



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2026 – 06:08 PM EDT

PDB ID : 9PT4 / pdb_00009pt4
EMDB ID : EMD-71830
Title : Cryo-EM structure of GPR84-Gi complex bound to OX04529
Authors : Zhang, X.; Zhang, C.
Deposited on : 2025-07-27
Resolution : 3.03 Å(reported)

This is a wwPDB EM Validation Summary 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:

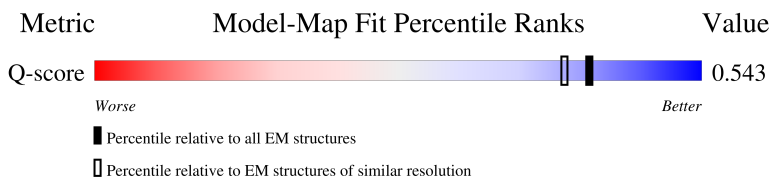
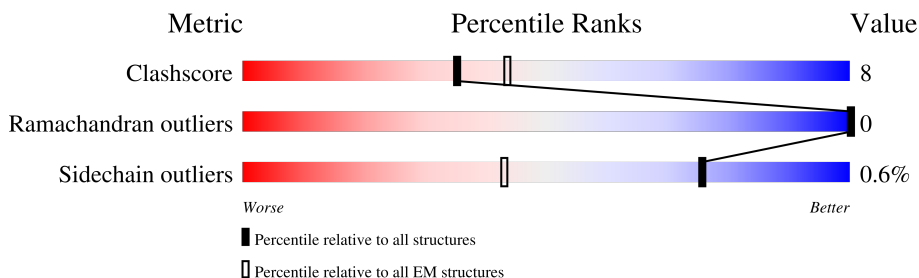
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.03 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	13929 (2.53 - 3.53)

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	R	615	
2	A	354	
3	B	376	
4	G	71	

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Mol	Chain	Length	Quality of chain
5	N	266	 A horizontal bar chart showing the quality of chain N. The bar is divided into three segments: green (70%), yellow (16%), and grey (13%). A red dot is at the start of the green segment, and a black dot is at the end of the grey segment.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8506 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 G-protein coupled receptor 84.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	285	Total	C	N	O	S	0	0
			2153	1430	360	350	13		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-52	ASP	-	expression tag	UNP Q9NQS5
R	-51	TYR	-	expression tag	UNP Q9NQS5
R	-50	LYS	-	expression tag	UNP Q9NQS5
R	-49	ASP	-	expression tag	UNP Q9NQS5
R	-48	ASP	-	expression tag	UNP Q9NQS5
R	-47	ASP	-	expression tag	UNP Q9NQS5
R	-46	ASP	-	expression tag	UNP Q9NQS5
R	-45	HIS	-	expression tag	UNP Q9NQS5
R	-44	HIS	-	expression tag	UNP Q9NQS5
R	-43	HIS	-	expression tag	UNP Q9NQS5
R	-42	HIS	-	expression tag	UNP Q9NQS5
R	-41	HIS	-	expression tag	UNP Q9NQS5
R	-40	HIS	-	expression tag	UNP Q9NQS5
R	-39	HIS	-	expression tag	UNP Q9NQS5
R	-38	HIS	-	expression tag	UNP Q9NQS5
R	-37	GLY	-	expression tag	UNP Q9NQS5
R	-36	GLN	-	expression tag	UNP Q9NQS5
R	-35	PRO	-	expression tag	UNP Q9NQS5
R	-34	GLY	-	expression tag	UNP Q9NQS5
R	-33	ASN	-	expression tag	UNP Q9NQS5
R	-32	GLY	-	expression tag	UNP Q9NQS5
R	-31	SER	-	expression tag	UNP Q9NQS5
R	-30	ALA	-	expression tag	UNP Q9NQS5
R	-29	PHE	-	expression tag	UNP Q9NQS5
R	-28	LEU	-	expression tag	UNP Q9NQS5
R	-27	LEU	-	expression tag	UNP Q9NQS5
R	-26	ALA	-	expression tag	UNP Q9NQS5
R	-25	PRO	-	expression tag	UNP Q9NQS5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-24	ASN	-	expression tag	UNP Q9NQS5
R	-23	GLY	-	expression tag	UNP Q9NQS5
R	-22	SER	-	expression tag	UNP Q9NQS5
R	-21	HIS	-	expression tag	UNP Q9NQS5
R	-20	ALA	-	expression tag	UNP Q9NQS5
R	-19	PRO	-	expression tag	UNP Q9NQS5
R	-18	ASP	-	expression tag	UNP Q9NQS5
R	-17	HIS	-	expression tag	UNP Q9NQS5
R	-16	ASN	-	expression tag	UNP Q9NQS5
R	-15	VAL	-	expression tag	UNP Q9NQS5
R	-14	THR	-	expression tag	UNP Q9NQS5
R	-13	GLN	-	expression tag	UNP Q9NQS5
R	-12	GLN	-	expression tag	UNP Q9NQS5
R	-11	ARG	-	expression tag	UNP Q9NQS5
R	-10	ASP	-	expression tag	UNP Q9NQS5
R	-9	GLU	-	expression tag	UNP Q9NQS5
R	-8	GLU	-	expression tag	UNP Q9NQS5
R	-7	ASN	-	expression tag	UNP Q9NQS5
R	-6	LEU	-	expression tag	UNP Q9NQS5
R	-5	TYR	-	expression tag	UNP Q9NQS5
R	-4	PHE	-	expression tag	UNP Q9NQS5
R	-3	GLN	-	expression tag	UNP Q9NQS5
R	-2	GLY	-	expression tag	UNP Q9NQS5
R	-1	VAL	-	expression tag	UNP Q9NQS5
R	0	ASP	-	expression tag	UNP Q9NQS5
R	388	HIS	-	expression tag	UNP Q9NQS5
R	389	MET	-	expression tag	UNP Q9NQS5
R	390	GLY	-	expression tag	UNP Q9NQS5
R	391	SER	-	expression tag	UNP Q9NQS5
R	392	SER	-	expression tag	UNP Q9NQS5
R	393	GLY	-	expression tag	UNP Q9NQS5
R	394	GLY	-	expression tag	UNP Q9NQS5
R	395	GLY	-	expression tag	UNP Q9NQS5
R	396	GLY	-	expression tag	UNP Q9NQS5
R	397	SER	-	expression tag	UNP Q9NQS5
R	398	GLY	-	expression tag	UNP Q9NQS5
R	399	GLY	-	expression tag	UNP Q9NQS5
R	400	GLY	-	expression tag	UNP Q9NQS5
R	401	GLY	-	expression tag	UNP Q9NQS5
R	402	SER	-	expression tag	UNP Q9NQS5
R	403	SER	-	expression tag	UNP Q9NQS5
R	404	GLY	-	expression tag	UNP Q9NQS5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	405	VAL	-	expression tag	UNP Q9NQS5
R	406	PHE	-	expression tag	UNP Q9NQS5
R	407	THR	-	expression tag	UNP Q9NQS5
R	408	LEU	-	expression tag	UNP Q9NQS5
R	409	GLU	-	expression tag	UNP Q9NQS5
R	410	ASP	-	expression tag	UNP Q9NQS5
R	411	PHE	-	expression tag	UNP Q9NQS5
R	412	VAL	-	expression tag	UNP Q9NQS5
R	413	GLY	-	expression tag	UNP Q9NQS5
R	414	ASP	-	expression tag	UNP Q9NQS5
R	415	TRP	-	expression tag	UNP Q9NQS5
R	416	GLU	-	expression tag	UNP Q9NQS5
R	417	GLN	-	expression tag	UNP Q9NQS5
R	418	THR	-	expression tag	UNP Q9NQS5
R	419	ALA	-	expression tag	UNP Q9NQS5
R	420	ALA	-	expression tag	UNP Q9NQS5
R	421	TYR	-	expression tag	UNP Q9NQS5
R	422	ASN	-	expression tag	UNP Q9NQS5
R	423	LEU	-	expression tag	UNP Q9NQS5
R	424	ASP	-	expression tag	UNP Q9NQS5
R	425	GLN	-	expression tag	UNP Q9NQS5
R	426	VAL	-	expression tag	UNP Q9NQS5
R	427	LEU	-	expression tag	UNP Q9NQS5
R	428	GLU	-	expression tag	UNP Q9NQS5
R	429	GLN	-	expression tag	UNP Q9NQS5
R	430	GLY	-	expression tag	UNP Q9NQS5
R	431	GLY	-	expression tag	UNP Q9NQS5
R	432	VAL	-	expression tag	UNP Q9NQS5
R	433	SER	-	expression tag	UNP Q9NQS5
R	434	SER	-	expression tag	UNP Q9NQS5
R	435	LEU	-	expression tag	UNP Q9NQS5
R	436	LEU	-	expression tag	UNP Q9NQS5
R	437	GLN	-	expression tag	UNP Q9NQS5
R	438	ASN	-	expression tag	UNP Q9NQS5
R	439	LEU	-	expression tag	UNP Q9NQS5
R	440	ALA	-	expression tag	UNP Q9NQS5
R	441	VAL	-	expression tag	UNP Q9NQS5
R	442	SER	-	expression tag	UNP Q9NQS5
R	443	VAL	-	expression tag	UNP Q9NQS5
R	444	THR	-	expression tag	UNP Q9NQS5
R	445	PRO	-	expression tag	UNP Q9NQS5
R	446	ILE	-	expression tag	UNP Q9NQS5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	447	GLN	-	expression tag	UNP Q9NQS5
R	448	ARG	-	expression tag	UNP Q9NQS5
R	449	ILE	-	expression tag	UNP Q9NQS5
R	450	VAL	-	expression tag	UNP Q9NQS5
R	451	ARG	-	expression tag	UNP Q9NQS5
R	452	SER	-	expression tag	UNP Q9NQS5
R	453	GLY	-	expression tag	UNP Q9NQS5
R	454	GLU	-	expression tag	UNP Q9NQS5
R	455	ASN	-	expression tag	UNP Q9NQS5
R	456	ALA	-	expression tag	UNP Q9NQS5
R	457	LEU	-	expression tag	UNP Q9NQS5
R	458	LYS	-	expression tag	UNP Q9NQS5
R	459	ILE	-	expression tag	UNP Q9NQS5
R	460	ASP	-	expression tag	UNP Q9NQS5
R	461	ILE	-	expression tag	UNP Q9NQS5
R	462	HIS	-	expression tag	UNP Q9NQS5
R	463	VAL	-	expression tag	UNP Q9NQS5
R	464	ILE	-	expression tag	UNP Q9NQS5
R	465	ILE	-	expression tag	UNP Q9NQS5
R	466	PRO	-	expression tag	UNP Q9NQS5
R	467	TYR	-	expression tag	UNP Q9NQS5
R	468	GLU	-	expression tag	UNP Q9NQS5
R	469	GLY	-	expression tag	UNP Q9NQS5
R	470	LEU	-	expression tag	UNP Q9NQS5
R	471	SER	-	expression tag	UNP Q9NQS5
R	472	ALA	-	expression tag	UNP Q9NQS5
R	473	ASP	-	expression tag	UNP Q9NQS5
R	474	GLN	-	expression tag	UNP Q9NQS5
R	475	MET	-	expression tag	UNP Q9NQS5
R	476	ALA	-	expression tag	UNP Q9NQS5
R	477	GLN	-	expression tag	UNP Q9NQS5
R	478	ILE	-	expression tag	UNP Q9NQS5
R	479	GLU	-	expression tag	UNP Q9NQS5
R	480	GLU	-	expression tag	UNP Q9NQS5
R	481	VAL	-	expression tag	UNP Q9NQS5
R	482	PHE	-	expression tag	UNP Q9NQS5
R	483	LYS	-	expression tag	UNP Q9NQS5
R	484	VAL	-	expression tag	UNP Q9NQS5
R	485	VAL	-	expression tag	UNP Q9NQS5
R	486	TYR	-	expression tag	UNP Q9NQS5
R	487	PRO	-	expression tag	UNP Q9NQS5
R	488	VAL	-	expression tag	UNP Q9NQS5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	489	ASP	-	expression tag	UNP Q9NQS5
R	490	ASP	-	expression tag	UNP Q9NQS5
R	491	HIS	-	expression tag	UNP Q9NQS5
R	492	HIS	-	expression tag	UNP Q9NQS5
R	493	PHE	-	expression tag	UNP Q9NQS5
R	494	LYS	-	expression tag	UNP Q9NQS5
R	495	VAL	-	expression tag	UNP Q9NQS5
R	496	ILE	-	expression tag	UNP Q9NQS5
R	497	LEU	-	expression tag	UNP Q9NQS5
R	498	PRO	-	expression tag	UNP Q9NQS5
R	499	TYR	-	expression tag	UNP Q9NQS5
R	500	GLY	-	expression tag	UNP Q9NQS5
R	501	THR	-	expression tag	UNP Q9NQS5
R	502	LEU	-	expression tag	UNP Q9NQS5
R	503	VAL	-	expression tag	UNP Q9NQS5
R	504	ILE	-	expression tag	UNP Q9NQS5
R	505	ASP	-	expression tag	UNP Q9NQS5
R	506	GLY	-	expression tag	UNP Q9NQS5
R	507	VAL	-	expression tag	UNP Q9NQS5
R	508	THR	-	expression tag	UNP Q9NQS5
R	509	PRO	-	expression tag	UNP Q9NQS5
R	510	ASN	-	expression tag	UNP Q9NQS5
R	511	MET	-	expression tag	UNP Q9NQS5
R	512	LEU	-	expression tag	UNP Q9NQS5
R	513	ASN	-	expression tag	UNP Q9NQS5
R	514	TYR	-	expression tag	UNP Q9NQS5
R	515	PHE	-	expression tag	UNP Q9NQS5
R	516	GLY	-	expression tag	UNP Q9NQS5
R	517	ARG	-	expression tag	UNP Q9NQS5
R	518	PRO	-	expression tag	UNP Q9NQS5
R	519	TYR	-	expression tag	UNP Q9NQS5
R	520	GLU	-	expression tag	UNP Q9NQS5
R	521	GLY	-	expression tag	UNP Q9NQS5
R	522	ILE	-	expression tag	UNP Q9NQS5
R	523	ALA	-	expression tag	UNP Q9NQS5
R	524	VAL	-	expression tag	UNP Q9NQS5
R	525	PHE	-	expression tag	UNP Q9NQS5
R	526	ASP	-	expression tag	UNP Q9NQS5
R	527	GLY	-	expression tag	UNP Q9NQS5
R	528	LYS	-	expression tag	UNP Q9NQS5
R	529	LYS	-	expression tag	UNP Q9NQS5
R	530	ILE	-	expression tag	UNP Q9NQS5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	531	THR	-	expression tag	UNP Q9NQS5
R	532	VAL	-	expression tag	UNP Q9NQS5
R	533	THR	-	expression tag	UNP Q9NQS5
R	534	GLY	-	expression tag	UNP Q9NQS5
R	535	THR	-	expression tag	UNP Q9NQS5
R	536	LEU	-	expression tag	UNP Q9NQS5
R	537	TRP	-	expression tag	UNP Q9NQS5
R	538	ASN	-	expression tag	UNP Q9NQS5
R	539	GLY	-	expression tag	UNP Q9NQS5
R	540	ASN	-	expression tag	UNP Q9NQS5
R	541	LYS	-	expression tag	UNP Q9NQS5
R	542	ILE	-	expression tag	UNP Q9NQS5
R	543	ILE	-	expression tag	UNP Q9NQS5
R	544	ASP	-	expression tag	UNP Q9NQS5
R	545	GLU	-	expression tag	UNP Q9NQS5
R	546	ARG	-	expression tag	UNP Q9NQS5
R	547	LEU	-	expression tag	UNP Q9NQS5
R	548	ILE	-	expression tag	UNP Q9NQS5
R	549	THR	-	expression tag	UNP Q9NQS5
R	550	PRO	-	expression tag	UNP Q9NQS5
R	551	ASP	-	expression tag	UNP Q9NQS5
R	552	GLY	-	expression tag	UNP Q9NQS5
R	553	SER	-	expression tag	UNP Q9NQS5
R	554	MET	-	expression tag	UNP Q9NQS5
R	555	LEU	-	expression tag	UNP Q9NQS5
R	556	PHE	-	expression tag	UNP Q9NQS5
R	557	ARG	-	expression tag	UNP Q9NQS5
R	558	VAL	-	expression tag	UNP Q9NQS5
R	559	THR	-	expression tag	UNP Q9NQS5
R	560	ILE	-	expression tag	UNP Q9NQS5
R	561	ASN	-	expression tag	UNP Q9NQS5
R	562	SER	-	expression tag	UNP Q9NQS5

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	224	Total	C	N	O	S	0	0
			1694	1086	288	307	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	340	Total	C	N	O	S	0	0
			2534	1568	452	493	21		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

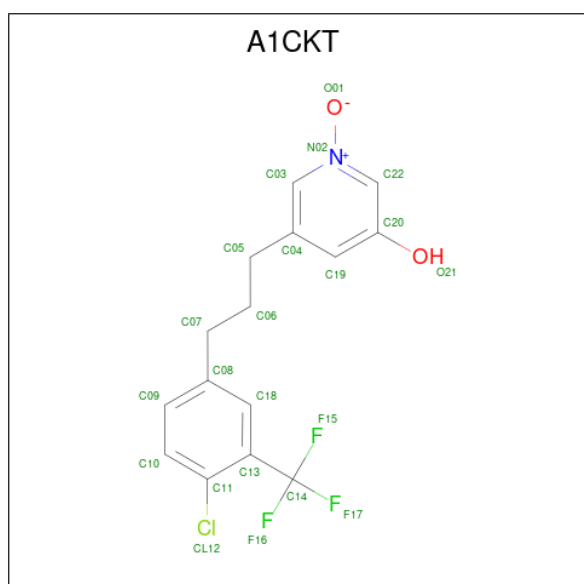
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	55	Total	C	N	O	S	0	0
			375	236	66	71	2		

- Molecule 5 is a protein called scFv16.

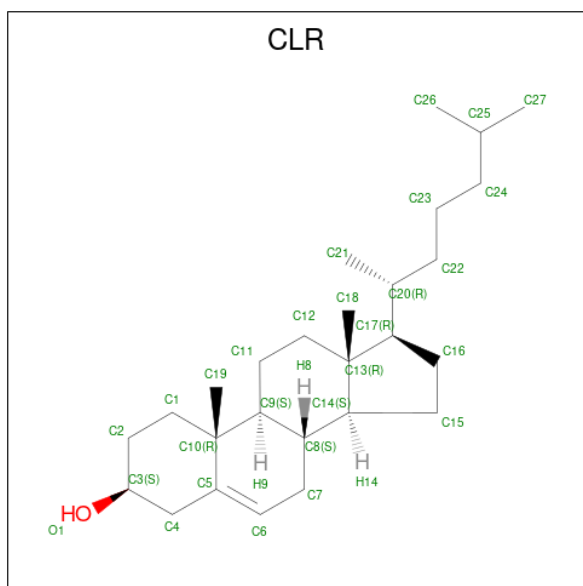
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	231	Total	C	N	O	S	0	0
			1700	1086	284	320	10		

- Molecule 6 is 5-[3-[4-chloranyl-3-(trifluoromethyl)phenyl]propyl]-1-oxidanyl-pyridi n-3-ol (CCD ID: A1CKT) (formula: C₁₅H₁₃ClF₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	R	1	Total	C	Cl	F	N	O	0
			22	15	1	3	1	2	

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

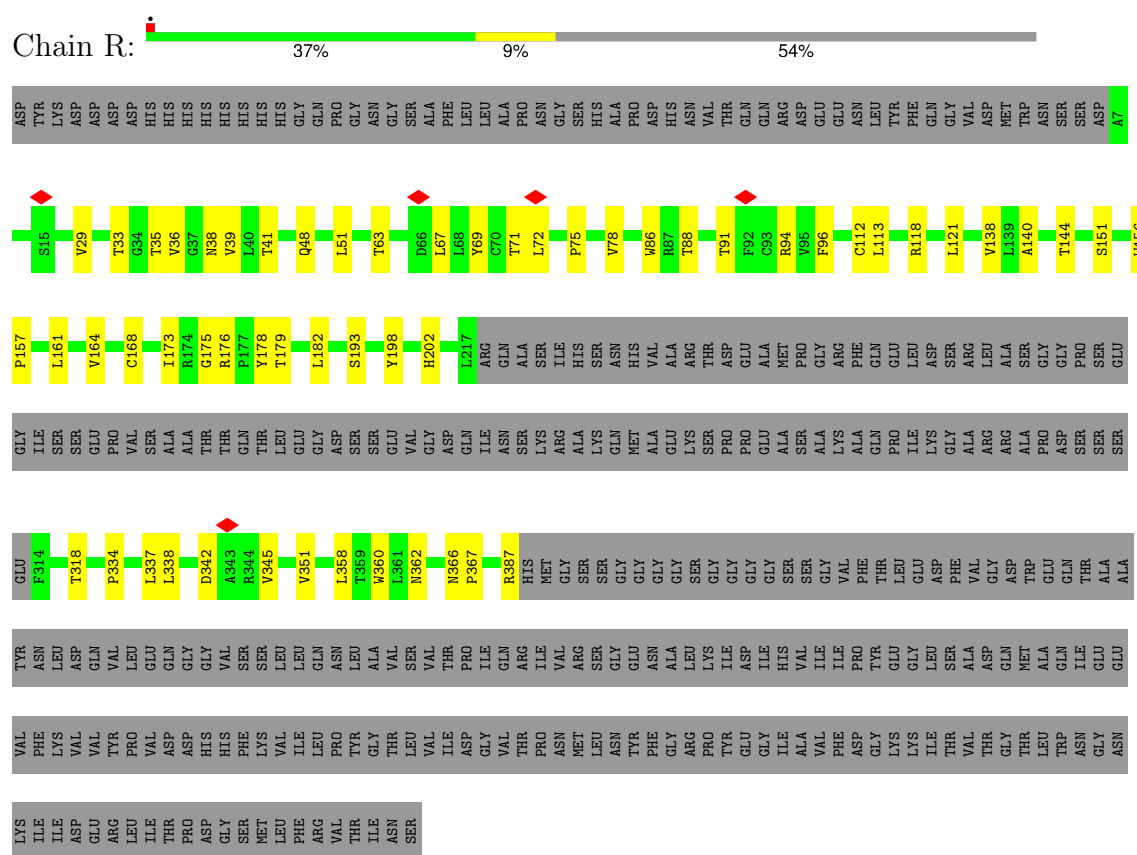


Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	

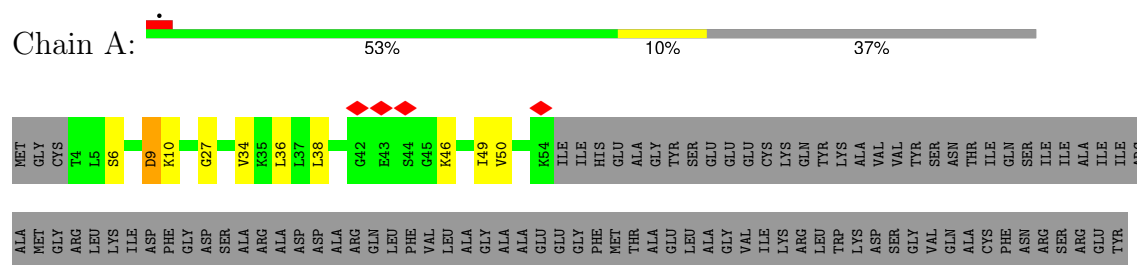
3 Residue-property plots

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.

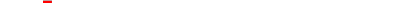
• Molecule 1: G-protein coupled receptor 84

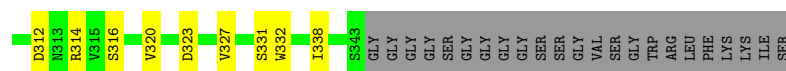


• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

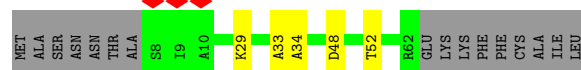




- Chain B:  73% 17% 10%



- Chain G: 



- Chain N:  70% 16% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218137	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-1.109	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	211.968, 211.968, 211.968	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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: A1CKT, CLR

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	R	0.15	0/2207	0.32	0/3024
2	A	0.22	0/1724	0.34	0/2329
3	B	0.23	0/2581	0.35	0/3509
4	G	0.13	0/381	0.24	0/523
5	N	0.22	0/1743	0.45	1/2374 (0.0%)
All	All	0.21	0/8636	0.36	1/11759 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	237	PRO	N-CA-C	-9.46	92.98	112.47

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	R	2153	0	2174	37	0
2	A	1694	0	1610	23	0
3	B	2534	0	2392	43	0
4	G	375	0	335	5	0
5	N	1700	0	1582	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	22	0	0	1	0
7	R	28	0	46	2	0
All	All	8506	0	8139	131	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 8.

The worst 5 of 131 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)
3:B:58:ILE:HG12	3:B:74:SER:OG	1.72	0.89
1:R:86:TRP:HB2	1:R:161:LEU:HD13	1.69	0.73
2:A:325:CYS:SG	2:A:326:SER:N	2.59	0.73
5:N:94:TYR:O	5:N:114:GLY:HA2	1.90	0.71
3:B:152:LEU:HD11	3:B:158:VAL:HG23	1.71	0.71

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	R	281/615 (46%)	273 (97%)	8 (3%)	0	100	100
2	A	220/354 (62%)	219 (100%)	1 (0%)	0	100	100
3	B	338/376 (90%)	326 (96%)	12 (4%)	0	100	100
4	G	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
5	N	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
All	All	1119/1682 (66%)	1088 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	R	220/514 (43%)	220 (100%)	0	100	100
2	A	167/305 (55%)	165 (99%)	2 (1%)	63	79
3	B	264/306 (86%)	264 (100%)	0	100	100
4	G	31/58 (53%)	31 (100%)	0	100	100
5	N	172/215 (80%)	169 (98%)	3 (2%)	53	75
All	All	854/1398 (61%)	849 (99%)	5 (1%)	76	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	SER
2	A	9	ASP
5	N	175	LEU
5	N	236	TYR
5	N	239	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	322	HIS
5	N	39	GLN
5	N	195	ASN
5	N	180	GLN
2	A	213	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
6	A1CKT	R	601	-	23,23,23	0.96	1 (4%)	31,33,33	1.15	1 (3%)
7	CLR	R	602	-	31,31,31	0.42	0	48,48,48	0.61	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
6	A1CKT	R	601	-	-	6/12/12/12	0/2/2/2
7	CLR	R	602	-	-	6/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	A1CKT	C11-CL12	2.10	1.78	1.73

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	601	A1CKT	C20-C19-C04	-3.19	118.03	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

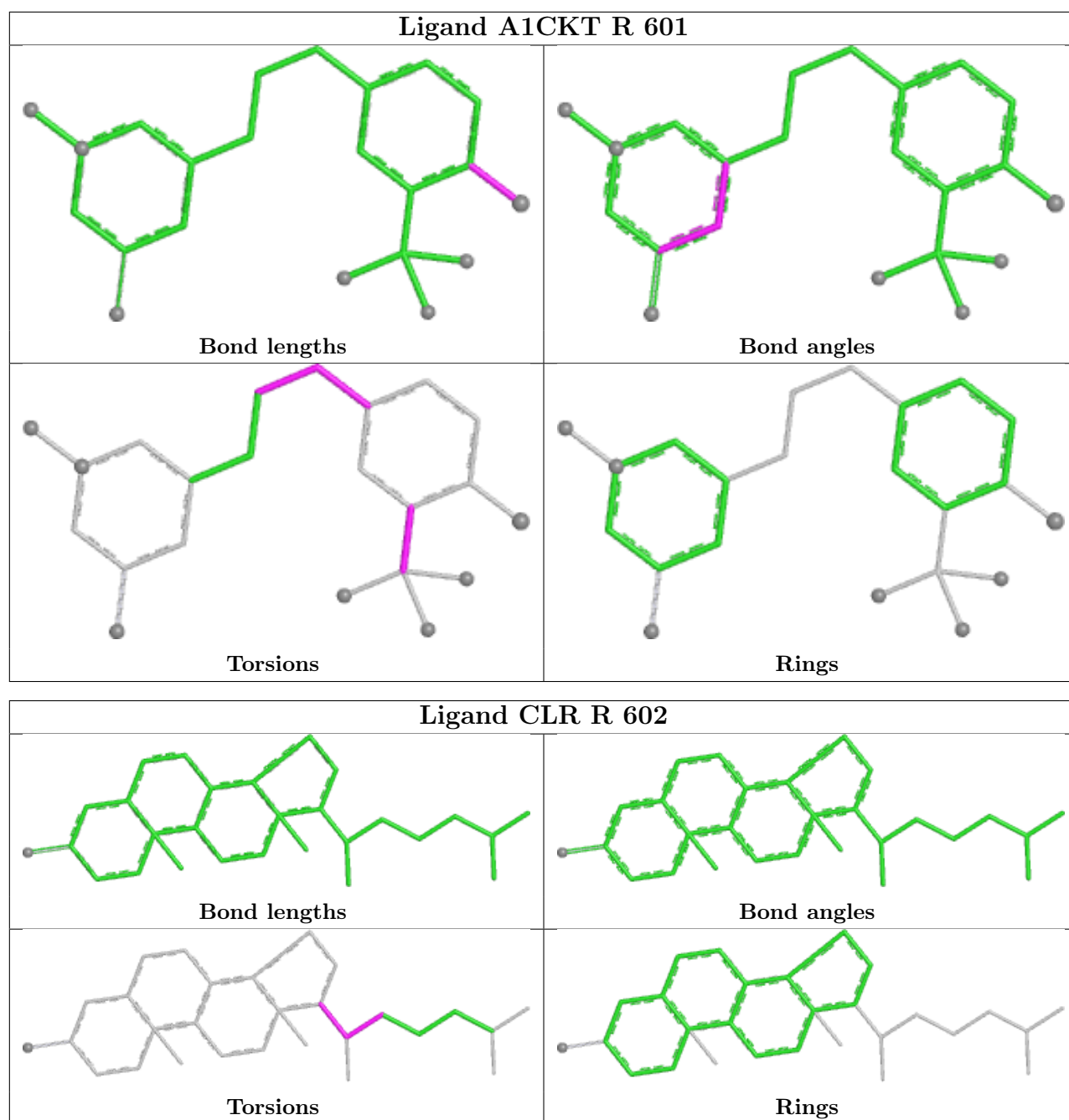
Mol	Chain	Res	Type	Atoms
6	R	601	A1CKT	C11-C13-C14-F15
6	R	601	A1CKT	C11-C13-C14-F16
6	R	601	A1CKT	C11-C13-C14-F17
7	R	602	CLR	C17-C20-C22-C23
6	R	601	A1CKT	C05-C06-C07-C08

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	A1CKT	1	0
7	R	602	CLR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

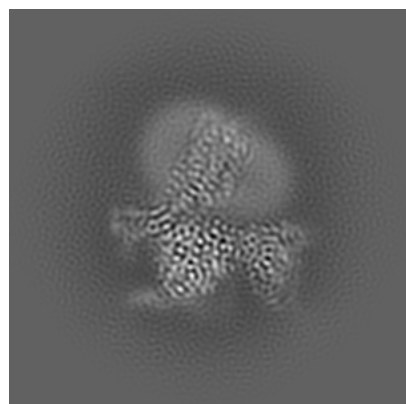
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71830. These allow visual inspection of the internal detail of the map and identification of artifacts.

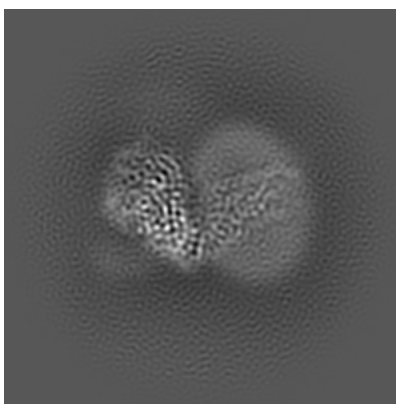
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

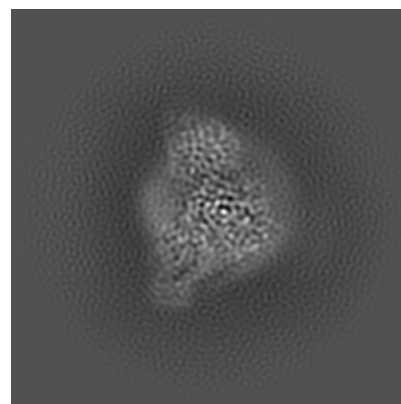
6.1.1 Primary map



X

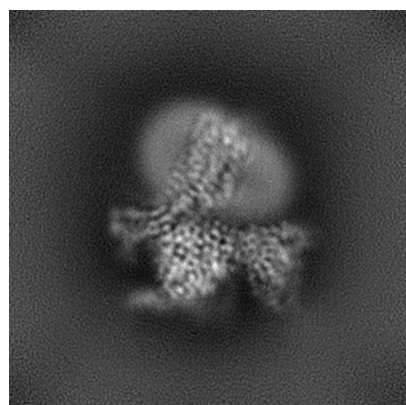


Y

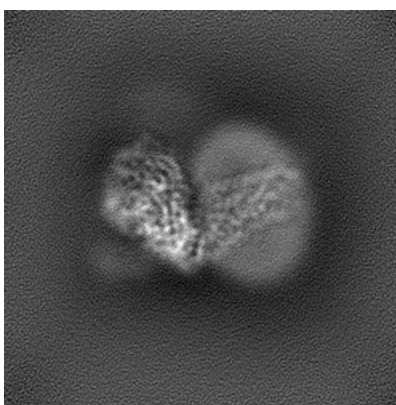


Z

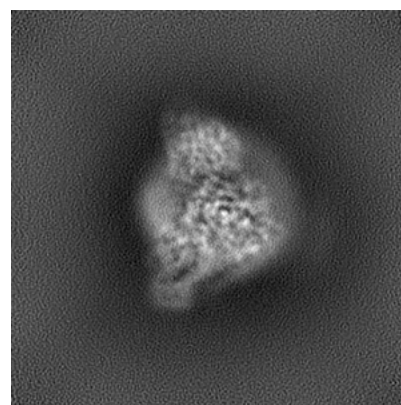
6.1.2 Raw map



X



Y

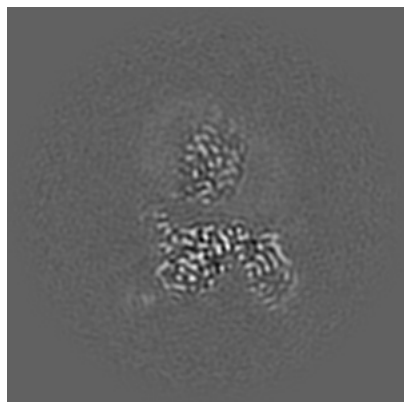


Z

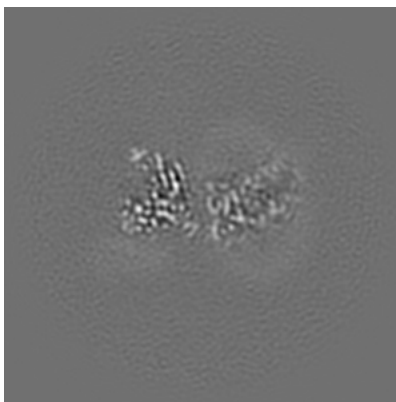
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

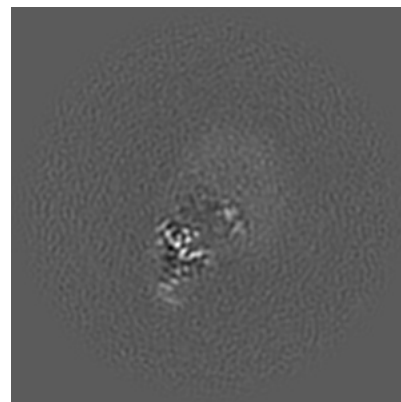
6.2.1 Primary map



X Index: 128

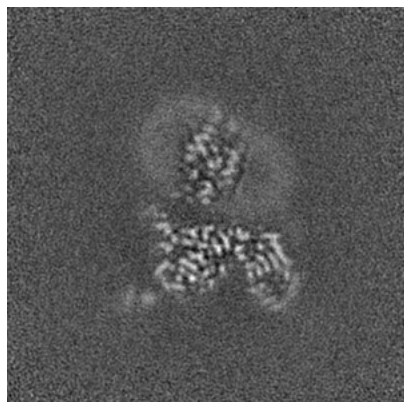


Y Index: 128

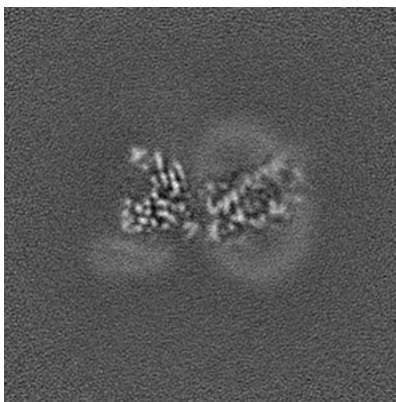


Z Index: 128

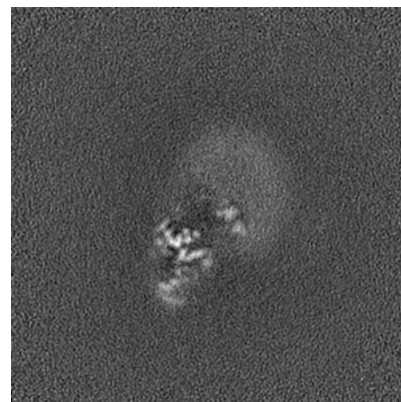
6.2.2 Raw map



X Index: 128



Y Index: 128

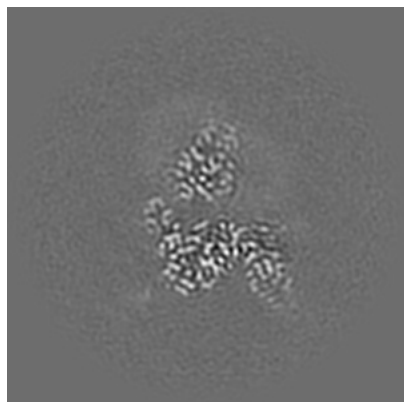


Z Index: 128

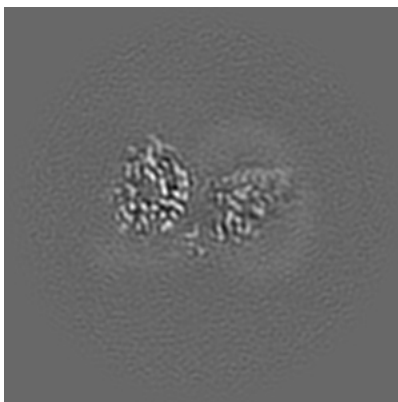
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

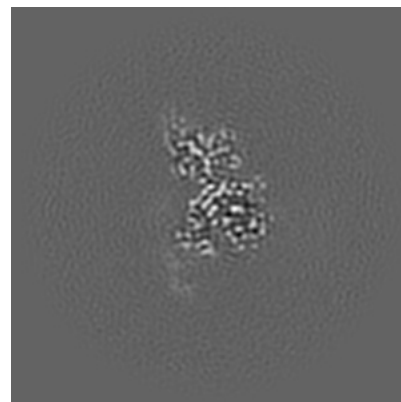
6.3.1 Primary map



X Index: 124

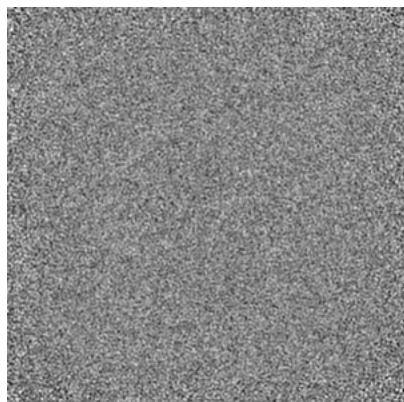


Y Index: 119

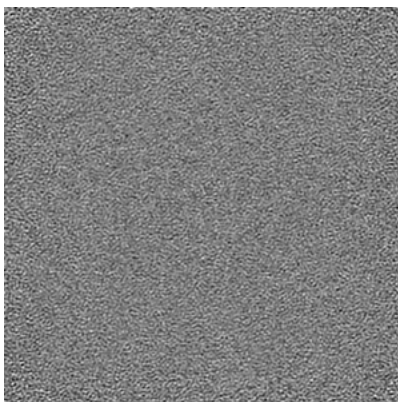


Z Index: 103

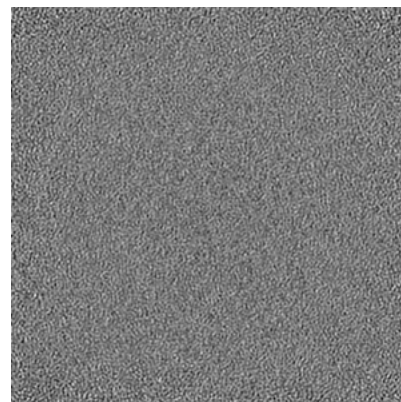
6.3.2 Raw map



X Index: 0



Y Index: 0

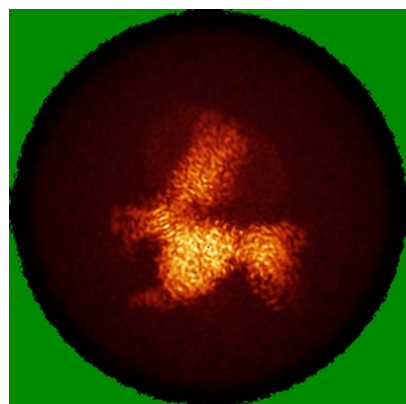


Z Index: 0

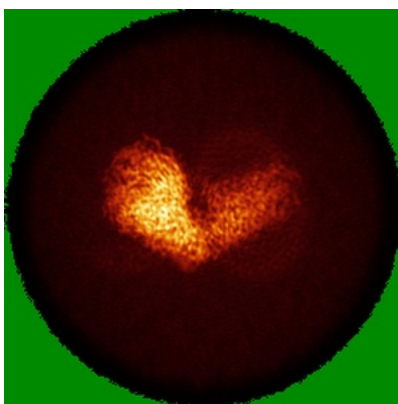
The images above show the largest variance slices of the map in three orthogonal directions.

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

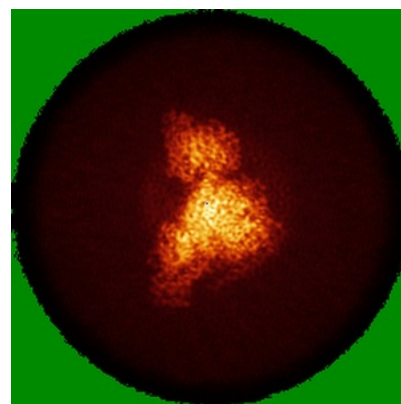
6.4.1 Primary map



X

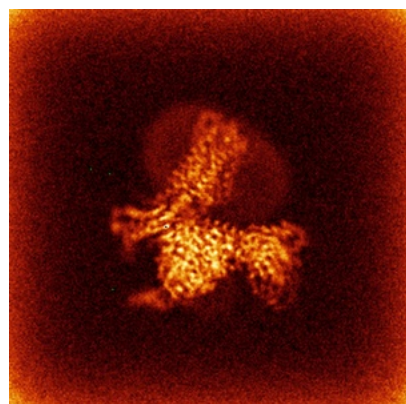


Y

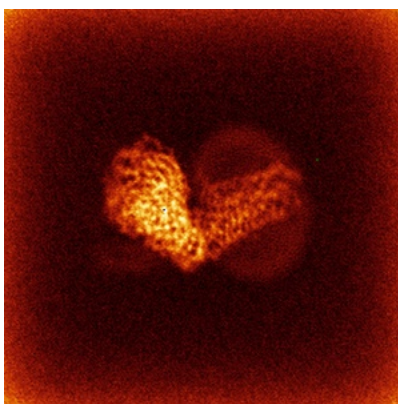


Z

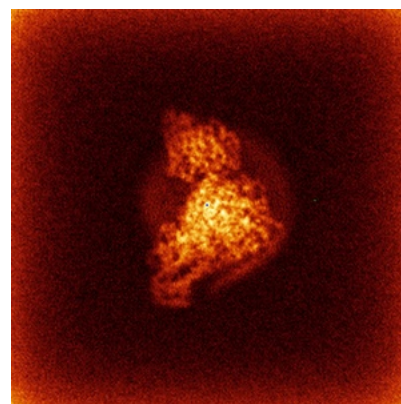
6.4.2 Raw map



X



Y



Z

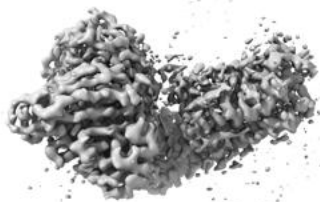
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

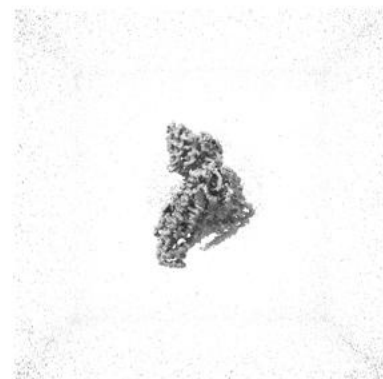
6.5.2 Raw map



X



Y



Z

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.

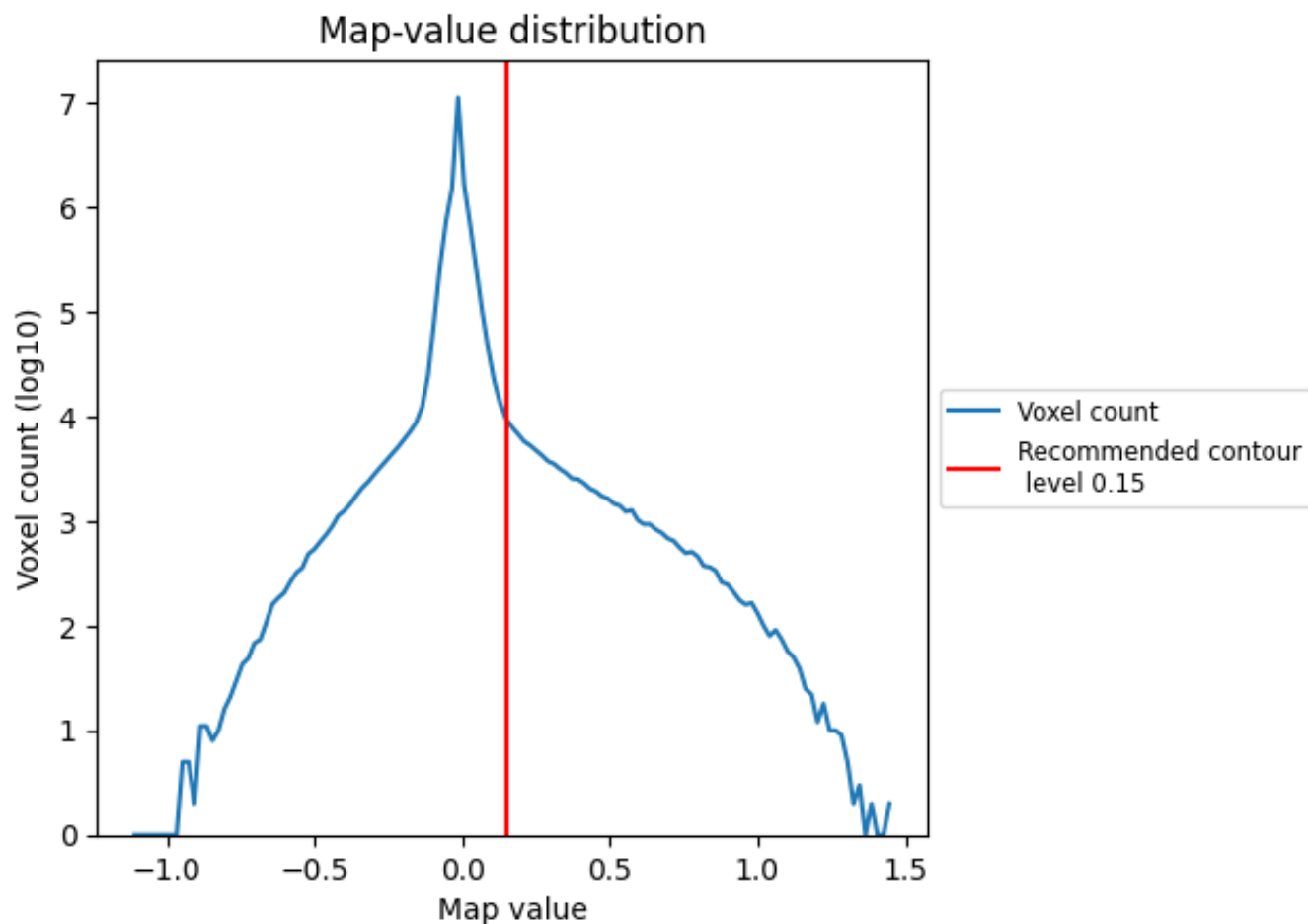
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

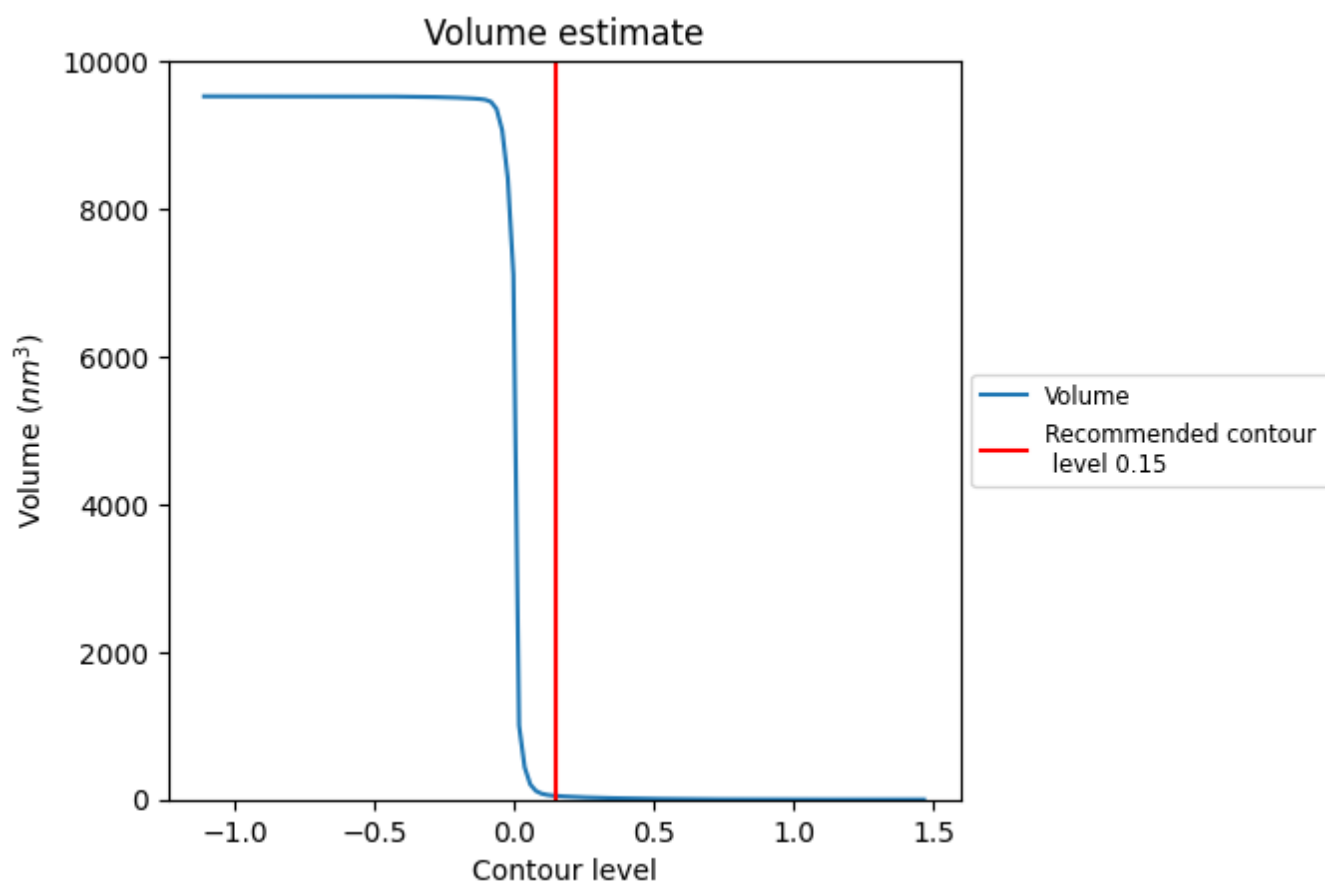
This section contains the results of statistical analysis of the map.

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.

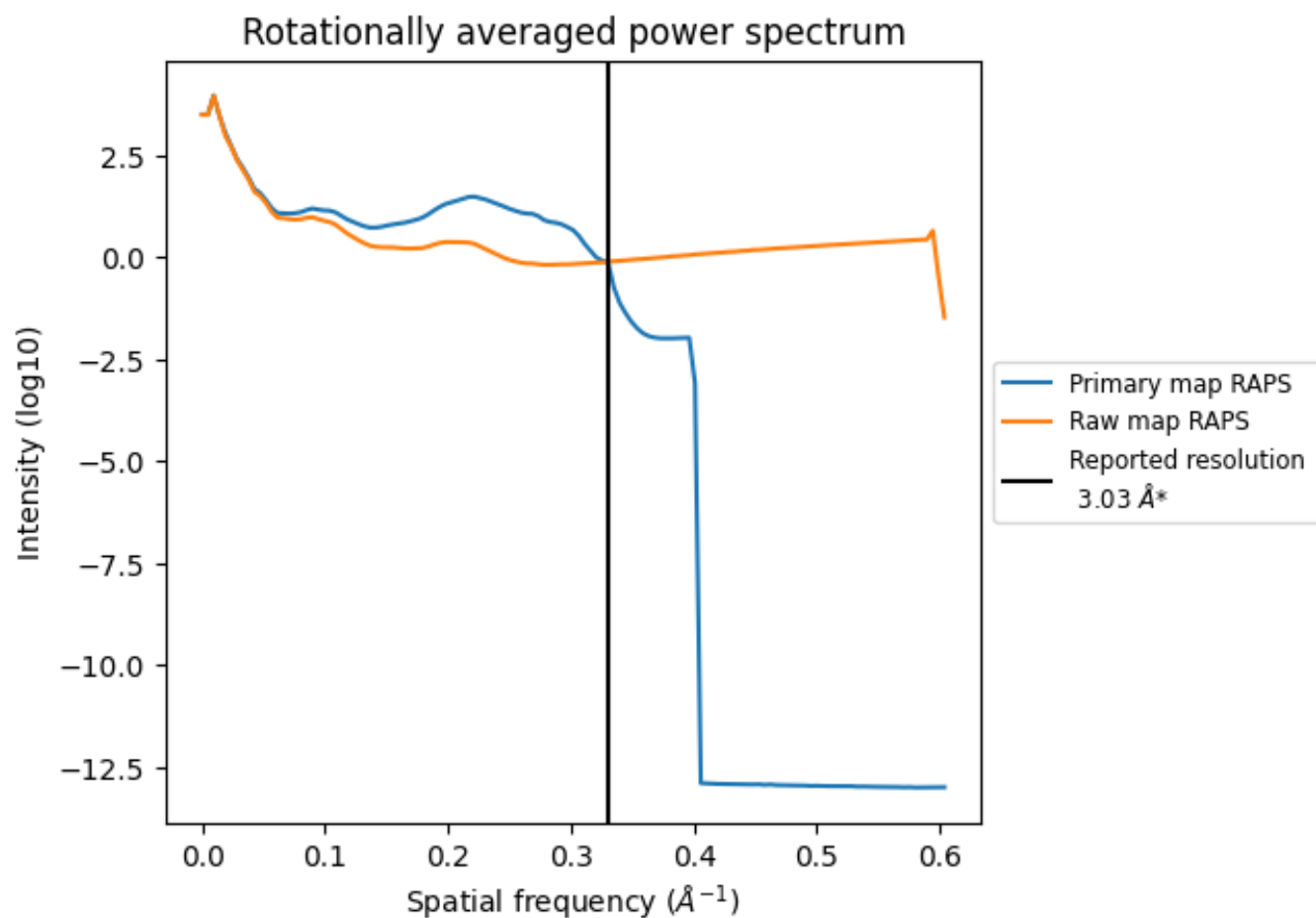
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm³; this corresponds to an approximate mass of 45 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 ⓘ

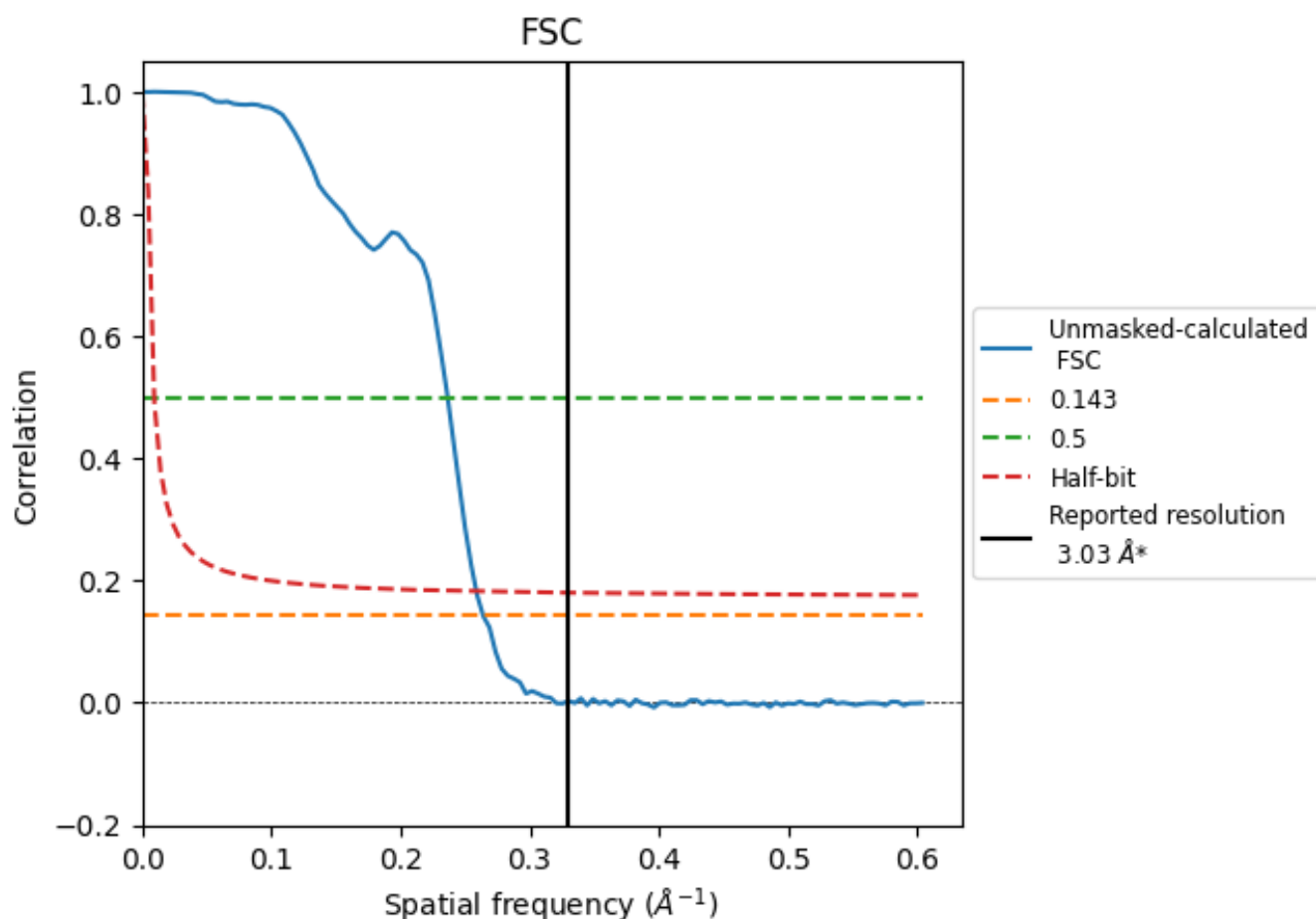


*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

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 0.330 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

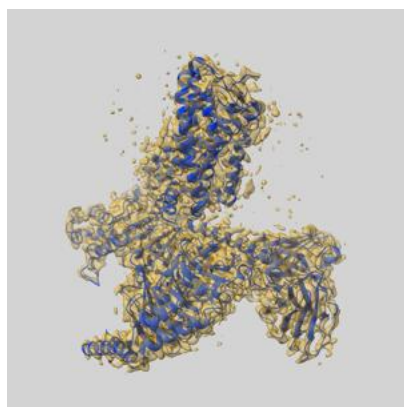
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	4.23	3.87

*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 3.79 differs from the reported value 3.03 by more than 10 %

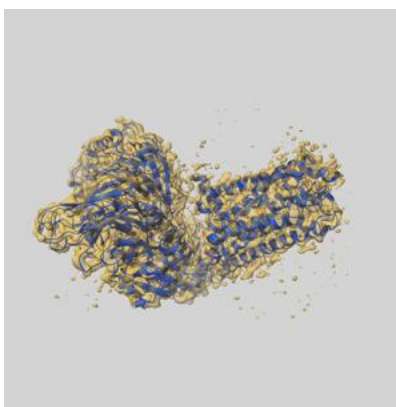
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71830 and PDB model 9PT4. Per-residue inclusion information can be found in section [3](#) on page [13](#).

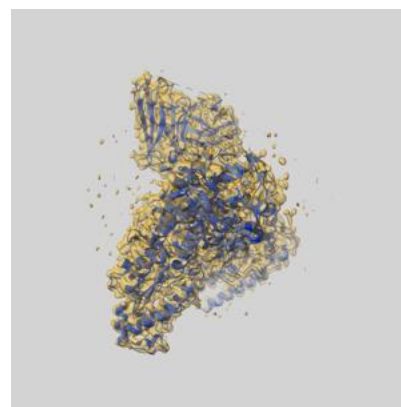
9.1 Map-model overlay [i](#)



X



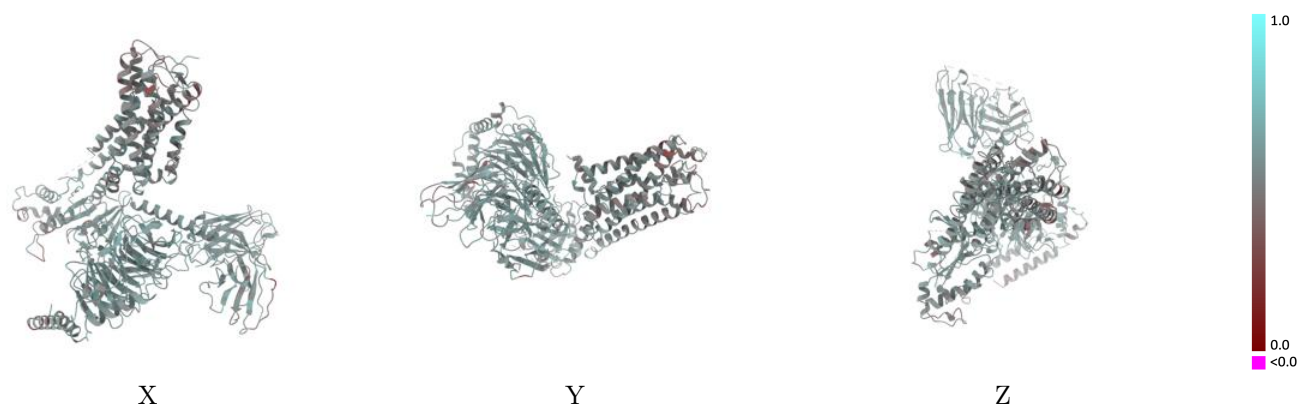
Y



Z

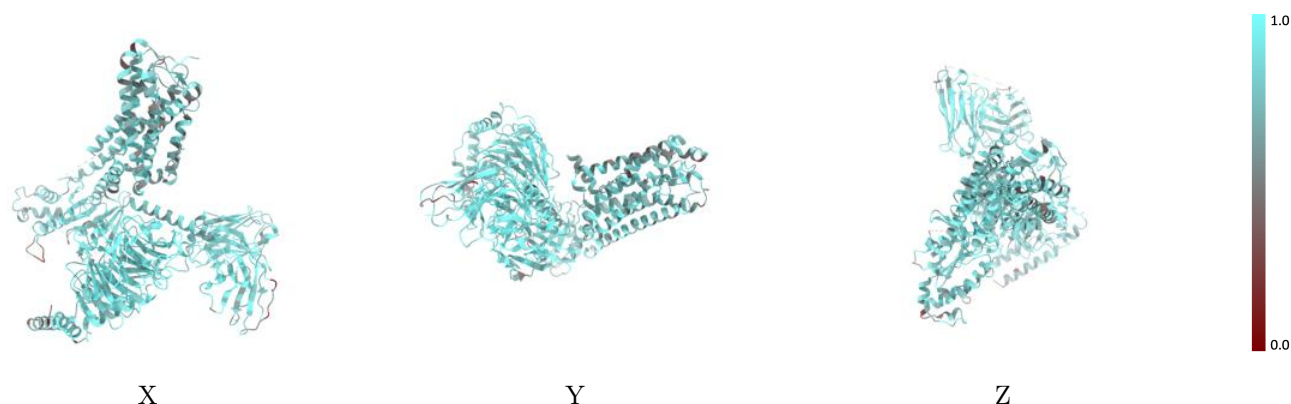
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



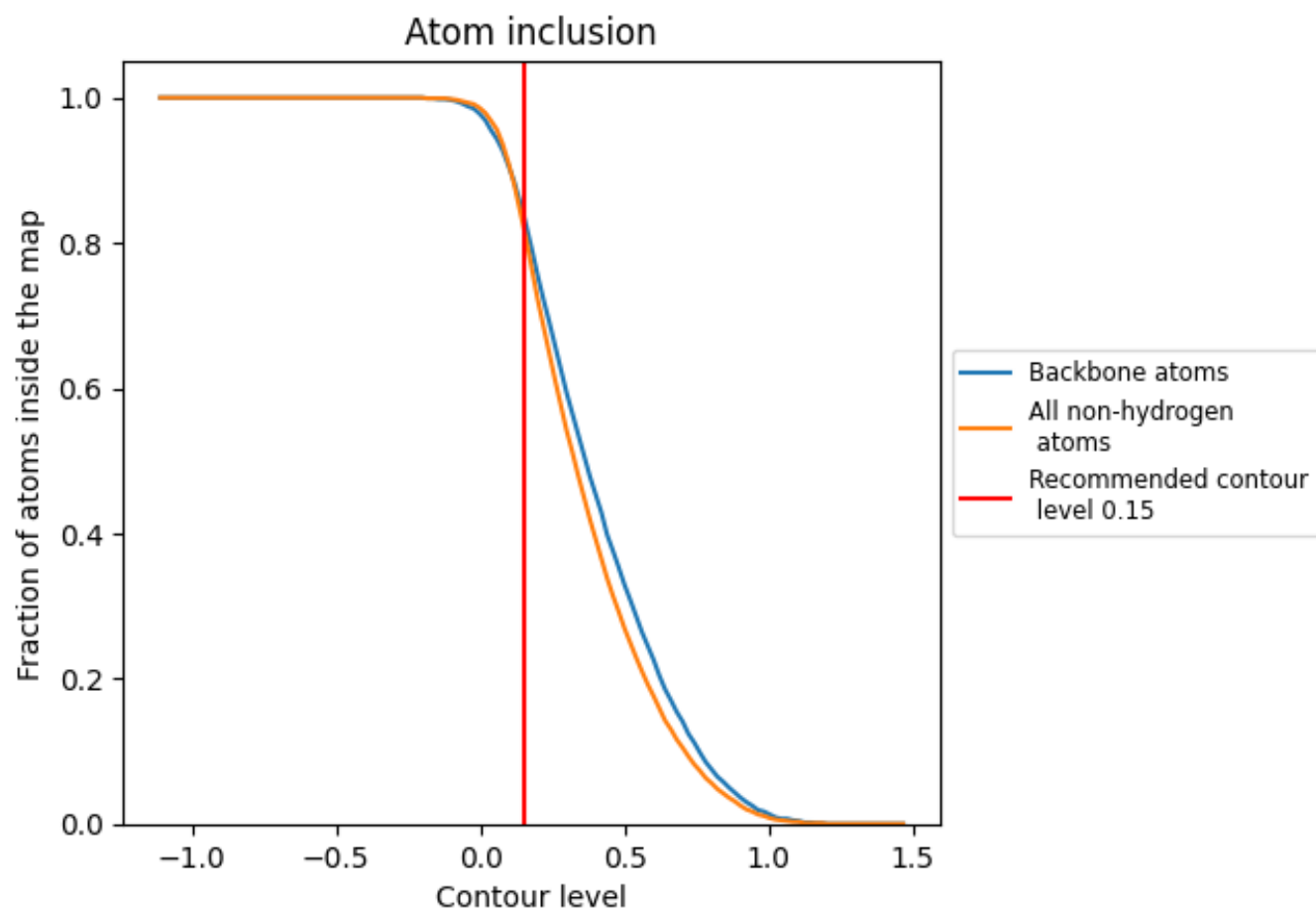
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.5430
A	0.8030	0.5380
B	0.8780	0.5720
G	0.8030	0.5400
N	0.8460	0.5520
R	0.7580	0.5050

