



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:49 PM UTC

PDB ID : 8AQS / pdb_00008aqs
EMDB ID : EMD-15588
Title : BA.4/5 SARS-CoV-2 Spike bound to human ACE2 (local)
Authors : Lau, K.; Ni, D.; Beckert, B.; Nazarov, S.; Myasnikov, A.; Pojer, F.; Stahlberg, H.; Uchikawa, E.
Deposited on : 2022-08-13
Resolution : 2.92 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

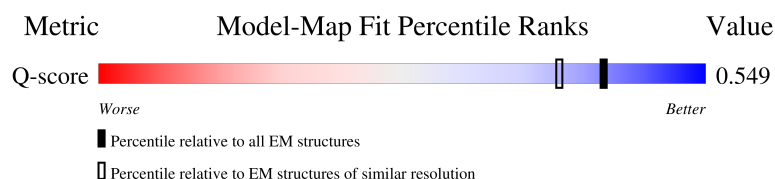
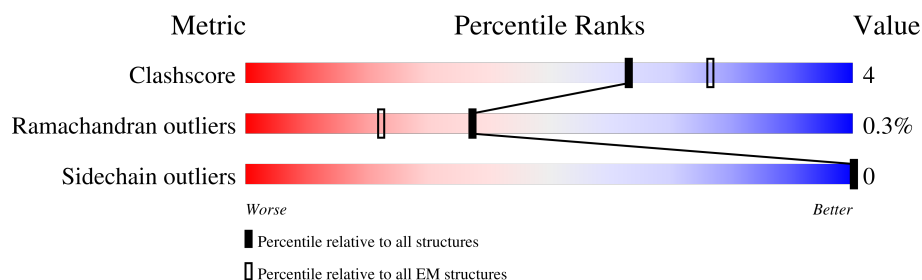
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	1288	
2	B	886	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6493 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	193	Total	C	N	O	S	0	0
			1543	994	261	280	8		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ALA	-	expression tag	UNP P10104
A	1260	TRP	-	expression tag	UNP P10104
A	1261	SER	-	expression tag	UNP P10104
A	1262	HIS	-	expression tag	UNP P10104
A	1263	PRO	-	expression tag	UNP P10104
A	1264	GLN	-	expression tag	UNP P10104
A	1265	PHE	-	expression tag	UNP P10104
A	1266	GLU	-	expression tag	UNP P10104
A	1267	LYS	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	595	Total	C	N	O	S	1	0
			4864	3113	806	916	29		

There are 287 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP Q9BYF1
B	-14	GLY	-	expression tag	UNP Q9BYF1
B	-13	THR	-	expression tag	UNP Q9BYF1
B	-12	LEU	-	expression tag	UNP Q9BYF1
B	-11	SER	-	expression tag	UNP Q9BYF1
B	-10	ALA	-	expression tag	UNP Q9BYF1
B	-9	PRO	-	expression tag	UNP Q9BYF1
B	-8	PRO	-	expression tag	UNP Q9BYF1
B	-7	CYS	-	expression tag	UNP Q9BYF1
B	-6	THR	-	expression tag	UNP Q9BYF1
B	-5	GLN	-	expression tag	UNP Q9BYF1
B	-4	ARG	-	expression tag	UNP Q9BYF1
B	-3	ILE	-	expression tag	UNP Q9BYF1
B	-2	LYS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	TRP	-	expression tag	UNP Q9BYF1
B	0	LYS	-	expression tag	UNP Q9BYF1
B	1	GLY	-	expression tag	UNP Q9BYF1
B	2	LEU	-	expression tag	UNP Q9BYF1
B	3	LEU	-	expression tag	UNP Q9BYF1
B	4	LEU	-	expression tag	UNP Q9BYF1
B	5	THR	-	expression tag	UNP Q9BYF1
B	6	ALA	-	expression tag	UNP Q9BYF1
B	7	SER	-	expression tag	UNP Q9BYF1
B	8	LEU	-	expression tag	UNP Q9BYF1
B	9	LEU	-	expression tag	UNP Q9BYF1
B	10	ASN	-	expression tag	UNP Q9BYF1
B	11	PHE	-	expression tag	UNP Q9BYF1
B	12	TRP	-	expression tag	UNP Q9BYF1
B	13	ASN	-	expression tag	UNP Q9BYF1
B	14	LEU	-	expression tag	UNP Q9BYF1
B	15	PRO	-	expression tag	UNP Q9BYF1
B	16	THR	-	expression tag	UNP Q9BYF1
B	17	THR	-	expression tag	UNP Q9BYF1
B	18	ALA	-	expression tag	UNP Q9BYF1
B	616	GLY	GLN	conflict	UNP Q9BYF1
B	618	LEU	ILE	conflict	UNP Q9BYF1
B	619	GLU	LYS	conflict	UNP Q9BYF1
B	621	LEU	-	expression tag	UNP Q9BYF1
B	622	PHE	-	expression tag	UNP Q9BYF1
B	623	GLN	-	expression tag	UNP Q9BYF1
B	624	GLY	-	expression tag	UNP Q9BYF1
B	625	PRO	-	expression tag	UNP Q9BYF1
B	626	MET	-	expression tag	UNP Q9BYF1
B	627	ASP	-	expression tag	UNP Q9BYF1
B	628	GLU	-	expression tag	UNP Q9BYF1
B	629	PRO	-	expression tag	UNP Q9BYF1
B	630	ARG	-	expression tag	UNP Q9BYF1
B	631	GLY	-	expression tag	UNP Q9BYF1
B	632	PRO	-	expression tag	UNP Q9BYF1
B	633	THR	-	expression tag	UNP Q9BYF1
B	634	ILE	-	expression tag	UNP Q9BYF1
B	635	LYS	-	expression tag	UNP Q9BYF1
B	636	PRO	-	expression tag	UNP Q9BYF1
B	637	CYS	-	expression tag	UNP Q9BYF1
B	638	PRO	-	expression tag	UNP Q9BYF1
B	639	PRO	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	640	CYS	-	expression tag	UNP Q9BYF1
B	641	LYS	-	expression tag	UNP Q9BYF1
B	642	CYS	-	expression tag	UNP Q9BYF1
B	643	PRO	-	expression tag	UNP Q9BYF1
B	644	ALA	-	expression tag	UNP Q9BYF1
B	645	PRO	-	expression tag	UNP Q9BYF1
B	646	ASN	-	expression tag	UNP Q9BYF1
B	647	LEU	-	expression tag	UNP Q9BYF1
B	648	LEU	-	expression tag	UNP Q9BYF1
B	649	GLY	-	expression tag	UNP Q9BYF1
B	650	GLY	-	expression tag	UNP Q9BYF1
B	651	PRO	-	expression tag	UNP Q9BYF1
B	652	SER	-	expression tag	UNP Q9BYF1
B	653	VAL	-	expression tag	UNP Q9BYF1
B	654	PHE	-	expression tag	UNP Q9BYF1
B	655	ILE	-	expression tag	UNP Q9BYF1
B	656	PHE	-	expression tag	UNP Q9BYF1
B	657	PRO	-	expression tag	UNP Q9BYF1
B	658	PRO	-	expression tag	UNP Q9BYF1
B	659	LYS	-	expression tag	UNP Q9BYF1
B	660	ILE	-	expression tag	UNP Q9BYF1
B	661	LYS	-	expression tag	UNP Q9BYF1
B	662	ASP	-	expression tag	UNP Q9BYF1
B	663	VAL	-	expression tag	UNP Q9BYF1
B	664	LEU	-	expression tag	UNP Q9BYF1
B	665	MET	-	expression tag	UNP Q9BYF1
B	666	ILE	-	expression tag	UNP Q9BYF1
B	667	SER	-	expression tag	UNP Q9BYF1
B	668	LEU	-	expression tag	UNP Q9BYF1
B	669	SER	-	expression tag	UNP Q9BYF1
B	670	PRO	-	expression tag	UNP Q9BYF1
B	671	ILE	-	expression tag	UNP Q9BYF1
B	672	VAL	-	expression tag	UNP Q9BYF1
B	673	THR	-	expression tag	UNP Q9BYF1
B	674	CYS	-	expression tag	UNP Q9BYF1
B	675	VAL	-	expression tag	UNP Q9BYF1
B	676	VAL	-	expression tag	UNP Q9BYF1
B	677	VAL	-	expression tag	UNP Q9BYF1
B	678	ASP	-	expression tag	UNP Q9BYF1
B	679	VAL	-	expression tag	UNP Q9BYF1
B	680	SER	-	expression tag	UNP Q9BYF1
B	681	GLU	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	ASP	-	expression tag	UNP Q9BYF1
B	683	ASP	-	expression tag	UNP Q9BYF1
B	684	PRO	-	expression tag	UNP Q9BYF1
B	685	ASP	-	expression tag	UNP Q9BYF1
B	686	VAL	-	expression tag	UNP Q9BYF1
B	687	GLN	-	expression tag	UNP Q9BYF1
B	688	ILE	-	expression tag	UNP Q9BYF1
B	689	SER	-	expression tag	UNP Q9BYF1
B	690	TRP	-	expression tag	UNP Q9BYF1
B	691	PHE	-	expression tag	UNP Q9BYF1
B	692	VAL	-	expression tag	UNP Q9BYF1
B	693	ASN	-	expression tag	UNP Q9BYF1
B	694	ASN	-	expression tag	UNP Q9BYF1
B	695	VAL	-	expression tag	UNP Q9BYF1
B	696	GLU	-	expression tag	UNP Q9BYF1
B	697	VAL	-	expression tag	UNP Q9BYF1
B	698	HIS	-	expression tag	UNP Q9BYF1
B	699	THR	-	expression tag	UNP Q9BYF1
B	700	ALA	-	expression tag	UNP Q9BYF1
B	701	GLN	-	expression tag	UNP Q9BYF1
B	702	THR	-	expression tag	UNP Q9BYF1
B	703	GLN	-	expression tag	UNP Q9BYF1
B	704	THR	-	expression tag	UNP Q9BYF1
B	705	HIS	-	expression tag	UNP Q9BYF1
B	706	ARG	-	expression tag	UNP Q9BYF1
B	707	GLU	-	expression tag	UNP Q9BYF1
B	708	ASP	-	expression tag	UNP Q9BYF1
B	709	TYR	-	expression tag	UNP Q9BYF1
B	710	ASN	-	expression tag	UNP Q9BYF1
B	711	SER	-	expression tag	UNP Q9BYF1
B	712	THR	-	expression tag	UNP Q9BYF1
B	713	LEU	-	expression tag	UNP Q9BYF1
B	714	ARG	-	expression tag	UNP Q9BYF1
B	715	VAL	-	expression tag	UNP Q9BYF1
B	716	VAL	-	expression tag	UNP Q9BYF1
B	717	SER	-	expression tag	UNP Q9BYF1
B	718	ALA	-	expression tag	UNP Q9BYF1
B	719	LEU	-	expression tag	UNP Q9BYF1
B	720	PRO	-	expression tag	UNP Q9BYF1
B	721	ILE	-	expression tag	UNP Q9BYF1
B	722	GLN	-	expression tag	UNP Q9BYF1
B	723	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	724	GLN	-	expression tag	UNP Q9BYF1
B	725	ASP	-	expression tag	UNP Q9BYF1
B	726	TRP	-	expression tag	UNP Q9BYF1
B	727	MET	-	expression tag	UNP Q9BYF1
B	728	SER	-	expression tag	UNP Q9BYF1
B	729	GLY	-	expression tag	UNP Q9BYF1
B	730	LYS	-	expression tag	UNP Q9BYF1
B	731	GLU	-	expression tag	UNP Q9BYF1
B	732	PHE	-	expression tag	UNP Q9BYF1
B	733	LYS	-	expression tag	UNP Q9BYF1
B	734	CYS	-	expression tag	UNP Q9BYF1
B	735	LYS	-	expression tag	UNP Q9BYF1
B	736	VAL	-	expression tag	UNP Q9BYF1
B	737	ASN	-	expression tag	UNP Q9BYF1
B	738	ASN	-	expression tag	UNP Q9BYF1
B	739	LYS	-	expression tag	UNP Q9BYF1
B	740	ASP	-	expression tag	UNP Q9BYF1
B	741	LEU	-	expression tag	UNP Q9BYF1
B	742	PRO	-	expression tag	UNP Q9BYF1
B	743	ALA	-	expression tag	UNP Q9BYF1
B	744	PRO	-	expression tag	UNP Q9BYF1
B	745	ILE	-	expression tag	UNP Q9BYF1
B	746	GLU	-	expression tag	UNP Q9BYF1
B	747	ARG	-	expression tag	UNP Q9BYF1
B	748	THR	-	expression tag	UNP Q9BYF1
B	749	ILE	-	expression tag	UNP Q9BYF1
B	750	SER	-	expression tag	UNP Q9BYF1
B	751	LYS	-	expression tag	UNP Q9BYF1
B	752	PRO	-	expression tag	UNP Q9BYF1
B	753	LYS	-	expression tag	UNP Q9BYF1
B	754	GLY	-	expression tag	UNP Q9BYF1
B	755	SER	-	expression tag	UNP Q9BYF1
B	756	VAL	-	expression tag	UNP Q9BYF1
B	757	ARG	-	expression tag	UNP Q9BYF1
B	758	ALA	-	expression tag	UNP Q9BYF1
B	759	PRO	-	expression tag	UNP Q9BYF1
B	760	GLN	-	expression tag	UNP Q9BYF1
B	761	VAL	-	expression tag	UNP Q9BYF1
B	762	TYR	-	expression tag	UNP Q9BYF1
B	763	VAL	-	expression tag	UNP Q9BYF1
B	764	LEU	-	expression tag	UNP Q9BYF1
B	765	PRO	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	766	PRO	-	expression tag	UNP Q9BYF1
B	767	PRO	-	expression tag	UNP Q9BYF1
B	768	GLU	-	expression tag	UNP Q9BYF1
B	769	GLU	-	expression tag	UNP Q9BYF1
B	770	GLU	-	expression tag	UNP Q9BYF1
B	771	MET	-	expression tag	UNP Q9BYF1
B	772	THR	-	expression tag	UNP Q9BYF1
B	773	LYS	-	expression tag	UNP Q9BYF1
B	774	LYS	-	expression tag	UNP Q9BYF1
B	775	GLN	-	expression tag	UNP Q9BYF1
B	776	VAL	-	expression tag	UNP Q9BYF1
B	777	THR	-	expression tag	UNP Q9BYF1
B	778	LEU	-	expression tag	UNP Q9BYF1
B	779	THR	-	expression tag	UNP Q9BYF1
B	780	CYS	-	expression tag	UNP Q9BYF1
B	781	MET	-	expression tag	UNP Q9BYF1
B	782	VAL	-	expression tag	UNP Q9BYF1
B	783	THR	-	expression tag	UNP Q9BYF1
B	784	ASP	-	expression tag	UNP Q9BYF1
B	785	PHE	-	expression tag	UNP Q9BYF1
B	786	MET	-	expression tag	UNP Q9BYF1
B	787	PRO	-	expression tag	UNP Q9BYF1
B	788	GLU	-	expression tag	UNP Q9BYF1
B	789	ASP	-	expression tag	UNP Q9BYF1
B	790	ILE	-	expression tag	UNP Q9BYF1
B	791	TYR	-	expression tag	UNP Q9BYF1
B	792	VAL	-	expression tag	UNP Q9BYF1
B	793	GLU	-	expression tag	UNP Q9BYF1
B	794	TRP	-	expression tag	UNP Q9BYF1
B	795	THR	-	expression tag	UNP Q9BYF1
B	796	ASN	-	expression tag	UNP Q9BYF1
B	797	ASN	-	expression tag	UNP Q9BYF1
B	798	GLY	-	expression tag	UNP Q9BYF1
B	799	LYS	-	expression tag	UNP Q9BYF1
B	800	THR	-	expression tag	UNP Q9BYF1
B	801	GLU	-	expression tag	UNP Q9BYF1
B	802	LEU	-	expression tag	UNP Q9BYF1
B	803	ASN	-	expression tag	UNP Q9BYF1
B	804	TYR	-	expression tag	UNP Q9BYF1
B	805	LYS	-	expression tag	UNP Q9BYF1
B	806	ASN	-	expression tag	UNP Q9BYF1
B	807	THR	-	expression tag	UNP Q9BYF1

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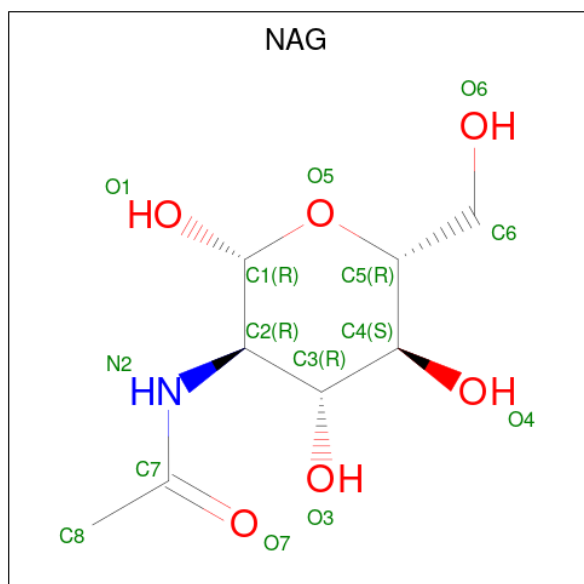
Chain	Residue	Modelled	Actual	Comment	Reference
B	808	GLU	-	expression tag	UNP Q9BYF1
B	809	PRO	-	expression tag	UNP Q9BYF1
B	810	VAL	-	expression tag	UNP Q9BYF1
B	811	LEU	-	expression tag	UNP Q9BYF1
B	812	ASP	-	expression tag	UNP Q9BYF1
B	813	SER	-	expression tag	UNP Q9BYF1
B	814	ASP	-	expression tag	UNP Q9BYF1
B	815	GLY	-	expression tag	UNP Q9BYF1
B	816	SER	-	expression tag	UNP Q9BYF1
B	817	TYR	-	expression tag	UNP Q9BYF1
B	818	PHE	-	expression tag	UNP Q9BYF1
B	819	MET	-	expression tag	UNP Q9BYF1
B	820	TYR	-	expression tag	UNP Q9BYF1
B	821	SER	-	expression tag	UNP Q9BYF1
B	822	LYS	-	expression tag	UNP Q9BYF1
B	823	LEU	-	expression tag	UNP Q9BYF1
B	824	ARG	-	expression tag	UNP Q9BYF1
B	825	VAL	-	expression tag	UNP Q9BYF1
B	826	GLU	-	expression tag	UNP Q9BYF1
B	827	LYS	-	expression tag	UNP Q9BYF1
B	828	LYS	-	expression tag	UNP Q9BYF1
B	829	ASN	-	expression tag	UNP Q9BYF1
B	830	TRP	-	expression tag	UNP Q9BYF1
B	831	VAL	-	expression tag	UNP Q9BYF1
B	832	GLU	-	expression tag	UNP Q9BYF1
B	833	ARG	-	expression tag	UNP Q9BYF1
B	834	ASN	-	expression tag	UNP Q9BYF1
B	835	SER	-	expression tag	UNP Q9BYF1
B	836	TYR	-	expression tag	UNP Q9BYF1
B	837	SER	-	expression tag	UNP Q9BYF1
B	838	CYS	-	expression tag	UNP Q9BYF1
B	839	SER	-	expression tag	UNP Q9BYF1
B	840	VAL	-	expression tag	UNP Q9BYF1
B	841	VAL	-	expression tag	UNP Q9BYF1
B	842	HIS	-	expression tag	UNP Q9BYF1
B	843	GLU	-	expression tag	UNP Q9BYF1
B	844	GLY	-	expression tag	UNP Q9BYF1
B	845	LEU	-	expression tag	UNP Q9BYF1
B	846	HIS	-	expression tag	UNP Q9BYF1
B	847	ASN	-	expression tag	UNP Q9BYF1
B	848	HIS	-	expression tag	UNP Q9BYF1
B	849	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	850	THR	-	expression tag	UNP Q9BYF1
B	851	THR	-	expression tag	UNP Q9BYF1
B	852	LYS	-	expression tag	UNP Q9BYF1
B	853	SER	-	expression tag	UNP Q9BYF1
B	854	PHE	-	expression tag	UNP Q9BYF1
B	855	SER	-	expression tag	UNP Q9BYF1
B	856	ARG	-	expression tag	UNP Q9BYF1
B	857	THR	-	expression tag	UNP Q9BYF1
B	858	PRO	-	expression tag	UNP Q9BYF1
B	859	GLY	-	expression tag	UNP Q9BYF1
B	860	LYS	-	expression tag	UNP Q9BYF1
B	861	HIS	-	expression tag	UNP Q9BYF1
B	862	HIS	-	expression tag	UNP Q9BYF1
B	863	HIS	-	expression tag	UNP Q9BYF1
B	864	HIS	-	expression tag	UNP Q9BYF1
B	865	HIS	-	expression tag	UNP Q9BYF1
B	866	HIS	-	expression tag	UNP Q9BYF1
B	867	HIS	-	expression tag	UNP Q9BYF1
B	868	HIS	-	expression tag	UNP Q9BYF1
B	869	HIS	-	expression tag	UNP Q9BYF1
B	870	HIS	-	expression tag	UNP Q9BYF1

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

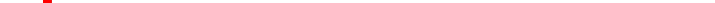
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	

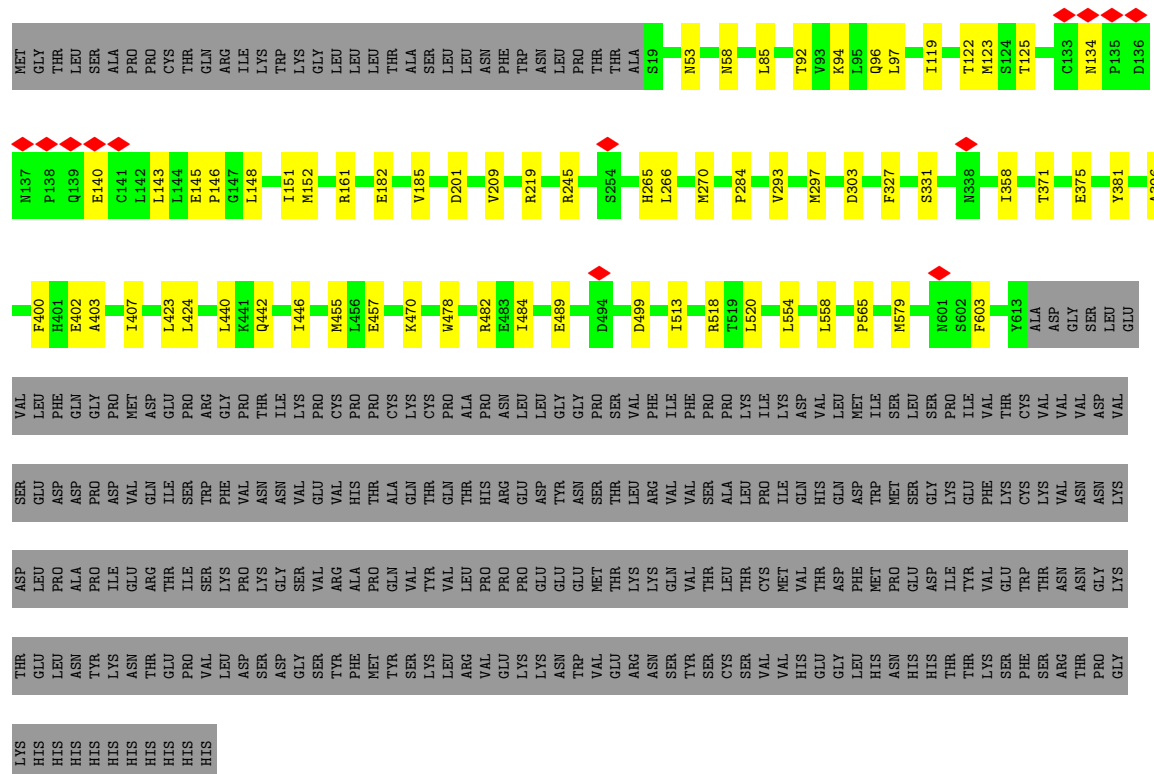
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	O	0
			1	1	

[illegible]

- Molecule 2: Processed angiotensin-converting enzyme 2

Chain B:  60% 7% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94718	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.294	Depositor
Minimum map value	-1.742	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	365.184, 365.184, 365.184	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0144, 1.0144, 1.0144	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: NAG, 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	0.12	0/1589	0.33	0/2163
2	B	0.11	0/5005	0.29	0/6800
All	All	0.11	0/6594	0.30	0/8963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1543	0	1466	13	0
2	B	4864	0	4642	40	0
3	A	14	0	13	1	0
3	B	70	0	65	0	0
4	B	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6493	0	6186	53	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 4.

All (53) 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:454:ARG:NH2	1:A:469:SER:O	2.31	0.62
2:B:145:GLU:HB2	2:B:146:PRO:HD3	1.83	0.58
2:B:331:SER:OG	2:B:358:ILE:O	2.23	0.56
1:A:350:VAL:HG12	1:A:422:ASN:HB3	1.88	0.56
2:B:143:LEU:HG	2:B:146:PRO:HD2	1.89	0.54
1:A:392:PHE:HD1	1:A:517:LEU:HB2	1.72	0.54
2:B:119:ILE:HG22	2:B:123:MET:HE2	1.91	0.53
2:B:53:ASN:O	2:B:58:ASN:ND2	2.39	0.52
1:A:343:ASN:HB2	3:A:1301:NAG:H2	1.91	0.52
1:A:372:ALA:HB3	1:A:373:PRO:HD3	1.90	0.52
2:B:245:ARG:NH2	2:B:603:PHE:O	2.43	0.52
2:B:201:ASP:OD2	2:B:219:ARG:NE	2.44	0.51
2:B:457:GLU:HG2	2:B:513:ILE:HD13	1.93	0.49
2:B:396:ALA:HB3	2:B:400:PHE:CE2	2.48	0.49
2:B:182:GLU:HA	2:B:185:VAL:HG12	1.95	0.48
2:B:293:VAL:HG12	2:B:297:MET:HG3	1.96	0.47
2:B:209:VAL:HG11	2:B:565:PRO:HB3	1.95	0.47
2:B:303:ASP:N	2:B:303:ASP:OD1	2.46	0.47
1:A:353:TRP:O	1:A:466:ARG:NH1	2.48	0.47
2:B:520:LEU:HD23	2:B:579:MET:HB3	1.96	0.46
2:B:455:MET:HG3	2:B:484:ILE:HD12	1.98	0.46
2:B:293:VAL:HG11	2:B:423:LEU:HD13	1.96	0.45
2:B:122:THR:HA	2:B:125:THR:HG22	1.98	0.45
2:B:97:LEU:HD23	2:B:97:LEU:HA	1.80	0.45
1:A:394:ASN:OD1	1:A:516:GLU:HB3	2.17	0.45
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.25	0.45
2:B:134:ASN:HD21	2:B:140:GLU:HB3	1.82	0.45
2:B:482:ARG:HH21	2:B:489:GLU:HG2	1.81	0.45
2:B:284:PRO:HG3	2:B:440:LEU:HD13	2.00	0.44
1:A:502:GLY:O	1:A:506:GLN:HG3	2.16	0.44
2:B:371:THR:O	2:B:375:GLU:HG2	2.18	0.44
2:B:143:LEU:HD23	2:B:143:LEU:H	1.82	0.44
2:B:402:GLU:HB2	2:B:518:ARG:HG3	2.00	0.44
2:B:381:TYR:CD1	2:B:558:LEU:HD22	2.52	0.44
1:A:365:TYR:CG	1:A:386:LYS:HG2	2.53	0.44
2:B:403:ALA:O	2:B:407:ILE:HG23	2.18	0.44
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.84	0.43
2:B:148:LEU:HA	2:B:151:ILE:HG22	1.99	0.43
2:B:161:ARG:HG3	2:B:265:HIS:HD2	1.84	0.43
2:B:161:ARG:HD3	2:B:266:LEU:HD23	2.00	0.43
2:B:478:TRP:NE1	2:B:499:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:MET:HE2	2:B:270:MET:HA	2.01	0.42
2:B:381:TYR:CE1	2:B:558:LEU:HD22	2.53	0.42
2:B:85:LEU:HD11	2:B:94:LYS:HG3	2.01	0.42
2:B:92:THR:O	2:B:96:GLN:HG3	2.21	0.41
2:B:424:LEU:HD23	2:B:424:LEU:HA	1.92	0.41
2:B:442:GLN:HG2	2:B:446:ILE:HD12	2.03	0.40
2:B:554:LEU:O	2:B:558:LEU:HG	2.21	0.40
1:A:354:ASN:O	1:A:398:ASP:HA	2.22	0.40
2:B:327:PHE:HE1	2:B:358:ILE:HG13	1.86	0.40
2:B:152:MET:HG3	2:B:270:MET:HE2	2.03	0.40
2:B:470:LYS:HB2	2:B:470:LYS:HE2	1.82	0.40
1:A:438:SER:OG	1:A:442:ASP:OD2	2.34	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	191/1288 (15%)	175 (92%)	14 (7%)	2 (1%)	12	37
2	B	594/886 (67%)	585 (98%)	9 (2%)	0	100	100
All	All	785/2174 (36%)	760 (97%)	23 (3%)	2 (0%)	37	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	ALA
1	A	486	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	A	166/1112 (15%)	166 (100%)	0	100	100
2	B	527/795 (66%)	527 (100%)	0	100	100
All	All	693/1907 (36%)	693 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	439	ASN
1	A	487	ASN
1	A	519	HIS
2	B	33	ASN
2	B	121	ASN
2	B	345	HIS
2	B	401	HIS
2	B	429	GLN
2	B	552	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	NAG	B	903	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	B	905	2	14,14,15	0.42	0	17,19,21	0.38	0
3	NAG	B	901	2	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	B	902	2	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	B	904	2	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.37	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
3	NAG	B	903	2	-	2/6/23/26	0/1/1/1
3	NAG	B	905	2	-	2/6/23/26	0/1/1/1
3	NAG	B	901	2	-	2/6/23/26	0/1/1/1
3	NAG	B	902	2	-	1/6/23/26	0/1/1/1
3	NAG	B	904	2	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	903	NAG	C4-C5-C6-O6
3	B	905	NAG	C4-C5-C6-O6
3	B	901	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	903	NAG	O5-C5-C6-O6
3	B	905	NAG	O5-C5-C6-O6
3	B	901	NAG	O5-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	904	NAG	O5-C5-C6-O6
3	B	904	NAG	C4-C5-C6-O6
3	B	904	NAG	C1-C2-N2-C7
3	B	904	NAG	C3-C2-N2-C7
3	B	902	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	NAG	1	0

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.

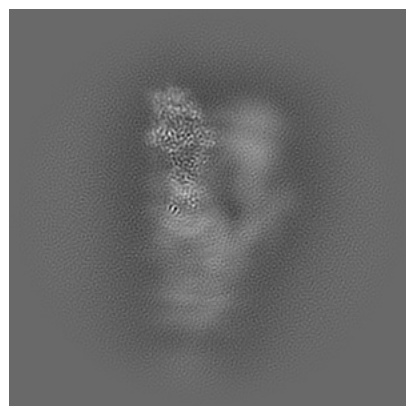
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15588. These allow visual inspection of the internal detail of the map and identification of artifacts.

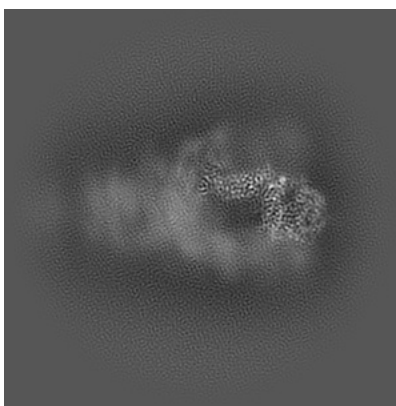
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

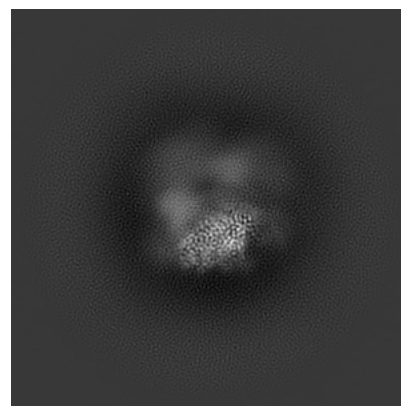
6.1.1 Primary map



X

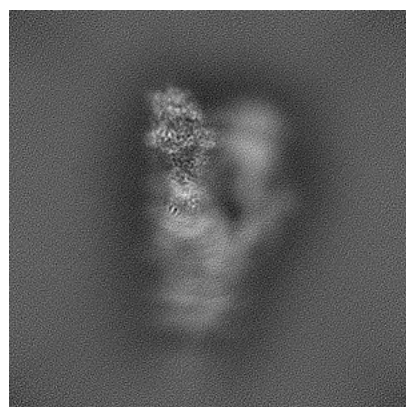


Y

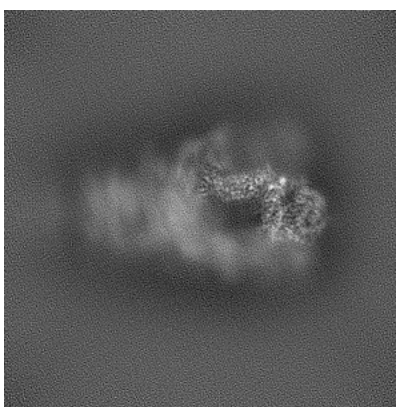


Z

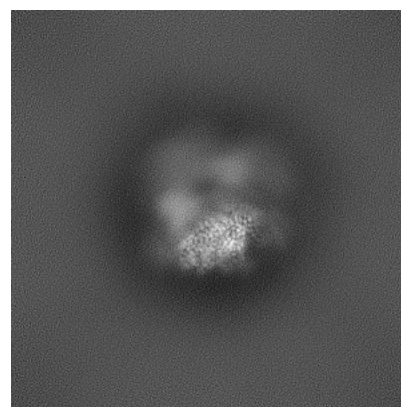
6.1.2 Raw map



X



Y

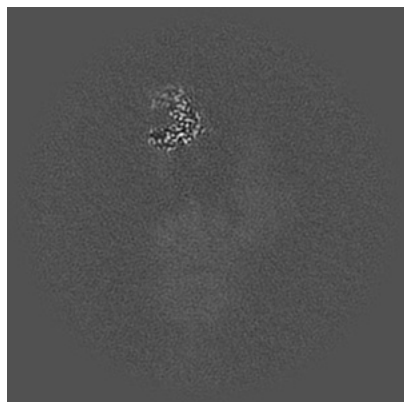


Z

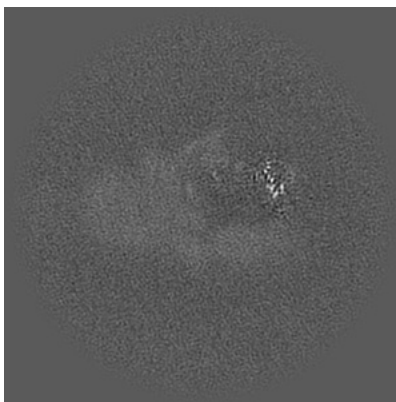
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

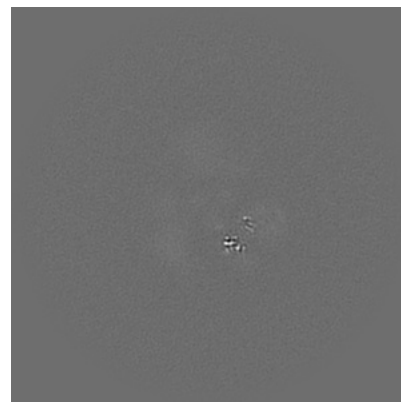
6.2.1 Primary map



X Index: 180

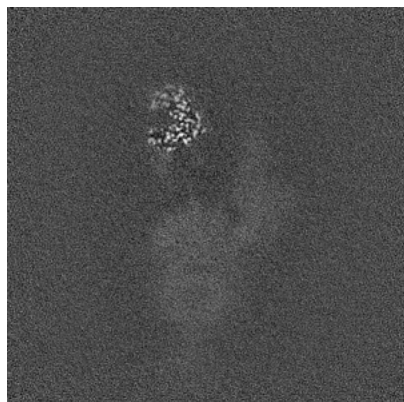


Y Index: 180

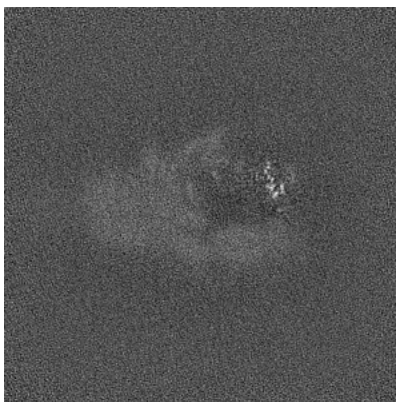


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

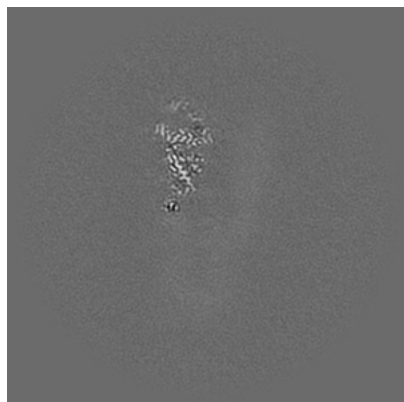


Z Index: 180

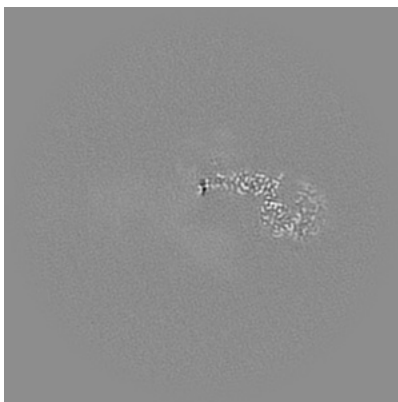
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

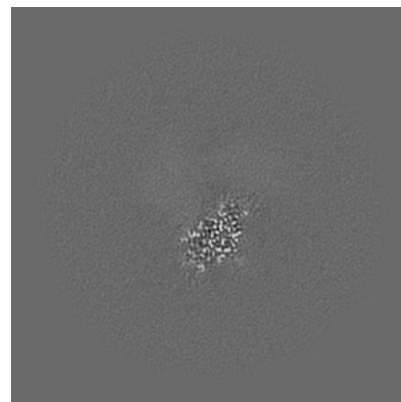
6.3.1 Primary map



X Index: 200

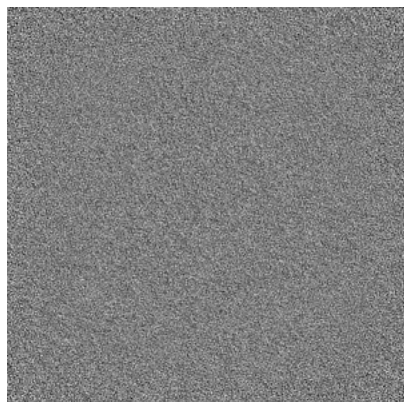


Y Index: 149

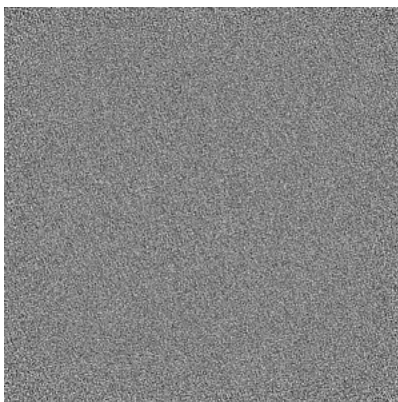


Z Index: 243

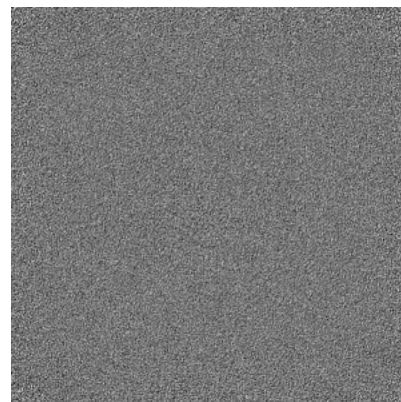
6.3.2 Raw map



X Index: 0



Y Index: 0

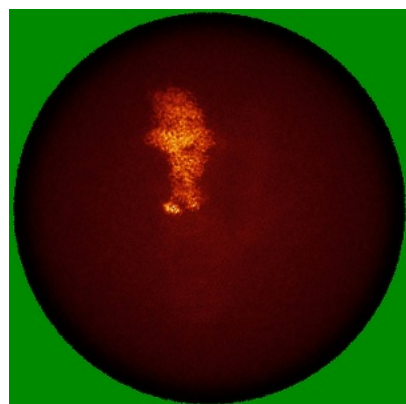


Z Index: 0

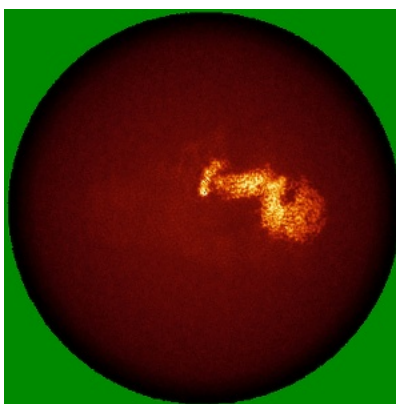
The images above show the largest variance slices of the map in three orthogonal directions.

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

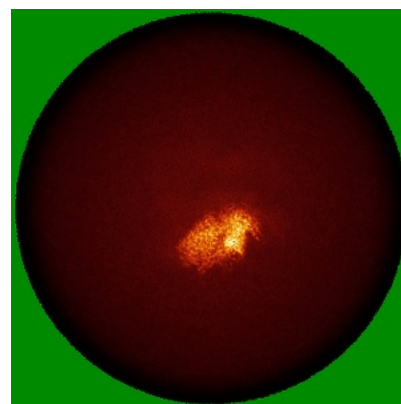
6.4.1 Primary map



X

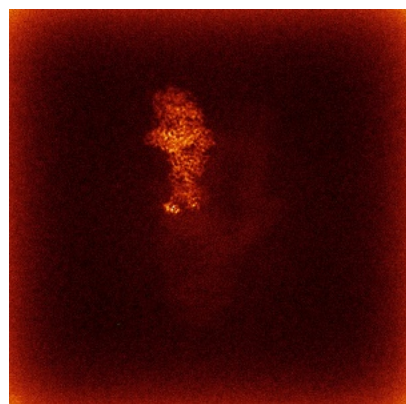


Y

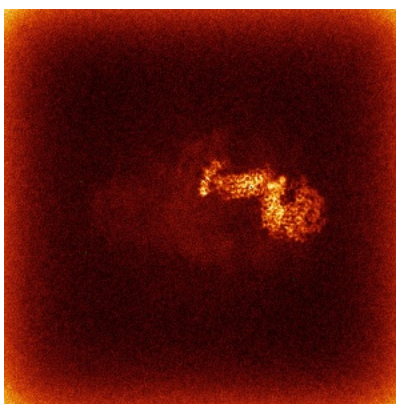


Z

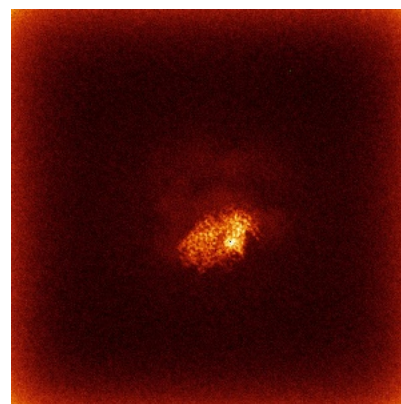
6.4.2 Raw map



X



Y

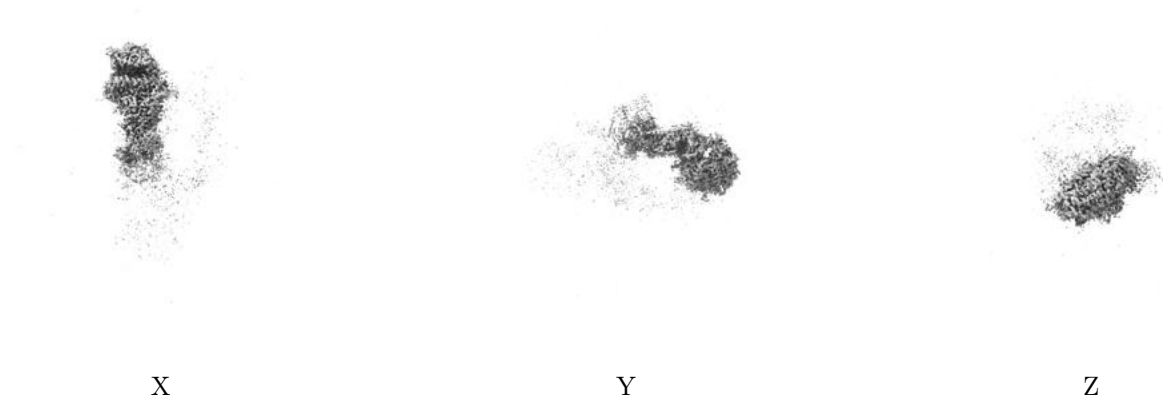


Z

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.

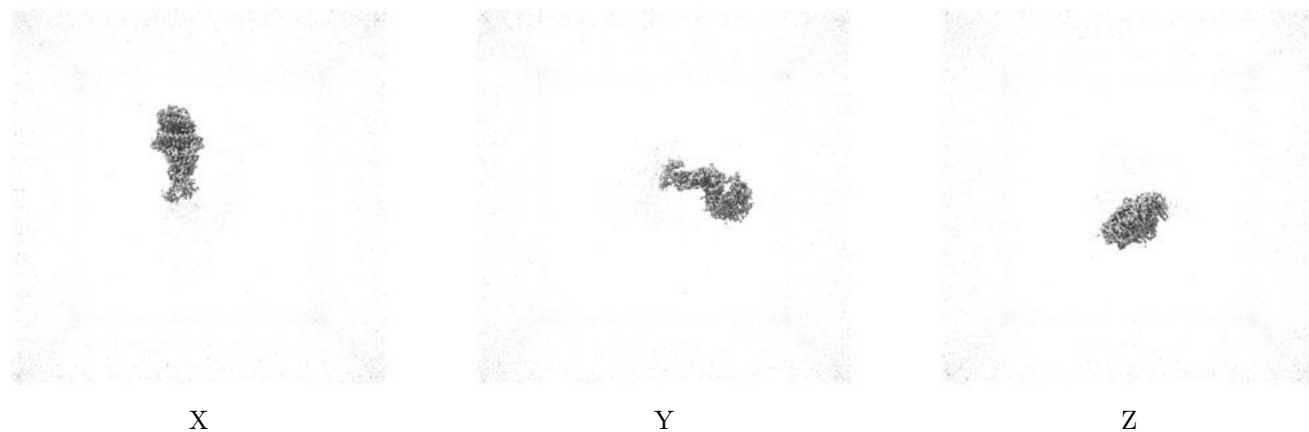
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

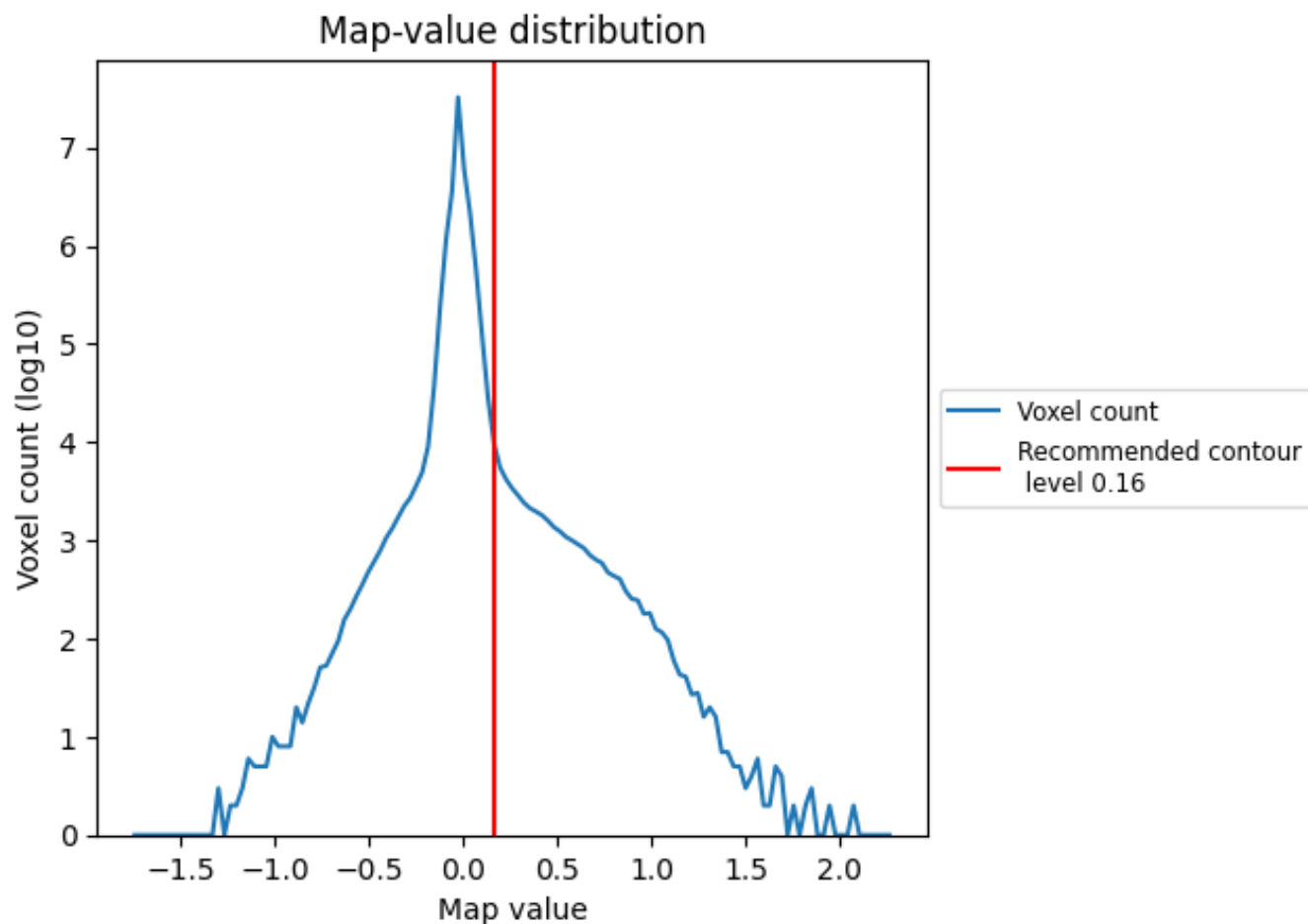
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

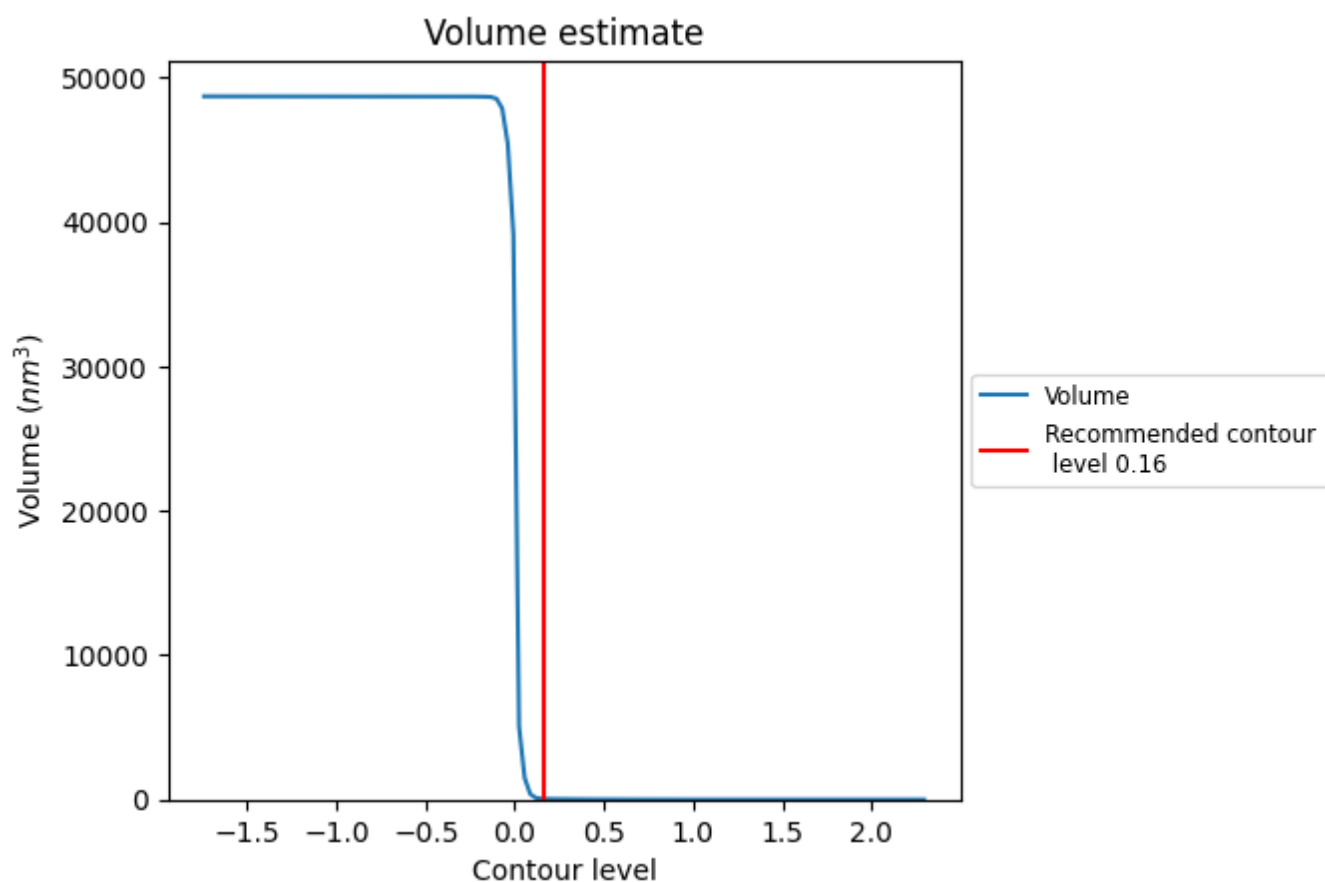
This section contains the results of statistical analysis of the map.

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.

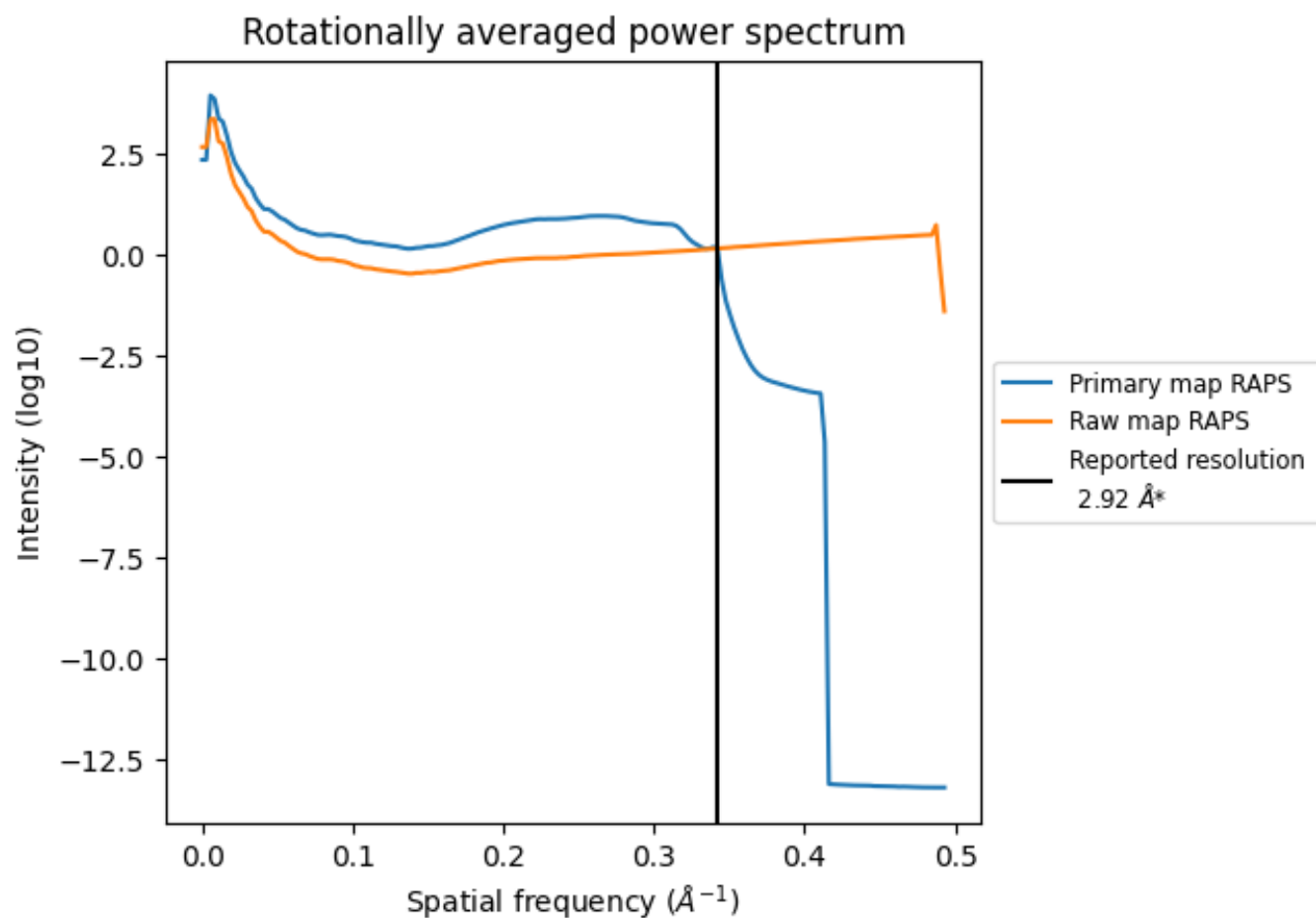
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm^3 ; this corresponds to an approximate mass of 48 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 ⓘ

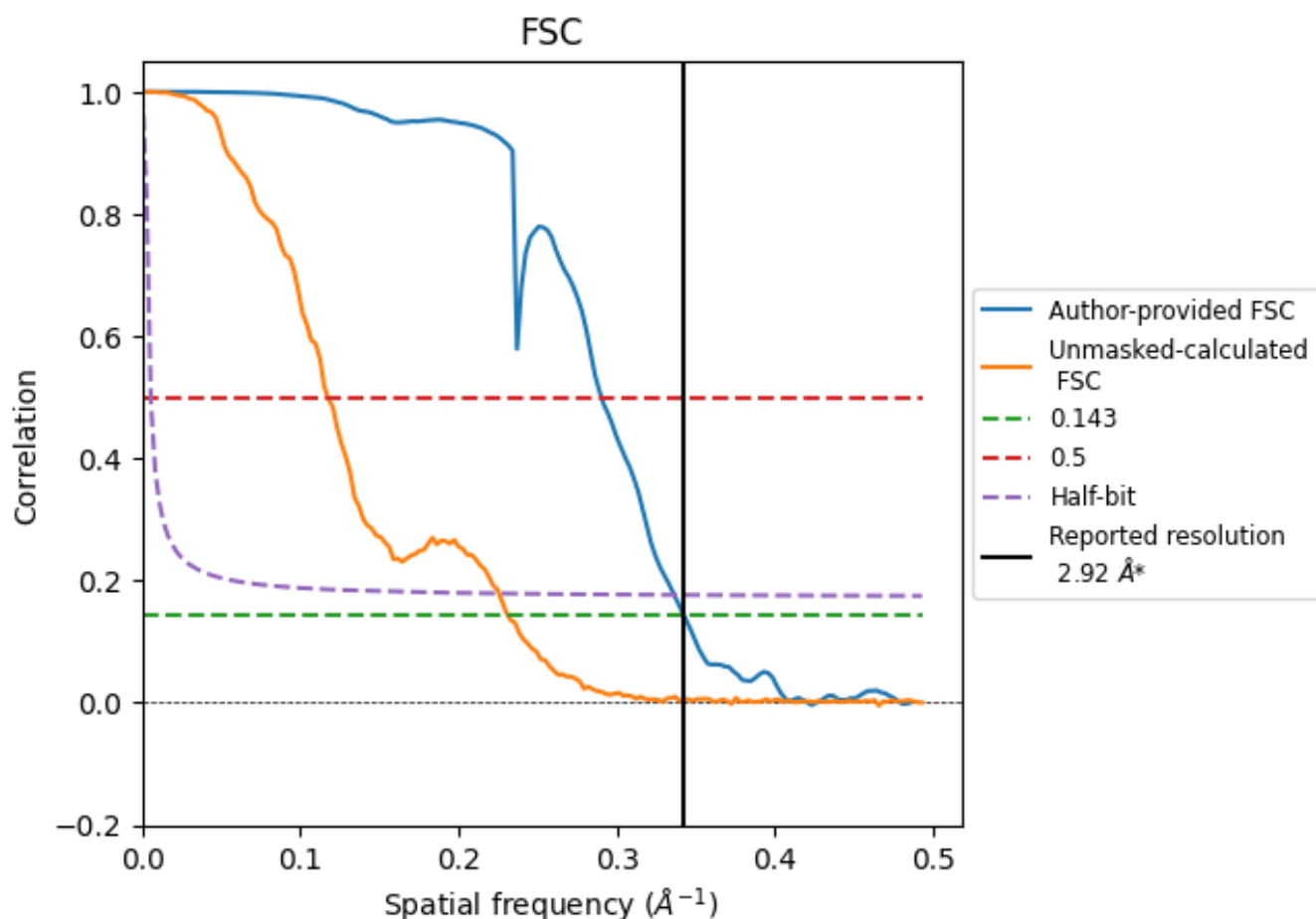


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

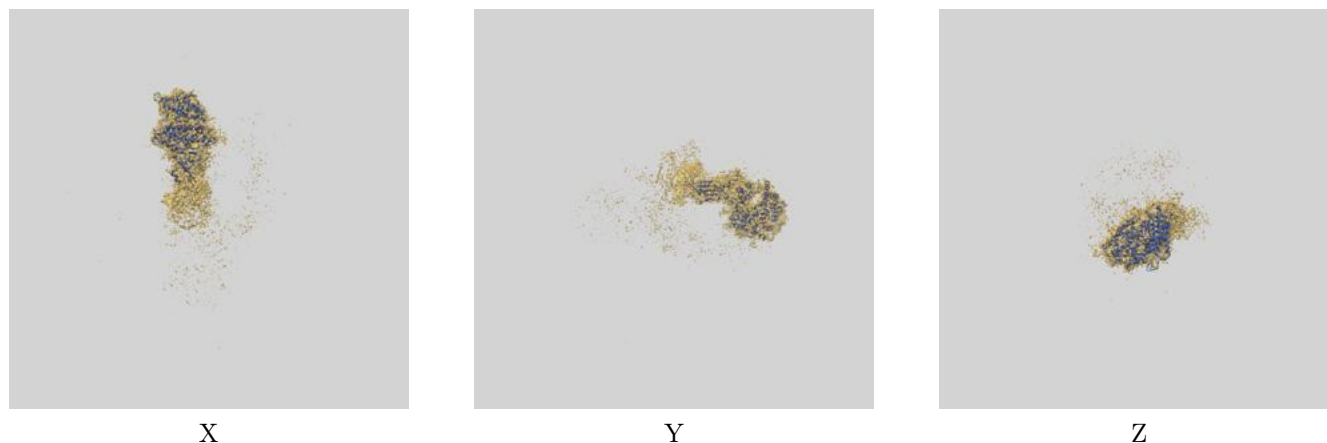
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.45	2.97
Unmasked-calculated*	4.33	8.53	4.43

*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 4.33 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

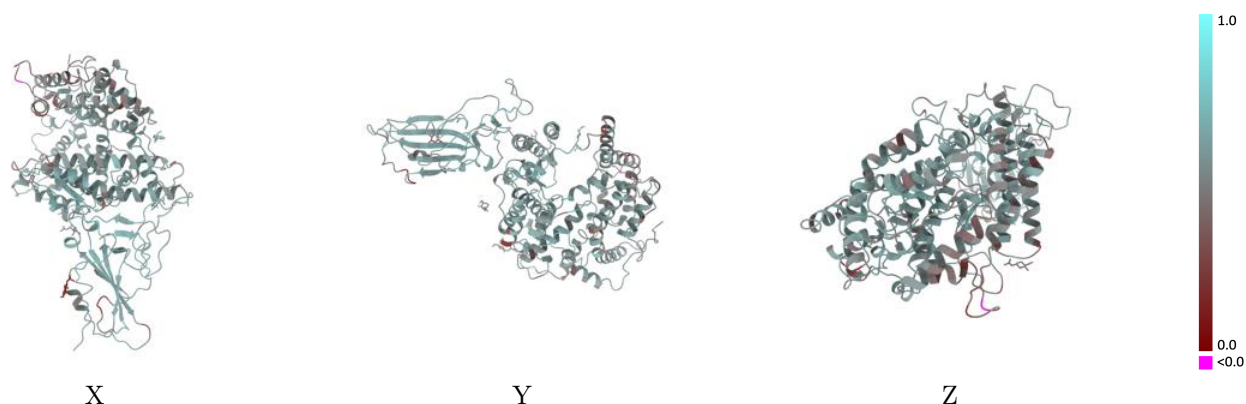
This section contains information regarding the fit between EMDB map EMD-15588 and PDB model 8AQS. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



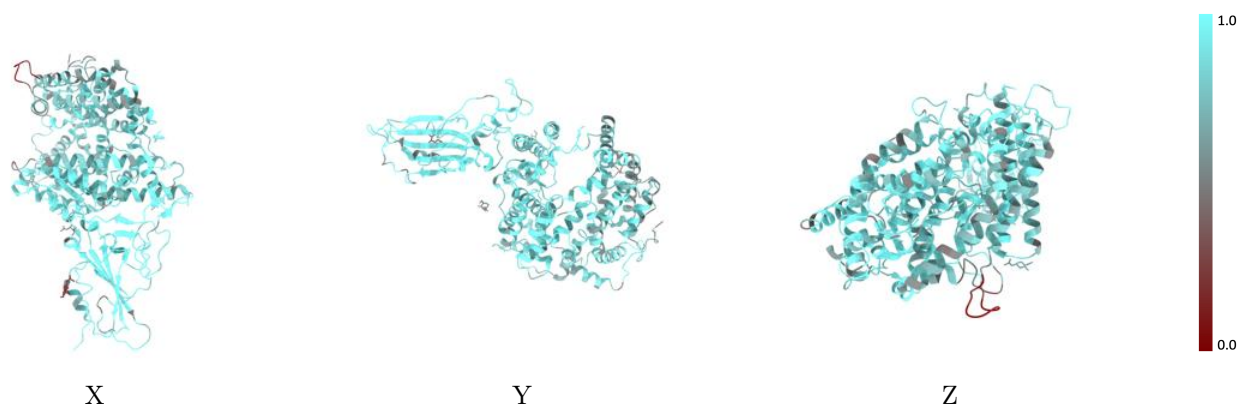
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



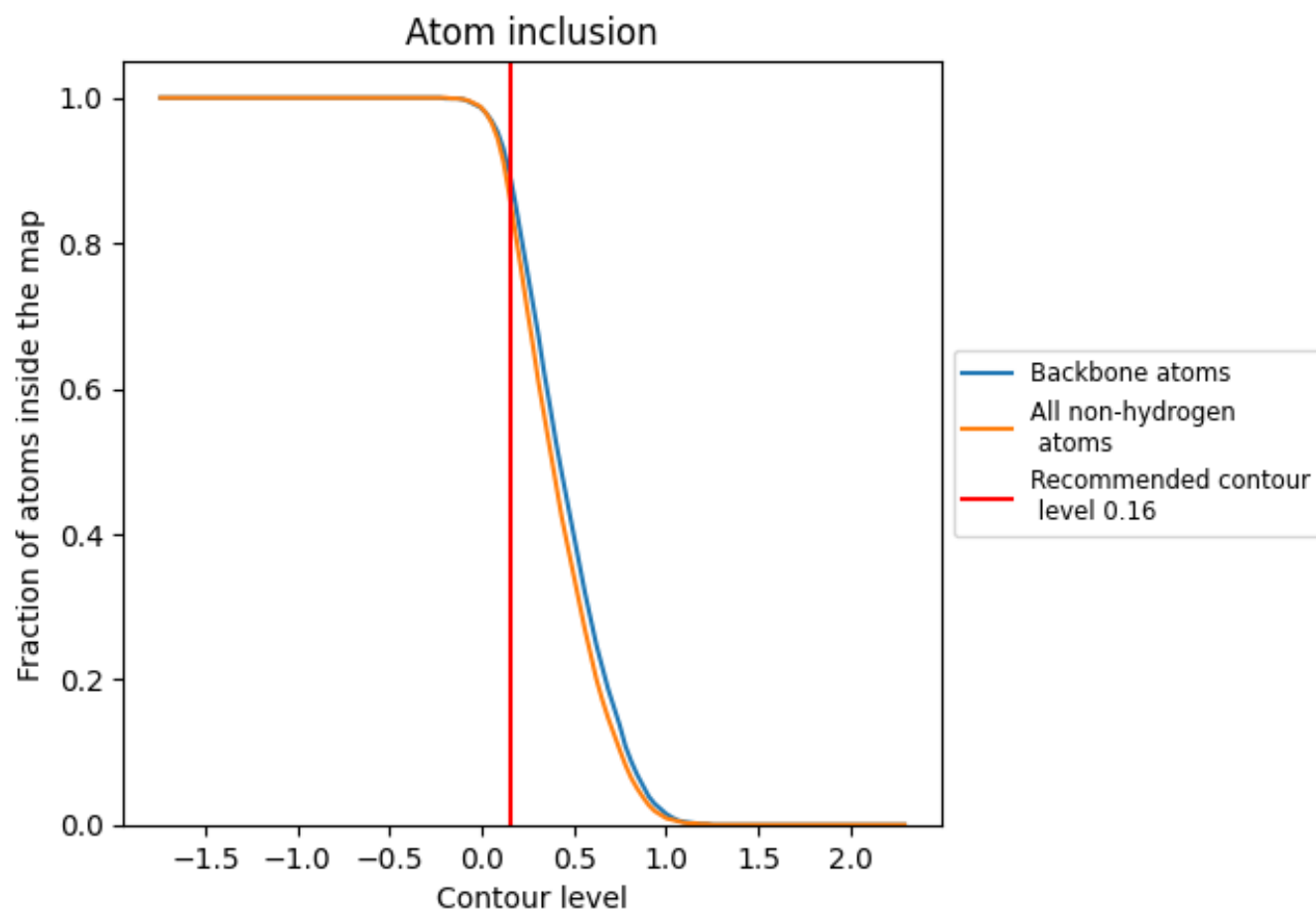
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.5490
A	0.8920	0.5650
B	0.8390	0.5440

