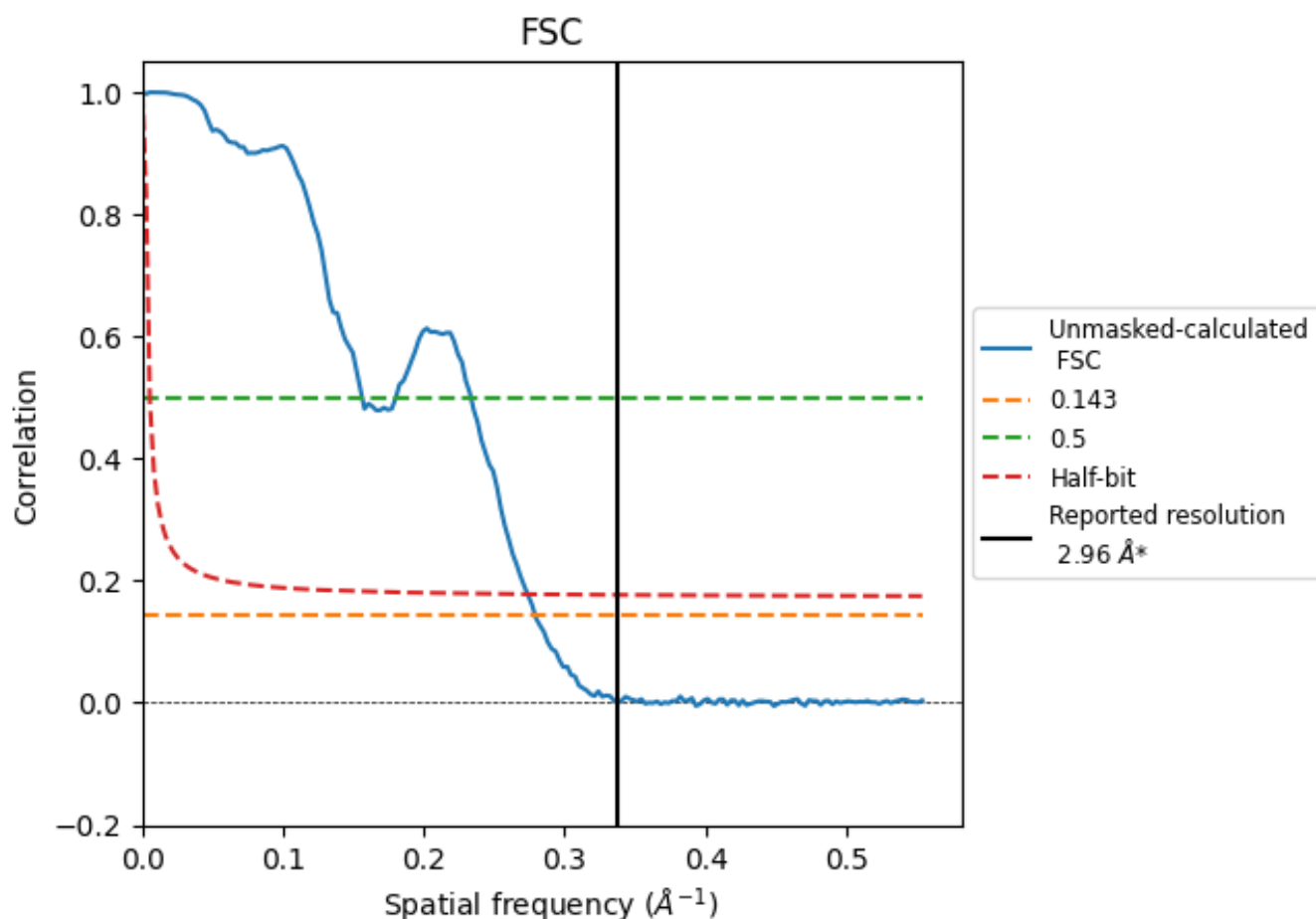


\*Reported resolution corresponds to spatial frequency of  $0.338 \text{ \AA}^{-1}$

## 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 0.338 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

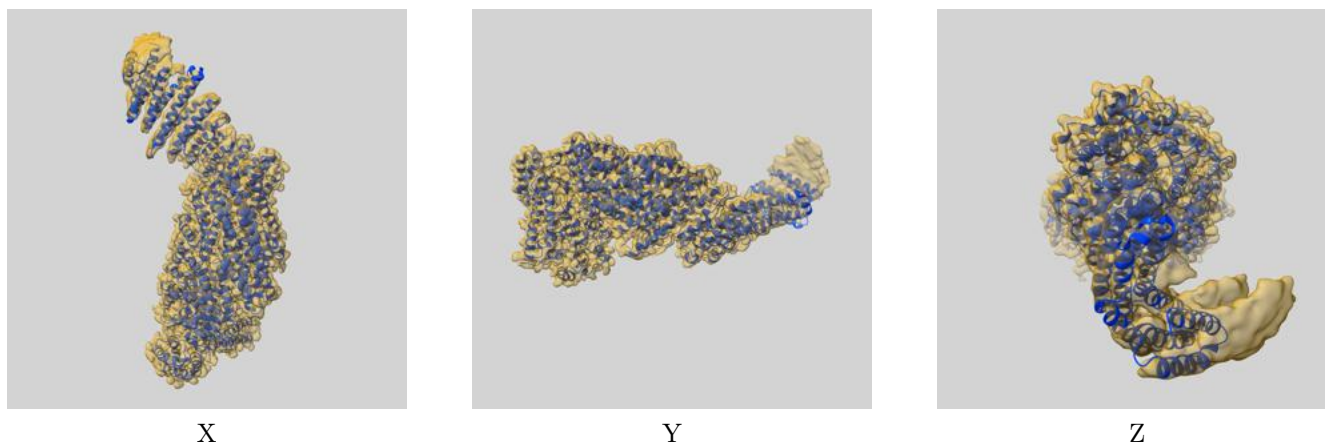
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	6.40	3.65

\*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 3.58 differs from the reported value 2.96 by more than 10 %

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

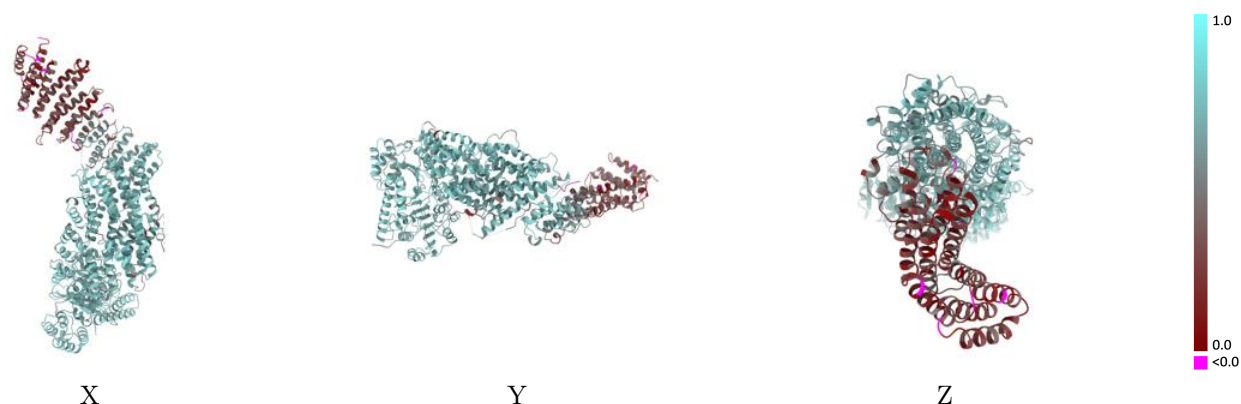
This section contains information regarding the fit between EMDB map EMD-52307 and PDB model 9HN5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



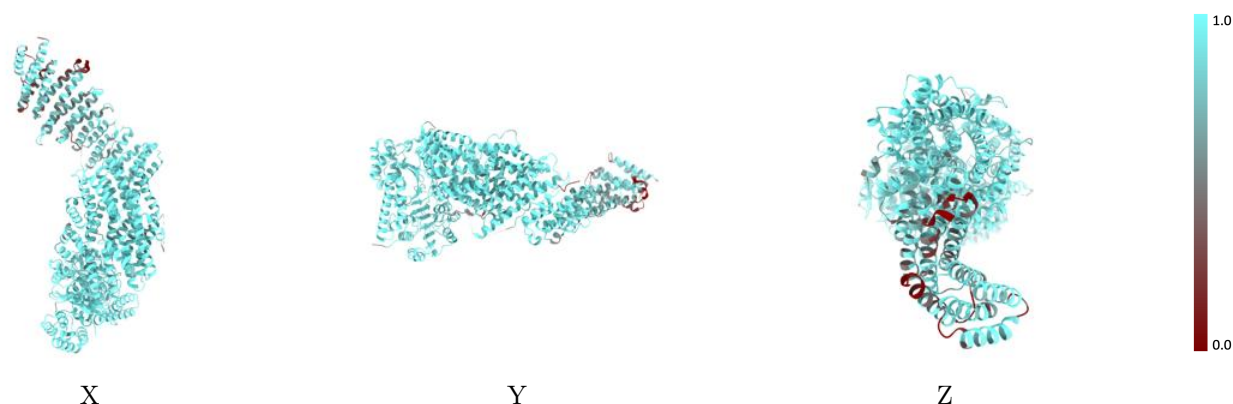
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



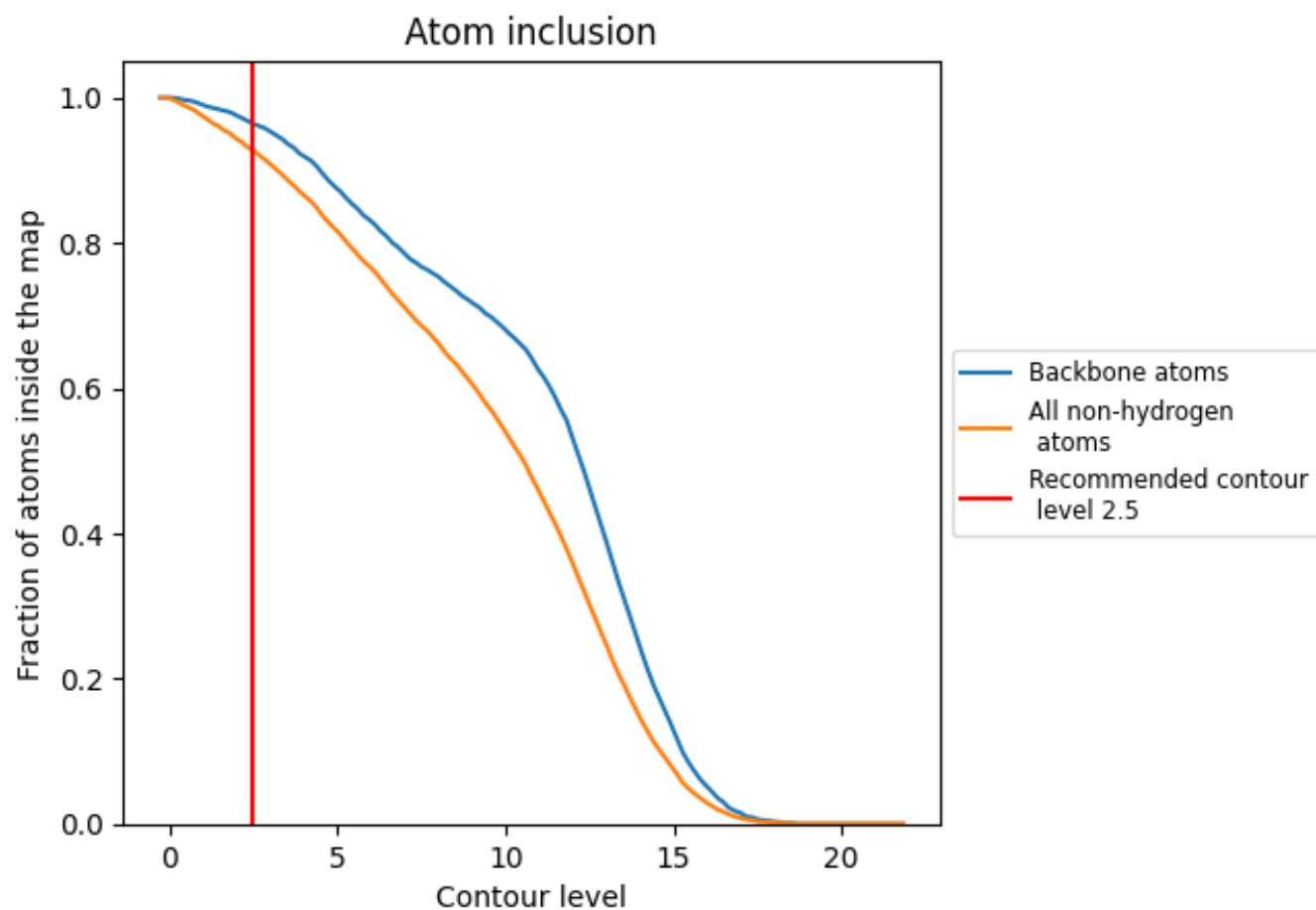
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9270	<div></div> 0.6050
A	<div></div> 0.9340	<div></div> 0.6110
B	<div></div> 0.6440	<div></div> 0.3810

