



Full wwPDB EM Validation Report ⓘ

Feb 12, 2025 – 02:14 PM JST

PDB ID : 8WLA
EMDB ID : EMD-37614
Title : Cryo-EM structure of the beta-1,3-glucan synthase FKS1-Rho1 complex
Authors : Li, J.L.; Zhu, A.Q.; Liu, J.X.; Dai, X.L.; Yan, C.Y.; Deng, D.; Wang, X.
Deposited on : 2023-09-29
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.dev113
MolProbity : 4.02b-467
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) : 2.40

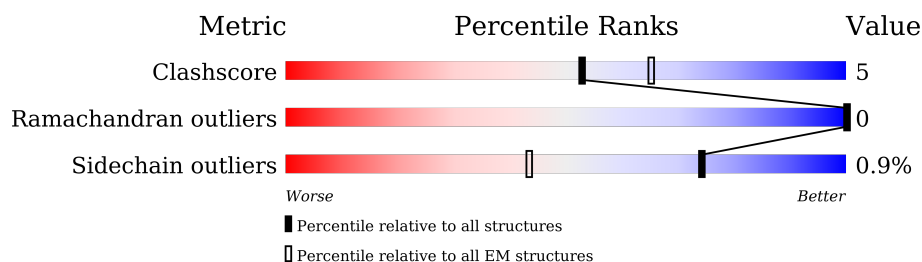
1 Overall quality at a glance

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)
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	209	
2	B	1876	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13360 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 GTP-binding protein RHO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	178	Total	C	N	O	S	0	0
			1383	873	234	269	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	HIS	GLN	engineered mutation	UNP P06780

- Molecule 2 is a protein called 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1492	Total	C	N	O	S	0	0
			11977	7799	2015	2090	73		

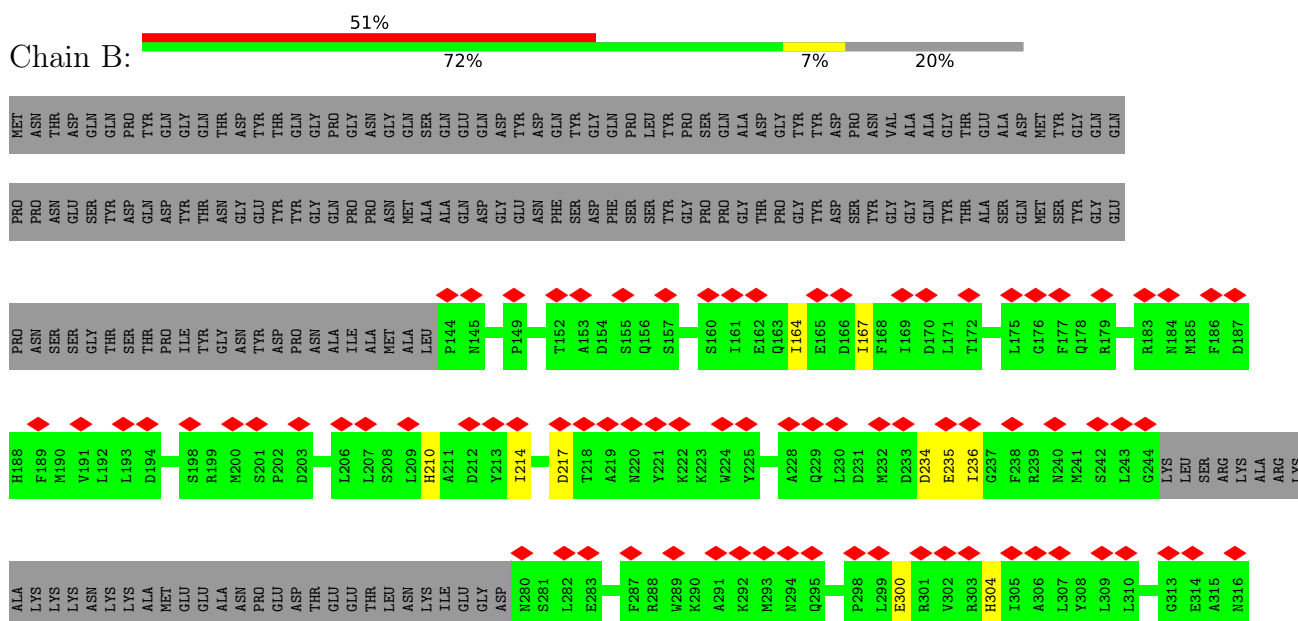
3 Residue-property plots

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: GTP-binding protein RHO1



• Molecule 2: 1,3-beta-glucan synthase component FKS1



L137	R138	Y139	E140	E141	Q142	T143	T144	N145	H146	P147	V148	A149	I150	V151	G152	A153	R154	E155	TVR	ILE	PHE	SER	GLU	ASN	SER	GLY	VAL	LEU	GLY	ASP	VAL	ALA	ALA	ALA	GLY	LYS	GLU	GLN	THR	F176	G177	L178	L179	F180	A181	R182	T183	L184	S185	Q186	E187	F188	G189	K190	LEU	HIS	TYR	GLY	H195
L1072	S1073	G1074	P1075	P1076	L1077	G1078	D1080	G1081	K1082	S1083	D1084	N1085	Q1086	N1087	H1088	A1089	F1092	Y1093	R1094	G1095	I1098	Q1099	L1100	I1101	D1102	A1103	N1104	Q1105	D1106	N1107	Y1108	L1109	E1110	E1111	C1112	L1113	K1114	I1115	R1116	L1119	A1120	E1121	F1122	E1123	E1124	L1125	N1126	V1127	E1128	Q1129	V1130	N1131	P1132	Y1133	A1134				
K997	F998	K999	F1000	L1001	V1002	S1003	M1004	L1007	A1008	K1009	F1010	K1011	P1012	L1015	E1016	E1019	L1022	R1023	A1024	Y1025	P1026	D1027	L1028	Q1029	I1030	A1031	Y1032	E1036	P1037	P1038	L1039	T1040	E1041	Y1048	L1051	I1052	D1053	G1054	H1055	C1056	E1057	I1058	L1059	D1060	R1065	P1066	K1067	F1068	R1069	V1070	Q1071								
I926	Q927	F928	K929	S930	A931	A932	P933	E934	Y935	T936	L937	R938	Y939	T940	S944	L945	Q948	T949	L950	Y951	I954	S955	G956	P957	M958	S961	R962	ALA	A963	I964	K965	L966	L967	Y968	R969	E974	Q977	M978	C980	G981	N982	A983	E984	L985	L986	E987	R988	E989	M993	R996									
R862	E863	D864	D865	Q866	F867	S868	R869	L873	E874	R875	L876	L879	V882	E883	W884	E885	C886	F887	W888	K889	D890	T891	K892	I893	L894	A895	E896	E897	T898	A899	A900	Y901	E902	G903	N904	E905	N906	GLU	ALA	GLU	LYS	GLU	ASP	ALA	LEU	SER	GLN	ILE	ASP	LEU	PRO	PHE	TYR	C925					
S798	Q799	ASP	ASP	ASN	ASN	PHE	E805	T806	E807	F808	F809	S813	E814	E816	R817	R818	I819	F822	A823	Q824	S825	L826	S827	T828	P829	T830	P831	E832	P833	W836	D837	N838	M839	P840	T841	F842	T843	W844	L845	T846	P847	H848	Y849	A850	E851	R852	L853	L854	L855	S856	L857	R858	E859	T860	T861				
I730	Y731	I734	L735	A736	T737	T738	D739	W740	E741	I742	K743	Y744	K745	V748	L749	I750	S751	Q752	W755	A756	I759	Y762	R763	E764	H765	L766	L767	A768	I769	D770	H771	Y772	Q773	K774	L775	L776	Y777	Q779	V780	P781	S782	A783	I784	E785	G786	K787	R788	T789	L790	R791	F795								
R657	C658	T659	G660	E661	Y662	W663	W664	G665	A666	W667	L668	C669	I675	W676	L679	A682	T683	I686	L687	F688	F689	L690	D691	T692	Y693	L694	W695	Y696	I697	W700	T701	S704	V705	G706	K707	S708	L711	G712	I713	S714	I715	W719	R720	F723	T724	R725	L726	P727	K728	R729									
P519	S520	K521	W522	A523	Q526	H527	L528	S529	R530	R531	F532	W533	F534	L535	I538	F539	G540	I541	N542	P545	I546	V549	F550	D553	K554	D555	Y558	S559	T560	H563	V564	V568	M569	F570	F571	V572	A575	I578	F579	F580	S581	I582	M583	P584	L585	G586	G587	L588	F589										
F452	M453	R454	I455	W456	H459	I460	S461	I462	F463	W464	M465	Y466	F467	M470	F474	M478	TVR	GLN	GLN	LEU	VAL	ASP	ASN	GLN	PRO	L488	A489	A490	Y491	K492	W493	A494	S495	C496	L497	L498	G499	G500	T501	V502	A503	S504	L505	I506	Q507	I508	V509	A510	T511	E514	W515	S516	F517	W518					
K386	I387	V388	G389	Y390	D391	L392	L393	N394	Q395	L396	F397	W398	Y399	P400	E401	G402	I403	A404	K405	I406	E409	D410	G411	T412	K413	L414	L417	E420	E421	R422	Y423	L424	R425	L426	G427	D428	W431	D432	D433	V434	F435	F436	K437	T438	Y439	K440	E441	T442	R443	T444	W445	L446	H447	L448					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.961	Depositor
Minimum map value	-1.330	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.229	Depositor
Map size (\AA)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1409	0.46	0/1916
2	B	0.28	0/12295	0.49	0/16696
All	All	0.28	0/13704	0.48	0/18612

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	11	ARG	Sidechain

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	1383	0	1351	10	0
2	B	11977	0	11777	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13360	0	13128	134	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 5.

All (134) 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)
2:B:662:TYR:CD2	2:B:663:TRP:CD1	2.34	1.14
2:B:1590:THR:CB	2:B:1858:TYR:OH	1.95	1.13
2:B:662:TYR:CD2	2:B:663:TRP:HD1	1.67	1.12
2:B:662:TYR:CE2	2:B:663:TRP:CD1	2.44	1.04
2:B:957:PHE:CE2	2:B:1101:ILE:HD13	1.92	1.04
2:B:957:PHE:CE2	2:B:1101:ILE:CD1	2.43	1.01
2:B:1000:PHE:HE1	2:B:1002:VAL:CG2	1.73	1.00
2:B:662:TYR:CE2	2:B:663:TRP:HD1	1.82	0.92
2:B:1000:PHE:CE1	2:B:1002:VAL:HG23	2.07	0.89
2:B:1000:PHE:CE1	2:B:1002:VAL:CG2	2.55	0.89
2:B:1668:ASN:HD22	2:B:1671:ARG:HG3	1.39	0.88
2:B:1657:PHE:HA	2:B:1660:VAL:HG12	1.54	0.86
2:B:1590:THR:CB	2:B:1858:TYR:HH	1.90	0.85
2:B:1653:VAL:CG1	2:B:1657:PHE:CE2	2.63	0.81
1:A:98:GLU:O	1:A:102:GLU:HG3	1.83	0.79
2:B:1668:ASN:ND2	2:B:1671:ARG:HG3	1.97	0.77
2:B:1657:PHE:O	2:B:1660:VAL:HG12	1.86	0.76
2:B:662:TYR:HD2	2:B:663:TRP:CD1	1.97	0.76
2:B:1641:VAL:O	2:B:1645:ILE:HG13	1.87	0.74
2:B:1499:PHE:CZ	2:B:1751:LEU:HD22	2.26	0.71
2:B:1653:VAL:HG12	2:B:1657:PHE:CE2	2.26	0.71
2:B:1657:PHE:CA	2:B:1660:VAL:HG12	2.21	0.70
2:B:948:GLN:N	2:B:948:GLN:OE1	2.25	0.70
2:B:957:PHE:CZ	2:B:1101:ILE:HD13	2.27	0.69
2:B:1596:VAL:CG1	2:B:1601:ARG:HH22	2.07	0.68
2:B:957:PHE:HE2	2:B:1101:ILE:CD1	2.07	0.66
2:B:1183:THR:HB	2:B:1375:VAL:HG21	1.78	0.66
2:B:1653:VAL:CG1	2:B:1657:PHE:HE2	2.06	0.66
2:B:1657:PHE:HA	2:B:1660:VAL:CG1	2.23	0.65
2:B:1596:VAL:CG1	2:B:1601:ARG:NH2	2.59	0.65
2:B:1000:PHE:HE1	2:B:1002:VAL:HG23	1.44	0.64
2:B:1367:TRP:O	2:B:1371:VAL:HG13	2.00	0.62
2:B:588:LEU:HD23	2:B:589:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:PHE:HE2	2:B:1101:ILE:HD12	1.63	0.61
2:B:957:PHE:CE2	2:B:1101:ILE:HD12	2.31	0.61
2:B:935:TYR:O	2:B:939:THR:HG23	2.01	0.61
2:B:1653:VAL:HG13	2:B:1657:PHE:CE2	2.35	0.61
2:B:346:GLU:N	2:B:346:GLU:OE1	2.35	0.60
2:B:777:TYR:O	2:B:779:GLN:NE2	2.34	0.60
2:B:1612:VAL:HG11	2:B:1653:VAL:HG21	1.84	0.60
2:B:1657:PHE:C	2:B:1660:VAL:HG12	2.22	0.59
2:B:1608:ALA:HB1	2:B:1657:PHE:CZ	2.38	0.58
2:B:210:HIS:CE1	2:B:214:ILE:HD11	2.40	0.57
2:B:664:TRP:HE1	2:B:668:LEU:HD12	1.70	0.57
2:B:846:THR:HB	2:B:1002:VAL:HG22	1.85	0.57
2:B:1651:VAL:HG22	2:B:1741:ALA:HA	1.85	0.56
2:B:837:ASP:N	2:B:837:ASP:OD1	2.38	0.56
2:B:1664:LEU:HD22	2:B:1840:LEU:HD23	1.87	0.56
2:B:1855:MET:SD	2:B:1855:MET:N	2.79	0.56
2:B:1843:PRO:HB2	2:B:1846:THR:CG2	2.36	0.55
2:B:234:ASP:OD1	2:B:235:GLU:N	2.39	0.55
2:B:662:TYR:CE2	2:B:663:TRP:NE1	2.73	0.55
2:B:662:TYR:HE2	2:B:663:TRP:CD1	2.17	0.54
2:B:1668:ASN:HD22	2:B:1671:ARG:CG	2.15	0.54
1:A:98:GLU:HG2	1:A:102:GLU:OE2	2.08	0.54
2:B:1657:PHE:O	2:B:1660:VAL:CG1	2.53	0.54
2:B:1294:HIS:HB2	2:B:1295:PRO:HD3	1.90	0.54
2:B:300:GLU:O	2:B:304:HIS:ND1	2.41	0.54
2:B:1858:TYR:O	2:B:1858:TYR:CG	2.60	0.54
2:B:1128:GLU:N	2:B:1128:GLU:OE1	2.38	0.54
2:B:1843:PRO:HB2	2:B:1846:THR:HG23	1.90	0.53
2:B:1495:ALA:HB3	2:B:1498:ASP:HB3	1.91	0.52
2:B:1503:TYR:CD1	2:B:1751:LEU:HD13	2.44	0.52
2:B:663:TRP:HB2	2:B:664:TRP:CE3	2.45	0.52
2:B:1341:VAL:HB	2:B:1342:PRO:HD3	1.92	0.52
2:B:657:ARG:O	2:B:1586:THR:HA	2.12	0.50
2:B:664:TRP:HB2	2:B:667:VAL:HG22	1.94	0.49
2:B:1596:VAL:HG11	2:B:1601:ARG:HH22	1.78	0.49
2:B:662:TYR:HE2	2:B:663:TRP:NE1	2.10	0.49
2:B:657:ARG:O	2:B:1586:THR:O	2.29	0.49
2:B:1590:THR:N	2:B:1858:TYR:OH	2.46	0.49
1:A:44:PHE:O	2:B:1011:LYS:NZ	2.34	0.49
2:B:745:LYS:O	2:B:748:VAL:HG12	2.13	0.49
2:B:1503:TYR:CD1	2:B:1751:LEU:CD1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1448:SER:O	2:B:1449:ALA:HB3	2.12	0.49
2:B:1727:SER:O	2:B:1731:THR:HG23	2.12	0.49
2:B:1649:VAL:O	2:B:1653:VAL:HG23	2.13	0.48
2:B:545:PRO:O	2:B:549:VAL:HG23	2.14	0.48
2:B:553:ASP:OD1	2:B:554:LYS:N	2.47	0.48
2:B:1664:LEU:CD2	2:B:1840:LEU:HD23	2.45	0.47
2:B:1733:LYS:O	2:B:1737:LEU:HG	2.14	0.47
2:B:236:ILE:HD13	2:B:605:THR:HG22	1.96	0.47
2:B:1673:LEU:O	2:B:1676:VAL:HG12	2.16	0.46
2:B:1000:PHE:HE1	2:B:1002:VAL:HG21	1.68	0.46
2:B:664:TRP:HB2	2:B:667:VAL:CG2	2.45	0.46
2:B:1371:VAL:O	2:B:1375:VAL:HG23	2.16	0.46
1:A:29:VAL:HG11	1:A:166:ALA:O	2.16	0.46
2:B:692:THR:HG21	2:B:1292:TYR:OH	2.15	0.46
2:B:1665:GLU:HG3	2:B:1672:MET:CA	2.46	0.45
1:A:75:ARG:N	1:A:76:PRO:HD2	2.32	0.45
2:B:1595:ARG:O	2:B:1837:VAL:HG23	2.16	0.45
2:B:1371:VAL:N	2:B:1372:PRO:HD2	2.32	0.45
2:B:1659:ILE:O	2:B:1663:VAL:HG23	2.17	0.45
1:A:9:ILE:HB	1:A:11:ARG:HH11	1.81	0.44
2:B:830:ILE:HG22	2:B:1241:TYR:CD1	2.53	0.44
2:B:1858:TYR:O	2:B:1858:TYR:CD2	2.70	0.44
1:A:178:ALA:O	1:A:182:ALA:N	2.50	0.44
2:B:462:ILE:HG21	2:B:633:TYR:CE1	2.53	0.43
2:B:664:TRP:CD1	2:B:664:TRP:O	2.71	0.43
1:A:84:VAL:HG23	1:A:118:ILE:HB	2.00	0.43
2:B:1371:VAL:HG22	2:B:1372:PRO:HD3	2.00	0.43
2:B:1641:VAL:O	2:B:1645:ILE:CG1	2.64	0.43
2:B:690:LEU:HD23	2:B:1365:VAL:HG11	2.01	0.43
2:B:217:ASP:OD2	2:B:1142:GLN:NE2	2.49	0.43
2:B:1653:VAL:HG12	2:B:1657:PHE:CD2	2.54	0.43
2:B:1522:TRP:CZ2	2:B:1526:VAL:HG11	2.54	0.42
2:B:641:VAL:HG13	2:B:642:LEU:N	2.35	0.42
2:B:785:GLU:N	2:B:785:GLU:OE1	2.52	0.42
2:B:657:ARG:HD2	2:B:1858:TYR:CD1	2.54	0.42
2:B:1725:GLN:N	2:B:1726:PRO:HD2	2.34	0.42
1:A:75:ARG:N	1:A:76:PRO:CD	2.83	0.42
2:B:1329:ILE:HG22	2:B:1330:TYR:N	2.34	0.42
2:B:1349:GLN:O	2:B:1352:VAL:HG22	2.20	0.42
2:B:1495:ALA:HB3	2:B:1498:ASP:CB	2.49	0.42
2:B:1608:ALA:HB1	2:B:1657:PHE:CE1	2.55	0.42

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:774:LYS:N	2:B:774:LYS:HD2	2.35	0.42
2:B:1499:PHE:CG	2:B:1758:ILE:HD11	2.54	0.42
2:B:1817:GLY:N	2:B:1818:PRO:HD2	2.35	0.42
1:A:9:ILE:HD11	1:A:183:SER:HB2	2.02	0.41
2:B:954:ILE:HD12	2:B:1028:LEU:HD11	2.02	0.41
2:B:1596:VAL:HG13	2:B:1601:ARG:NH2	2.35	0.41
2:B:1560:LEU:O	2:B:1563:ALA:HB3	2.20	0.41
2:B:1340:LEU:HD22	2:B:1340:LEU:H	1.85	0.41
2:B:164:ILE:O	2:B:167:ILE:HG22	2.20	0.41
2:B:1294:HIS:HB2	2:B:1295:PRO:CD	2.50	0.41
2:B:1662:TRP:CD1	2:B:1667:PHE:HA	2.55	0.41
2:B:1845:ASN:C	2:B:1846:THR:HG23	2.41	0.41
2:B:661:GLU:O	2:B:665:GLY:CA	2.69	0.41
2:B:1334:LYS:HG2	2:B:1335:PRO:HD2	2.02	0.41
2:B:1516:GLN:O	2:B:1518:HIS:CD2	2.74	0.41
2:B:1669:PHE:CE2	2:B:1673:LEU:HD11	2.55	0.41
2:B:1503:TYR:HD1	2:B:1751:LEU:CD1	2.34	0.40
2:B:580:PHE:HE1	2:B:588:LEU:HD21	1.86	0.40
2:B:1690:MET:O	2:B:1694:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/209 (84%)	171 (97%)	5 (3%)	0	100	100
2	B	1466/1876 (78%)	1437 (98%)	29 (2%)	0	100	100
All	All	1642/2085 (79%)	1608 (98%)	34 (2%)	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	151/180 (84%)	148 (98%)	3 (2%)	50	70
2	B	1264/1620 (78%)	1254 (99%)	10 (1%)	79	87
All	All	1415/1800 (79%)	1402 (99%)	13 (1%)	74	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	ARG
1	A	11	ARG
2	B	658	CYS
2	B	662	TYR
2	B	739	ASP
2	B	1010	PHE
2	B	1093	TYR
2	B	1328	CYS
2	B	1346	TYR
2	B	1467	HIS
2	B	1515	ASN
2	B	1658	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1518	HIS
2	B	1668	ASN
2	B	1748	HIS

5.3.3 RNA ⓘ

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.

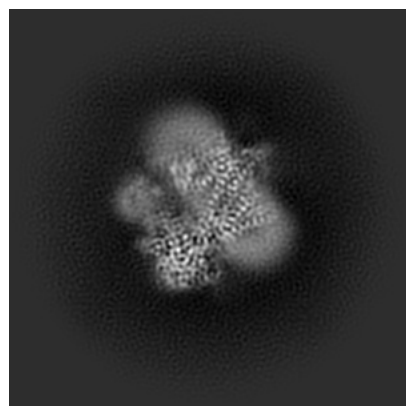
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37614. These allow visual inspection of the internal detail of the map and identification of artifacts.

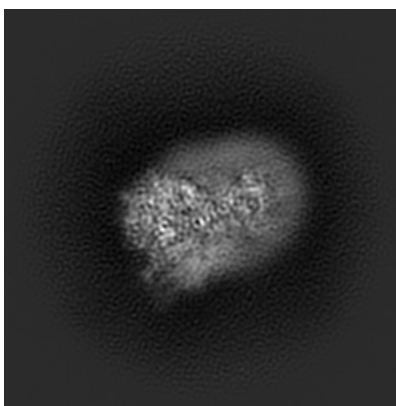
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

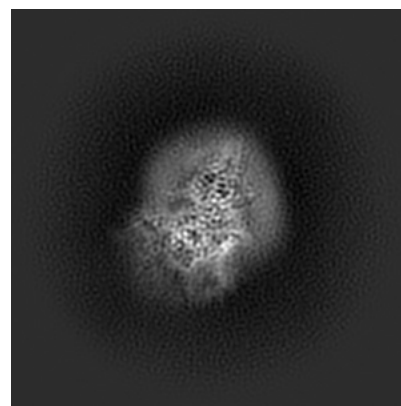
6.1.1 Primary map



X

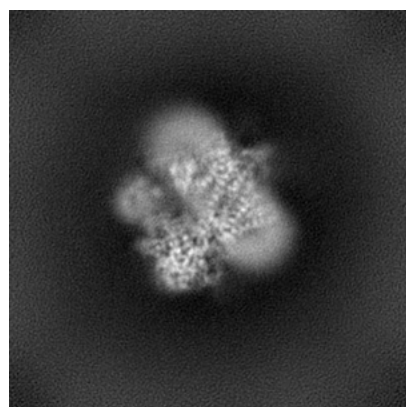


Y

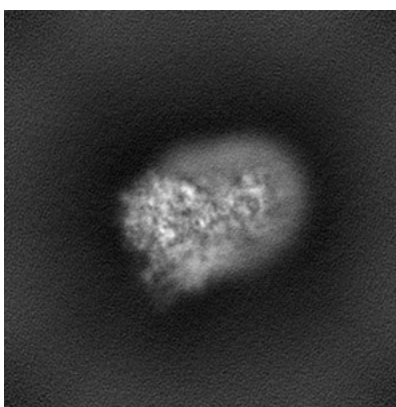


Z

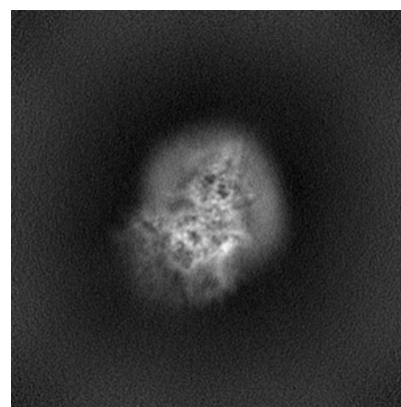
6.1.2 Raw map



X



Y

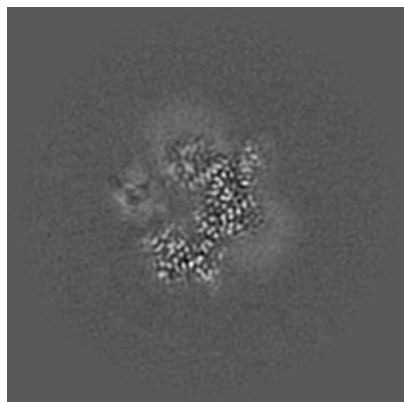


Z

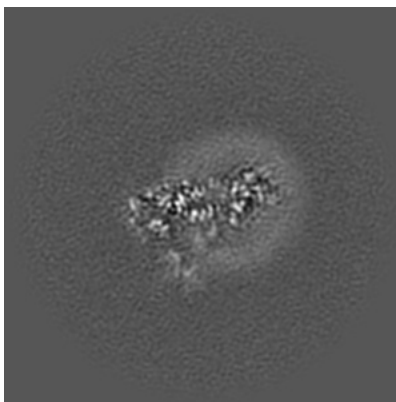
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

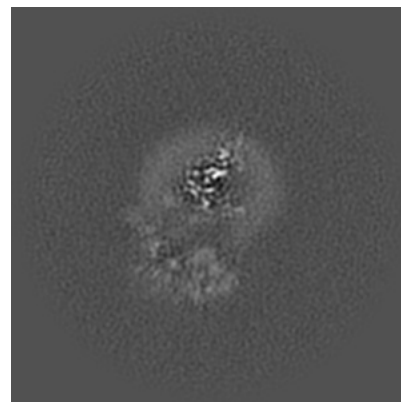
6.2.1 Primary map



X Index: 128

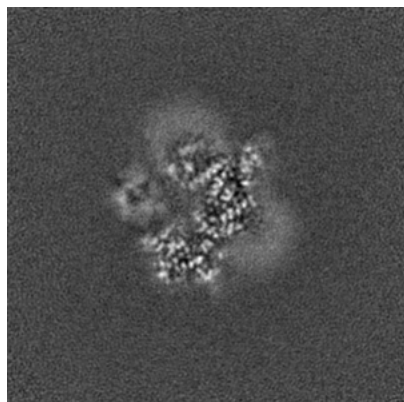


Y Index: 128

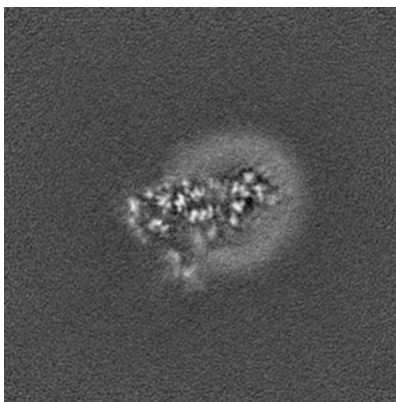


Z Index: 128

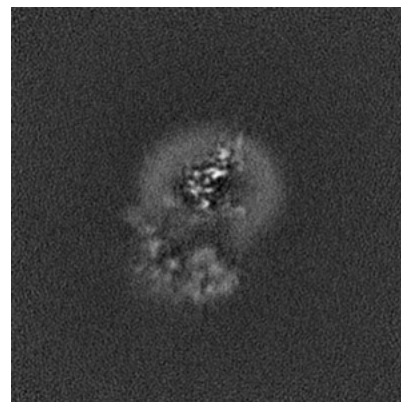
6.2.2 Raw map



X Index: 128



Y Index: 128

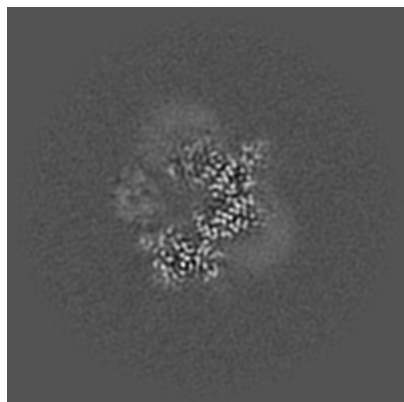


Z Index: 128

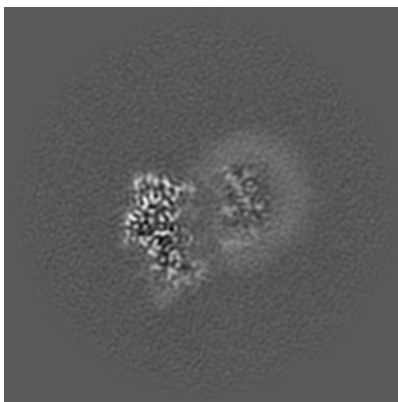
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

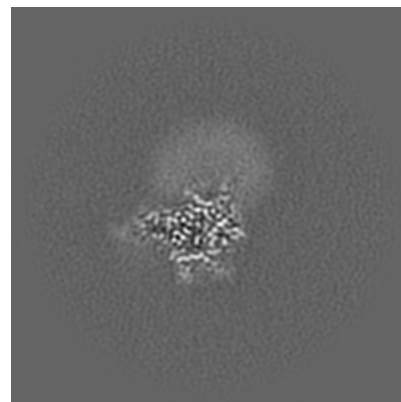
6.3.1 Primary map



X Index: 130

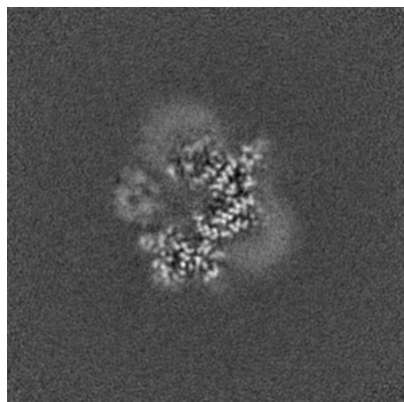


Y Index: 113

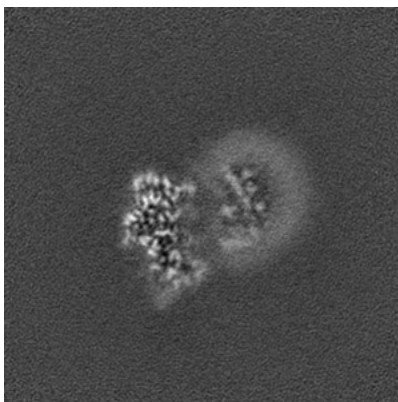


Z Index: 103

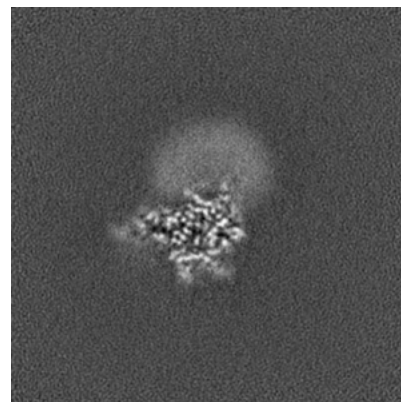
6.3.2 Raw map



X Index: 130



Y Index: 113

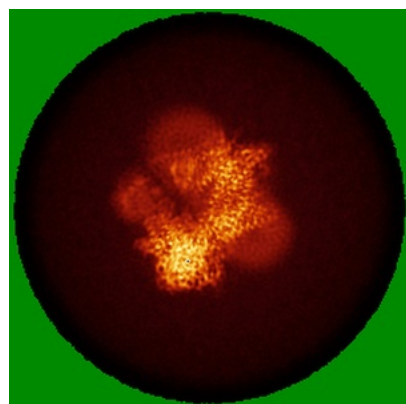


Z Index: 103

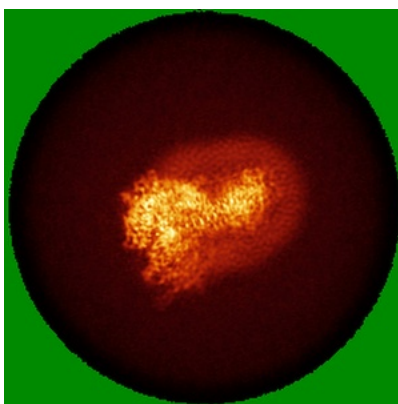
The images above show the largest variance slices of the map in three orthogonal directions.

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

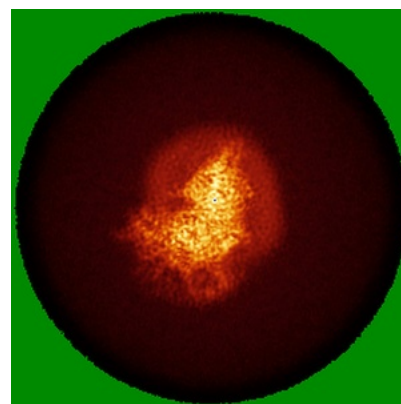
6.4.1 Primary map



X

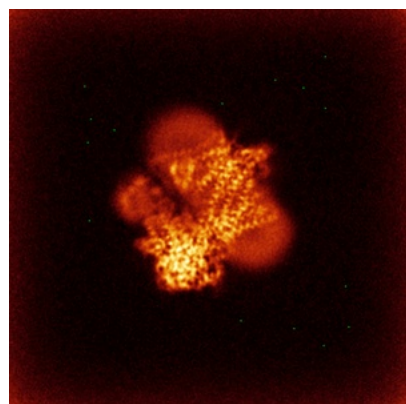


Y

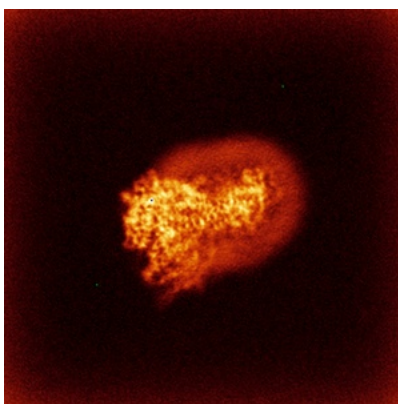


Z

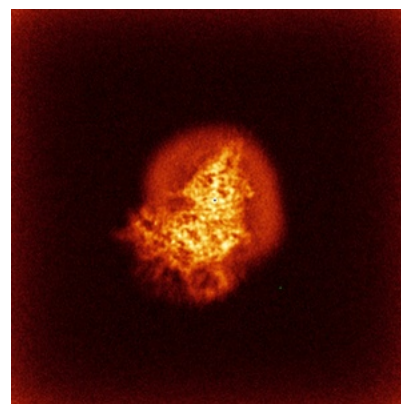
6.4.2 Raw map



X



Y

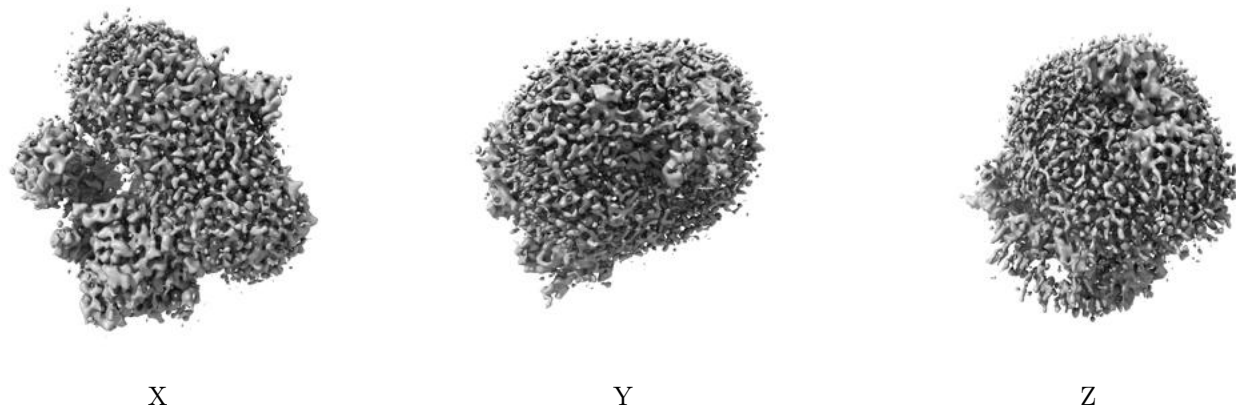


Z

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.

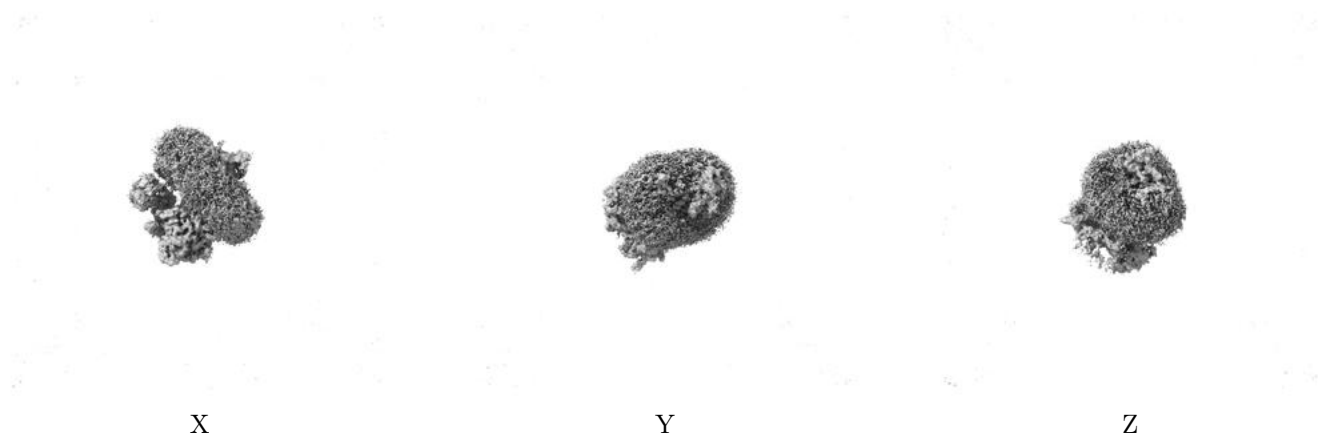
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.229. 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.

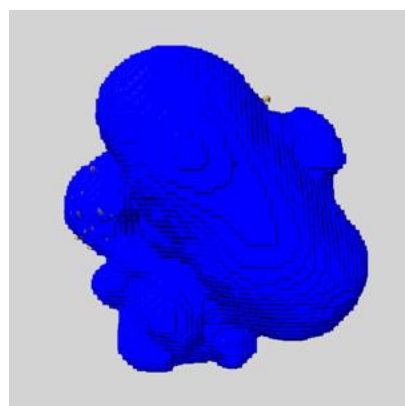
6.6 Mask visualisation [i](#)

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

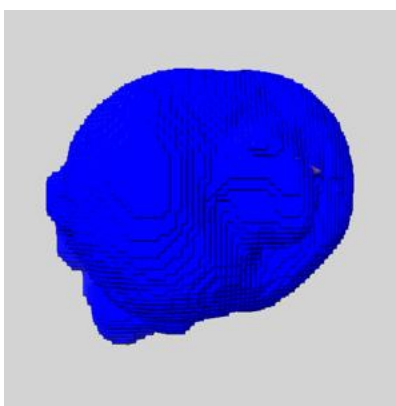
A mask typically either:

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

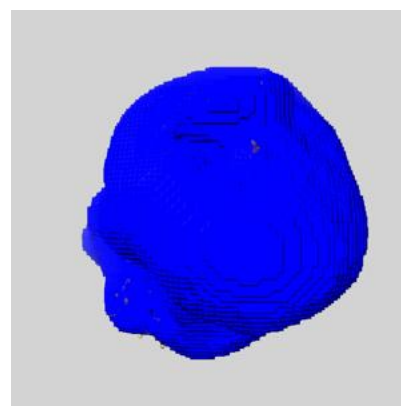
6.6.1 emd_37614_msk_1.map [i](#)



X



Y

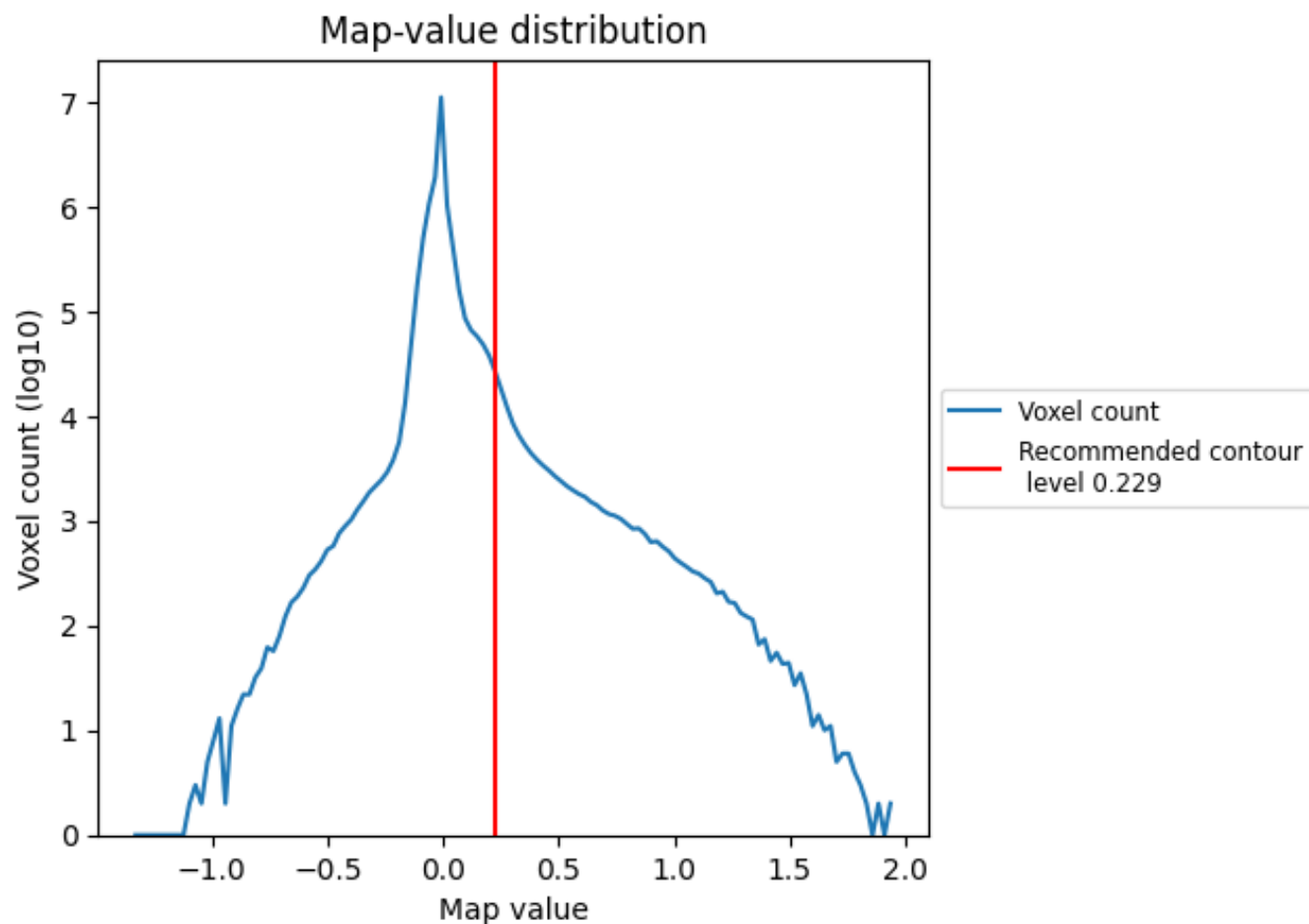


Z

7 Map analysis [i](#)

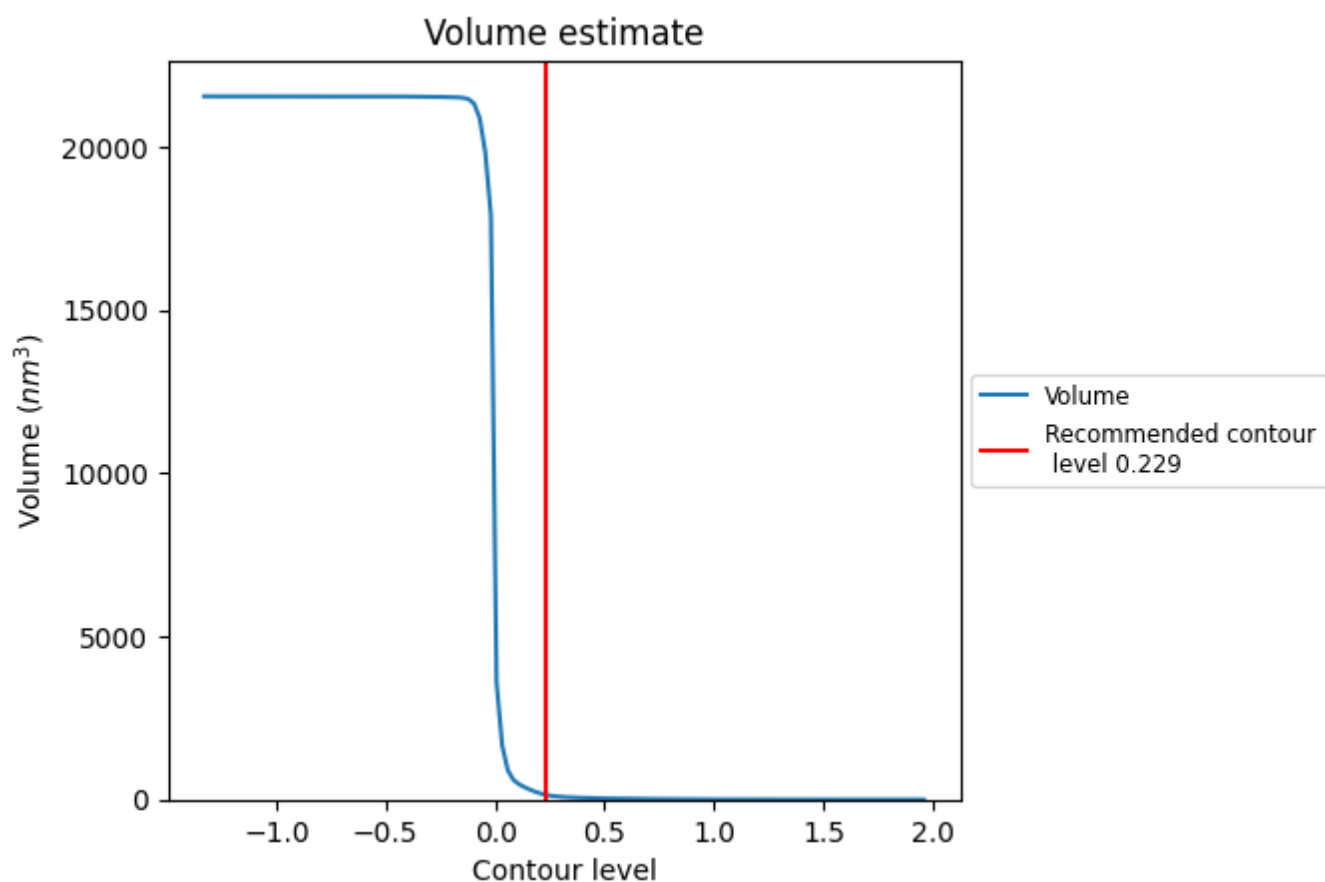
This section contains the results of statistical analysis of the map.

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.

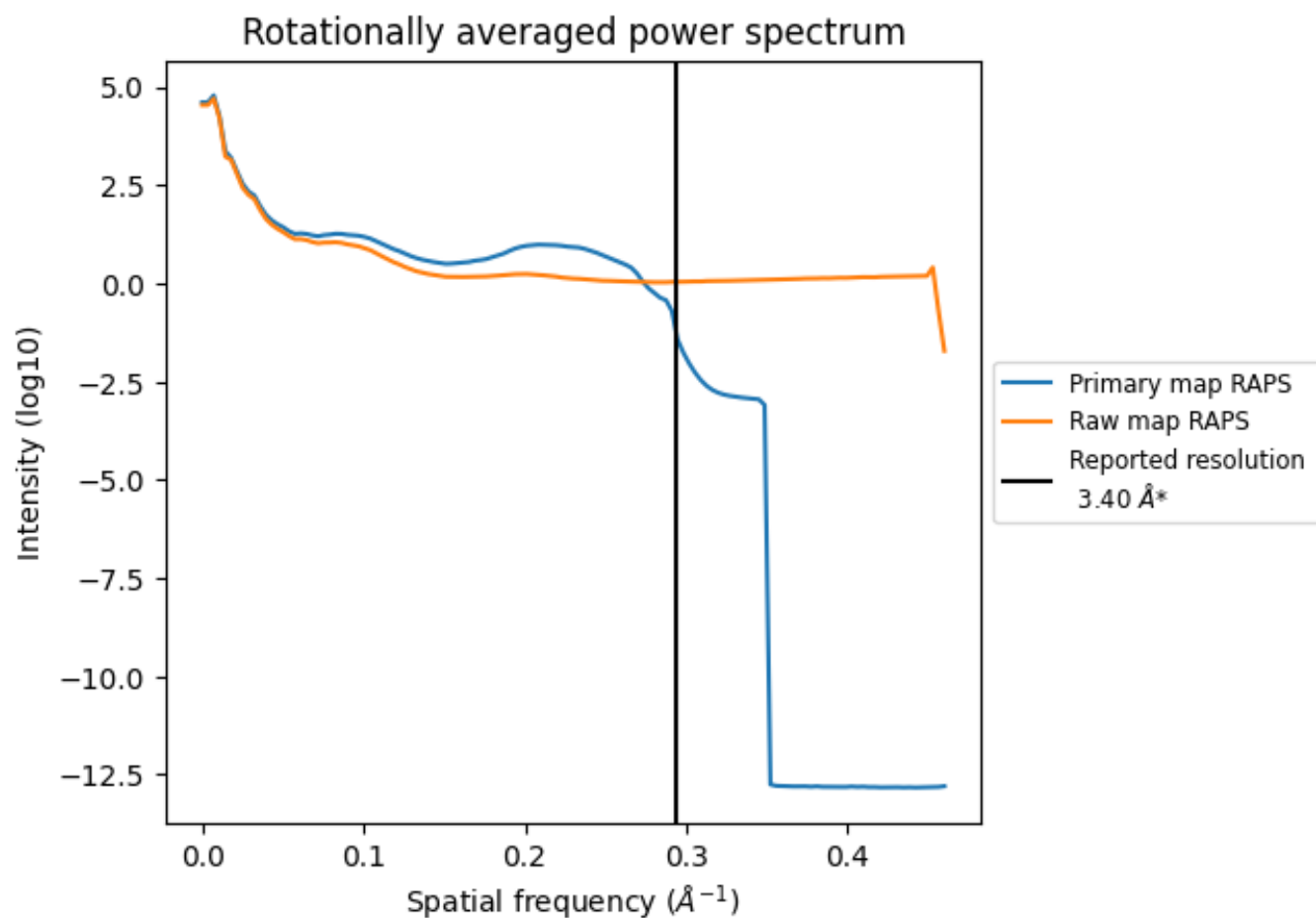
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 ⓘ

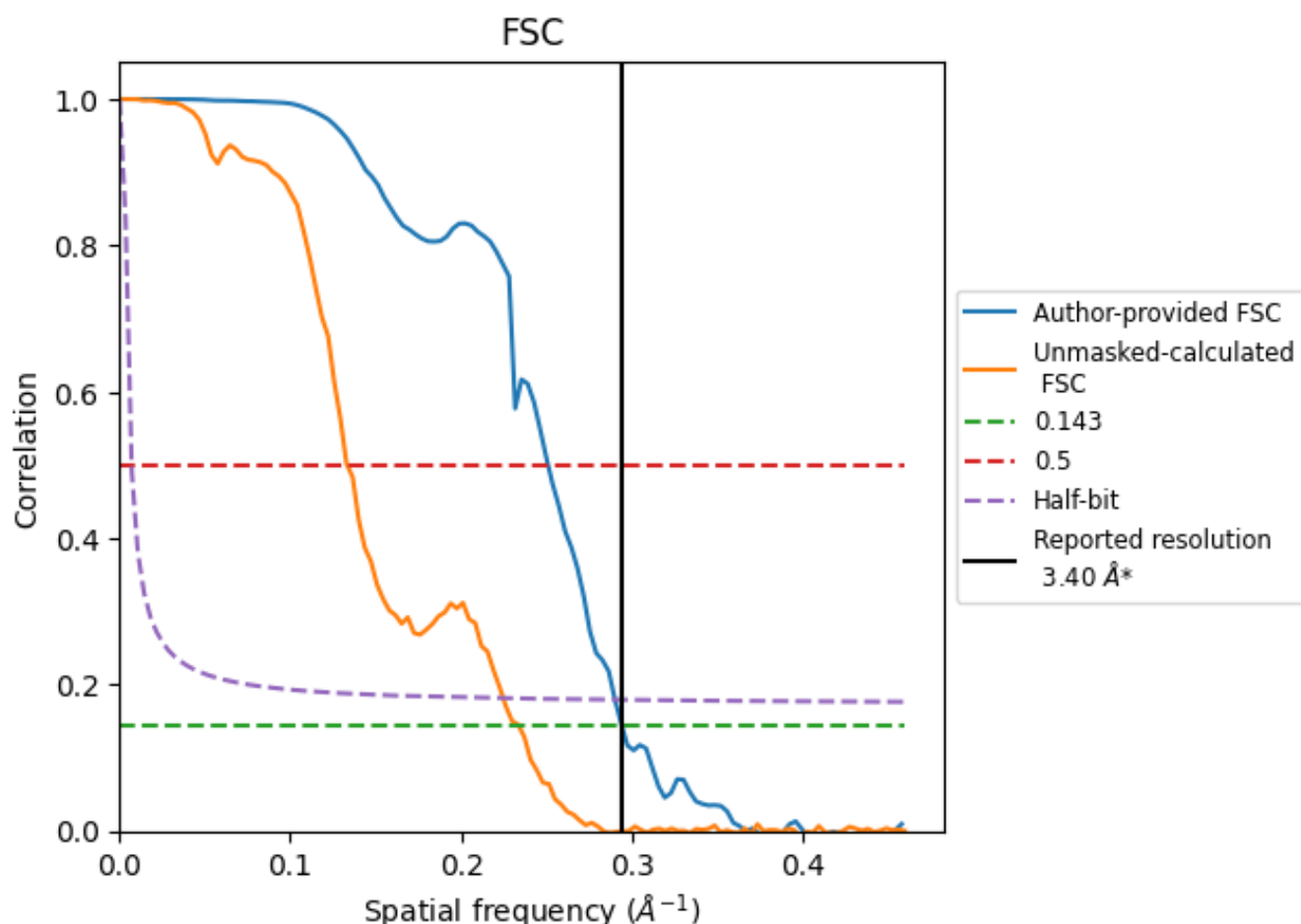


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

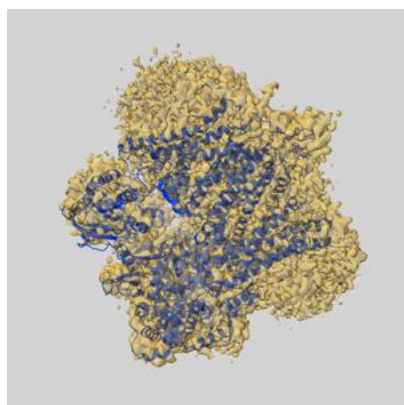
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.98	3.44
Unmasked-calculated*	4.27	7.50	4.45

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

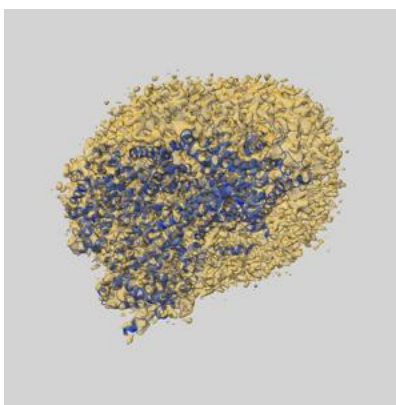
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37614 and PDB model 8WLA. Per-residue inclusion information can be found in section [3](#) on page [4](#).

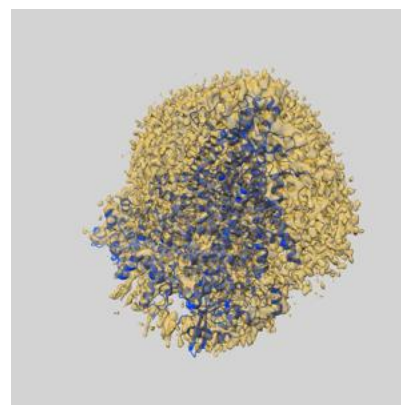
9.1 Map-model overlay [i](#)



X



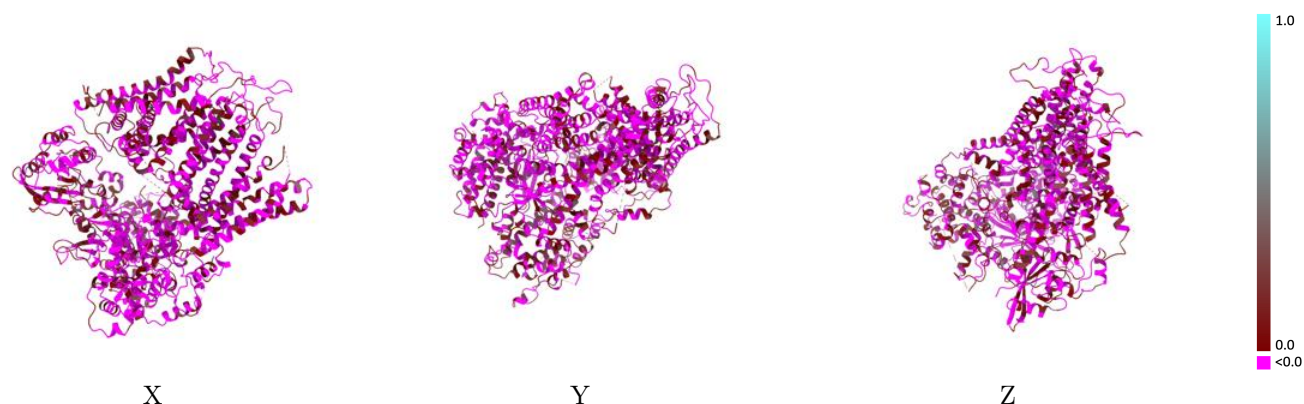
Y



Z

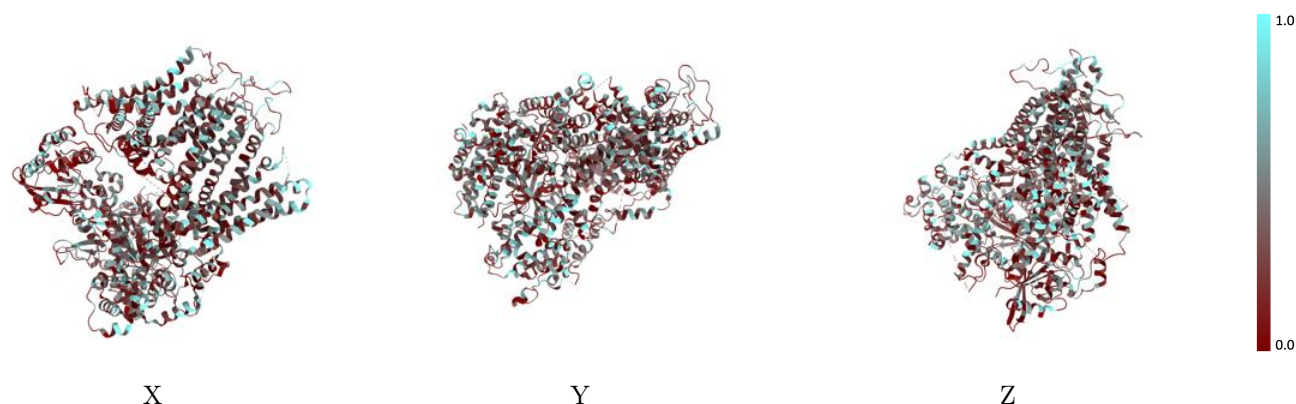
The images above show the 3D surface view of the map at the recommended contour level 0.229 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



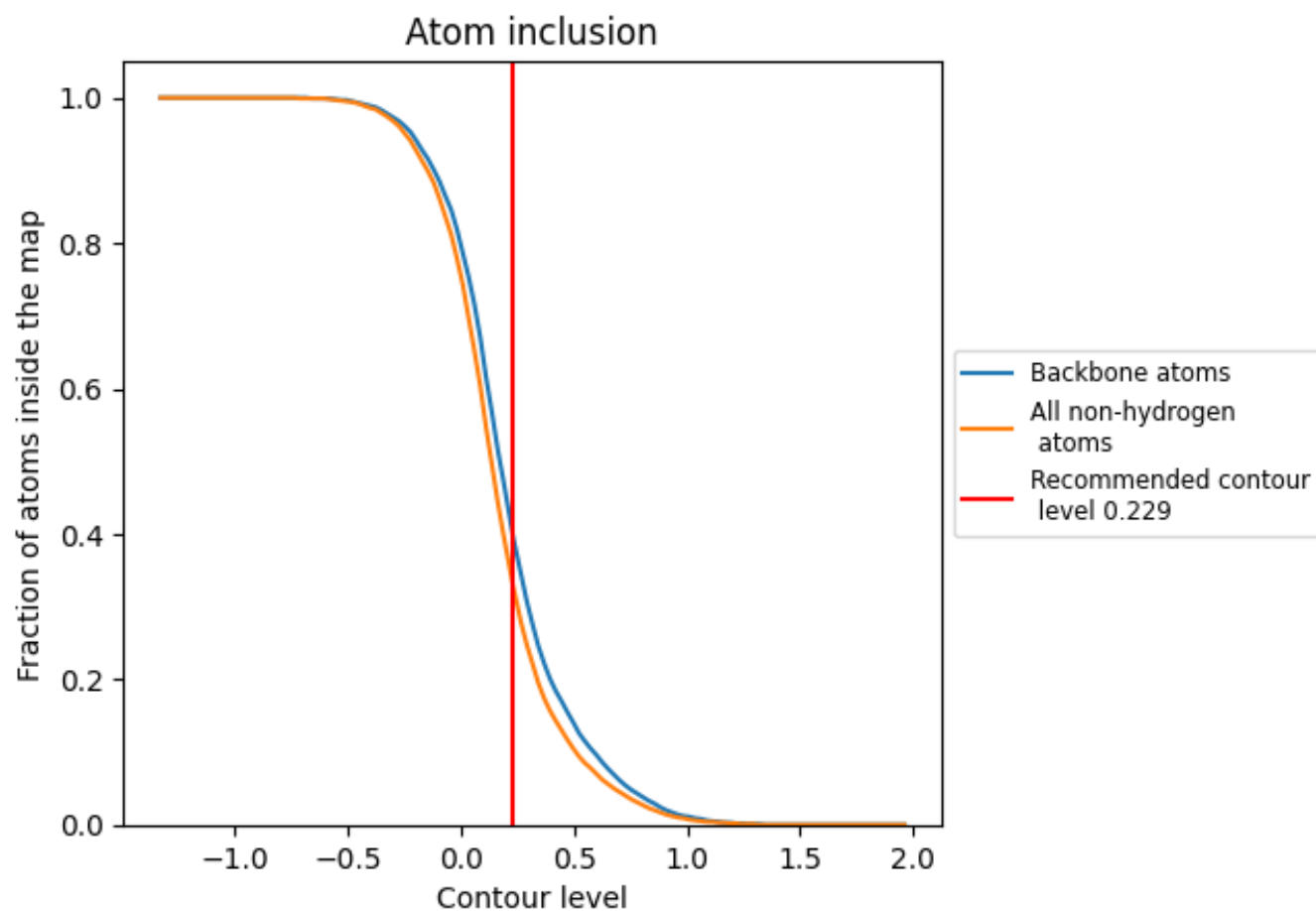
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.229).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 33% 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 (0.229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3290	<div></div> -0.0500
A	<div></div> 0.2520	<div></div> -0.0100
B	<div></div> 0.3380	<div></div> -0.0540

