



# wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 05:17 PM JST

PDB ID : 8IHF  
EMDB ID : EMD-35443  
Title : Cryo-EM structure of HCA2-Gi complex with MK6892  
Authors : Suzuki, S.; Nishikawa, K.; Suzuki, H.; Fujiyoshi, Y.  
Deposited on : 2023-02-22  
Resolution : 2.97 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.39

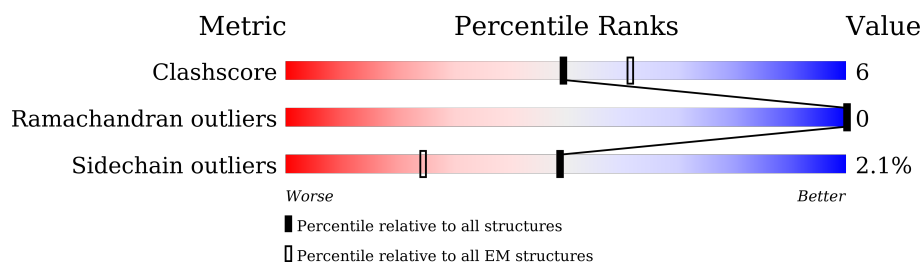
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	354	 51% 10% 38%
2	S	248	 77% 14% 9%
3	B	382	 77% 12% 11%
4	C	70	 79% 20%
5	R	658	 37% 7% 56%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8691 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1706	1086	285	324	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	GLY	engineered mutation	UNP P63096
A	219	ALA	THR	conflict	UNP P63096
A	288	GLN	PRO	conflict	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 2 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	226	Total	C	N	O	S	0	0
			1690	1075	277	329	9		

- 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	339	Total	C	N	O	S	0	0
			2485	1544	443	481	17		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P62874
B	-14	HIS	-	expression tag	UNP P62874
B	-13	HIS	-	expression tag	UNP P62874
B	-12	HIS	-	expression tag	UNP P62874
B	-11	HIS	-	expression tag	UNP P62874
B	-10	HIS	-	expression tag	UNP P62874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P62874
B	-8	HIS	-	expression tag	UNP P62874
B	-7	HIS	-	expression tag	UNP P62874
B	-6	GLU	-	expression tag	UNP P62874
B	-5	ASN	-	expression tag	UNP P62874
B	-4	LEU	-	expression tag	UNP P62874
B	-3	TYR	-	expression tag	UNP P62874
B	-2	PHE	-	expression tag	UNP P62874
B	-1	GLN	-	expression tag	UNP P62874
B	0	GLY	-	expression tag	UNP P62874
B	1	SER	-	expression tag	UNP P62874
B	341	GLY	-	expression tag	UNP P62874
B	342	GLY	-	expression tag	UNP P62874
B	343	SER	-	expression tag	UNP P62874
B	344	GLY	-	expression tag	UNP P62874
B	345	GLY	-	expression tag	UNP P62874
B	346	GLY	-	expression tag	UNP P62874
B	347	GLY	-	expression tag	UNP P62874
B	348	SER	-	expression tag	UNP P62874
B	349	GLY	-	expression tag	UNP P62874
B	350	GLY	-	expression tag	UNP P62874
B	351	SER	-	expression tag	UNP P62874
B	352	SER	-	expression tag	UNP P62874
B	353	SER	-	expression tag	UNP P62874
B	354	GLY	-	expression tag	UNP P62874
B	355	GLY	-	expression tag	UNP P62874
B	356	VAL	-	expression tag	UNP P62874
B	357	SER	-	expression tag	UNP P62874
B	358	GLY	-	expression tag	UNP P62874
B	359	TRP	-	expression tag	UNP P62874
B	360	ARG	-	expression tag	UNP P62874
B	361	LEU	-	expression tag	UNP P62874
B	362	PHE	-	expression tag	UNP P62874
B	363	LYS	-	expression tag	UNP P62874
B	364	LYS	-	expression tag	UNP P62874
B	365	ILE	-	expression tag	UNP P62874
B	366	SER	-	expression tag	UNP P62874

- 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	C	56	Total	C	N	O	S	0	0
			383	240	65	75	3		

- Molecule 5 is a protein called Soluble cytochrome b562,Hydroxycarboxylic acid receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	292	Total	C	N	O	S	0	0
			2385	1591	398	375	21		

There are 193 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-128	MET	-	initiating methionine	UNP P0ABE7
R	-127	LYS	-	expression tag	UNP P0ABE7
R	-126	THR	-	expression tag	UNP P0ABE7
R	-125	ILE	-	expression tag	UNP P0ABE7
R	-124	ILE	-	expression tag	UNP P0ABE7
R	-123	ALA	-	expression tag	UNP P0ABE7
R	-122	LEU	-	expression tag	UNP P0ABE7
R	-121	SER	-	expression tag	UNP P0ABE7
R	-120	TYR	-	expression tag	UNP P0ABE7
R	-119	ILE	-	expression tag	UNP P0ABE7
R	-118	PHE	-	expression tag	UNP P0ABE7
R	-117	CYS	-	expression tag	UNP P0ABE7
R	-116	LEU	-	expression tag	UNP P0ABE7
R	-115	VAL	-	expression tag	UNP P0ABE7
R	-114	PHE	-	expression tag	UNP P0ABE7
R	-113	ALA	-	expression tag	UNP P0ABE7
R	-112	ASP	-	expression tag	UNP P0ABE7
R	-111	TYR	-	expression tag	UNP P0ABE7
R	-110	LYS	-	expression tag	UNP P0ABE7
R	-109	ASP	-	expression tag	UNP P0ABE7
R	-108	ASP	-	expression tag	UNP P0ABE7
R	-107	ASP	-	expression tag	UNP P0ABE7
R	-106	ASP	-	expression tag	UNP P0ABE7
R	-105	LYS	-	expression tag	UNP P0ABE7
R	-98	TRP	MET	engineered mutation	UNP P0ABE7
R	-3	ILE	HIS	engineered mutation	UNP P0ABE7
R	1	LEU	-	linker	UNP P0ABE7
R	364	GLU	-	expression tag	UNP Q8TDS4
R	365	ASN	-	expression tag	UNP Q8TDS4
R	366	LEU	-	expression tag	UNP Q8TDS4
R	367	TYR	-	expression tag	UNP Q8TDS4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	368	PHE	-	expression tag	UNP Q8TDS4
R	369	GLN	-	expression tag	UNP Q8TDS4
R	370	GLY	-	expression tag	UNP Q8TDS4
R	371	SER	-	expression tag	UNP Q8TDS4
R	372	VAL	-	expression tag	UNP Q8TDS4
R	373	PHE	-	expression tag	UNP Q8TDS4
R	374	THR	-	expression tag	UNP Q8TDS4
R	375	LEU	-	expression tag	UNP Q8TDS4
R	376	GLU	-	expression tag	UNP Q8TDS4
R	377	ASP	-	expression tag	UNP Q8TDS4
R	378	PHE	-	expression tag	UNP Q8TDS4
R	379	VAL	-	expression tag	UNP Q8TDS4
R	380	GLY	-	expression tag	UNP Q8TDS4
R	381	ASP	-	expression tag	UNP Q8TDS4
R	382	TRP	-	expression tag	UNP Q8TDS4
R	383	GLU	-	expression tag	UNP Q8TDS4
R	384	GLN	-	expression tag	UNP Q8TDS4
R	385	THR	-	expression tag	UNP Q8TDS4
R	386	ALA	-	expression tag	UNP Q8TDS4
R	387	ALA	-	expression tag	UNP Q8TDS4
R	388	TYR	-	expression tag	UNP Q8TDS4
R	389	ASN	-	expression tag	UNP Q8TDS4
R	390	LEU	-	expression tag	UNP Q8TDS4
R	391	ASP	-	expression tag	UNP Q8TDS4
R	392	GLN	-	expression tag	UNP Q8TDS4
R	393	VAL	-	expression tag	UNP Q8TDS4
R	394	LEU	-	expression tag	UNP Q8TDS4
R	395	GLU	-	expression tag	UNP Q8TDS4
R	396	GLN	-	expression tag	UNP Q8TDS4
R	397	GLY	-	expression tag	UNP Q8TDS4
R	398	GLY	-	expression tag	UNP Q8TDS4
R	399	VAL	-	expression tag	UNP Q8TDS4
R	400	SER	-	expression tag	UNP Q8TDS4
R	401	SER	-	expression tag	UNP Q8TDS4
R	402	LEU	-	expression tag	UNP Q8TDS4
R	403	LEU	-	expression tag	UNP Q8TDS4
R	404	GLN	-	expression tag	UNP Q8TDS4
R	405	ASN	-	expression tag	UNP Q8TDS4
R	406	LEU	-	expression tag	UNP Q8TDS4
R	407	ALA	-	expression tag	UNP Q8TDS4
R	408	VAL	-	expression tag	UNP Q8TDS4
R	409	SER	-	expression tag	UNP Q8TDS4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	410	VAL	-	expression tag	UNP Q8TDS4
R	411	THR	-	expression tag	UNP Q8TDS4
R	412	PRO	-	expression tag	UNP Q8TDS4
R	413	ILE	-	expression tag	UNP Q8TDS4
R	414	GLN	-	expression tag	UNP Q8TDS4
R	415	ARG	-	expression tag	UNP Q8TDS4
R	416	ILE	-	expression tag	UNP Q8TDS4
R	417	VAL	-	expression tag	UNP Q8TDS4
R	418	ARG	-	expression tag	UNP Q8TDS4
R	419	SER	-	expression tag	UNP Q8TDS4
R	420	GLY	-	expression tag	UNP Q8TDS4
R	421	GLU	-	expression tag	UNP Q8TDS4
R	422	ASN	-	expression tag	UNP Q8TDS4
R	423	ALA	-	expression tag	UNP Q8TDS4
R	424	LEU	-	expression tag	UNP Q8TDS4
R	425	LYS	-	expression tag	UNP Q8TDS4
R	426	ILE	-	expression tag	UNP Q8TDS4
R	427	ASP	-	expression tag	UNP Q8TDS4
R	428	ILE	-	expression tag	UNP Q8TDS4
R	429	HIS	-	expression tag	UNP Q8TDS4
R	430	VAL	-	expression tag	UNP Q8TDS4
R	431	ILE	-	expression tag	UNP Q8TDS4
R	432	ILE	-	expression tag	UNP Q8TDS4
R	433	PRO	-	expression tag	UNP Q8TDS4
R	434	TYR	-	expression tag	UNP Q8TDS4
R	435	GLU	-	expression tag	UNP Q8TDS4
R	436	GLY	-	expression tag	UNP Q8TDS4
R	437	LEU	-	expression tag	UNP Q8TDS4
R	438	SER	-	expression tag	UNP Q8TDS4
R	439	ALA	-	expression tag	UNP Q8TDS4
R	440	ASP	-	expression tag	UNP Q8TDS4
R	441	GLN	-	expression tag	UNP Q8TDS4
R	442	MET	-	expression tag	UNP Q8TDS4
R	443	ALA	-	expression tag	UNP Q8TDS4
R	444	GLN	-	expression tag	UNP Q8TDS4
R	445	ILE	-	expression tag	UNP Q8TDS4
R	446	GLU	-	expression tag	UNP Q8TDS4
R	447	GLU	-	expression tag	UNP Q8TDS4
R	448	VAL	-	expression tag	UNP Q8TDS4
R	449	PHE	-	expression tag	UNP Q8TDS4
R	450	LYS	-	expression tag	UNP Q8TDS4
R	451	VAL	-	expression tag	UNP Q8TDS4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	452	VAL	-	expression tag	UNP Q8TDS4
R	453	TYR	-	expression tag	UNP Q8TDS4
R	454	PRO	-	expression tag	UNP Q8TDS4
R	455	VAL	-	expression tag	UNP Q8TDS4
R	456	ASP	-	expression tag	UNP Q8TDS4
R	457	ASP	-	expression tag	UNP Q8TDS4
R	458	HIS	-	expression tag	UNP Q8TDS4
R	459	HIS	-	expression tag	UNP Q8TDS4
R	460	PHE	-	expression tag	UNP Q8TDS4
R	461	LYS	-	expression tag	UNP Q8TDS4
R	462	VAL	-	expression tag	UNP Q8TDS4
R	463	ILE	-	expression tag	UNP Q8TDS4
R	464	LEU	-	expression tag	UNP Q8TDS4
R	465	PRO	-	expression tag	UNP Q8TDS4
R	466	TYR	-	expression tag	UNP Q8TDS4
R	467	GLY	-	expression tag	UNP Q8TDS4
R	468	THR	-	expression tag	UNP Q8TDS4
R	469	LEU	-	expression tag	UNP Q8TDS4
R	470	VAL	-	expression tag	UNP Q8TDS4
R	471	ILE	-	expression tag	UNP Q8TDS4
R	472	ASP	-	expression tag	UNP Q8TDS4
R	473	GLY	-	expression tag	UNP Q8TDS4
R	474	VAL	-	expression tag	UNP Q8TDS4
R	475	THR	-	expression tag	UNP Q8TDS4
R	476	PRO	-	expression tag	UNP Q8TDS4
R	477	ASN	-	expression tag	UNP Q8TDS4
R	478	MET	-	expression tag	UNP Q8TDS4
R	479	LEU	-	expression tag	UNP Q8TDS4
R	480	ASN	-	expression tag	UNP Q8TDS4
R	481	TYR	-	expression tag	UNP Q8TDS4
R	482	PHE	-	expression tag	UNP Q8TDS4
R	483	GLY	-	expression tag	UNP Q8TDS4
R	484	ARG	-	expression tag	UNP Q8TDS4
R	485	PRO	-	expression tag	UNP Q8TDS4
R	486	TYR	-	expression tag	UNP Q8TDS4
R	487	GLU	-	expression tag	UNP Q8TDS4
R	488	GLY	-	expression tag	UNP Q8TDS4
R	489	ILE	-	expression tag	UNP Q8TDS4
R	490	ALA	-	expression tag	UNP Q8TDS4
R	491	VAL	-	expression tag	UNP Q8TDS4
R	492	PHE	-	expression tag	UNP Q8TDS4
R	493	ASP	-	expression tag	UNP Q8TDS4

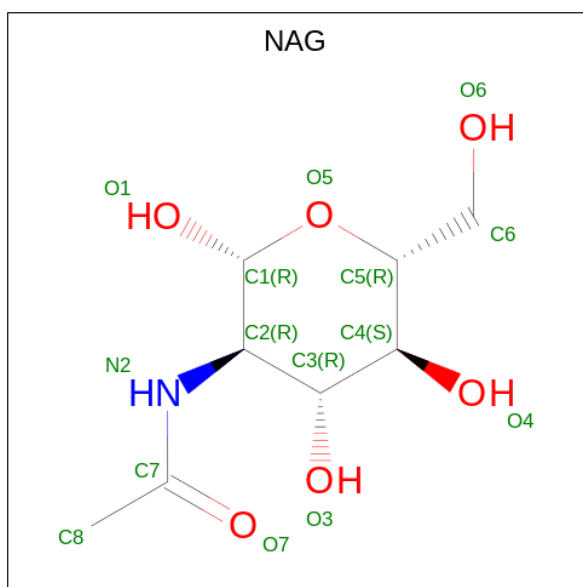
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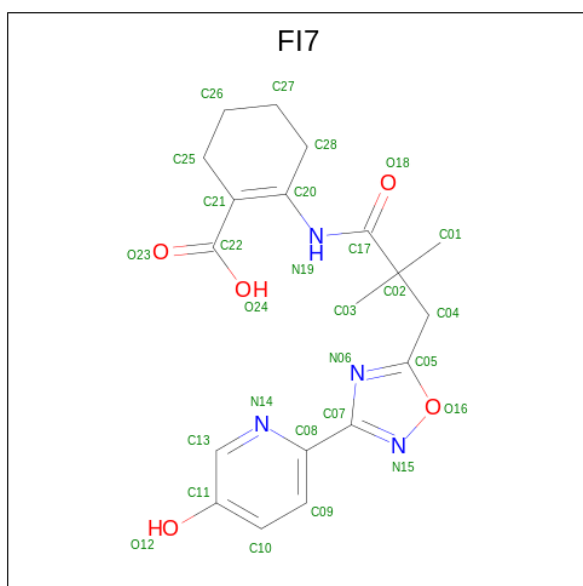
Chain	Residue	Modelled	Actual	Comment	Reference
R	494	GLY	-	expression tag	UNP Q8TDS4
R	495	LYS	-	expression tag	UNP Q8TDS4
R	496	LYS	-	expression tag	UNP Q8TDS4
R	497	ILE	-	expression tag	UNP Q8TDS4
R	498	THR	-	expression tag	UNP Q8TDS4
R	499	VAL	-	expression tag	UNP Q8TDS4
R	500	THR	-	expression tag	UNP Q8TDS4
R	501	GLY	-	expression tag	UNP Q8TDS4
R	502	THR	-	expression tag	UNP Q8TDS4
R	503	LEU	-	expression tag	UNP Q8TDS4
R	504	TRP	-	expression tag	UNP Q8TDS4
R	505	ASN	-	expression tag	UNP Q8TDS4
R	506	GLY	-	expression tag	UNP Q8TDS4
R	507	ASN	-	expression tag	UNP Q8TDS4
R	508	LYS	-	expression tag	UNP Q8TDS4
R	509	ILE	-	expression tag	UNP Q8TDS4
R	510	ILE	-	expression tag	UNP Q8TDS4
R	511	ASP	-	expression tag	UNP Q8TDS4
R	512	GLU	-	expression tag	UNP Q8TDS4
R	513	ARG	-	expression tag	UNP Q8TDS4
R	514	LEU	-	expression tag	UNP Q8TDS4
R	515	ILE	-	expression tag	UNP Q8TDS4
R	516	THR	-	expression tag	UNP Q8TDS4
R	517	PRO	-	expression tag	UNP Q8TDS4
R	518	ASP	-	expression tag	UNP Q8TDS4
R	519	GLY	-	expression tag	UNP Q8TDS4
R	520	SER	-	expression tag	UNP Q8TDS4
R	521	MET	-	expression tag	UNP Q8TDS4
R	522	LEU	-	expression tag	UNP Q8TDS4
R	523	PHE	-	expression tag	UNP Q8TDS4
R	524	ARG	-	expression tag	UNP Q8TDS4
R	525	VAL	-	expression tag	UNP Q8TDS4
R	526	THR	-	expression tag	UNP Q8TDS4
R	527	ILE	-	expression tag	UNP Q8TDS4
R	528	ASN	-	expression tag	UNP Q8TDS4
R	529	SER	-	expression tag	UNP Q8TDS4

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is 2-[[2,2-dimethyl-3-[3-(5-oxidanylpurin-2-yl)-1,2,4-oxadiazol-5-yl]propanoyl]amino]cyclohexene-1-carboxylic acid (three-letter code: FI7) (formula:  $C_{19}H_{22}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).

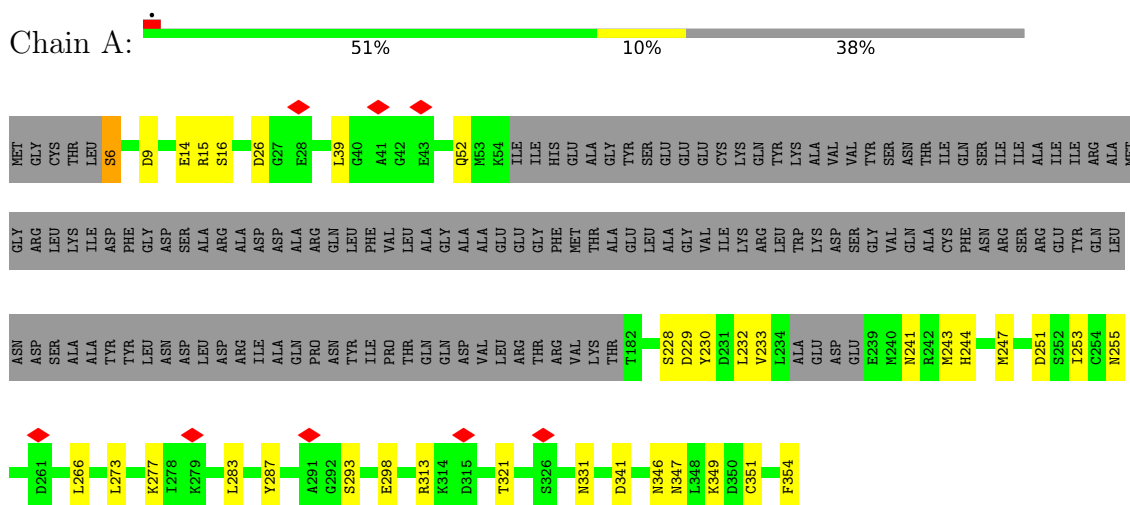


Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			28	19	4	5	

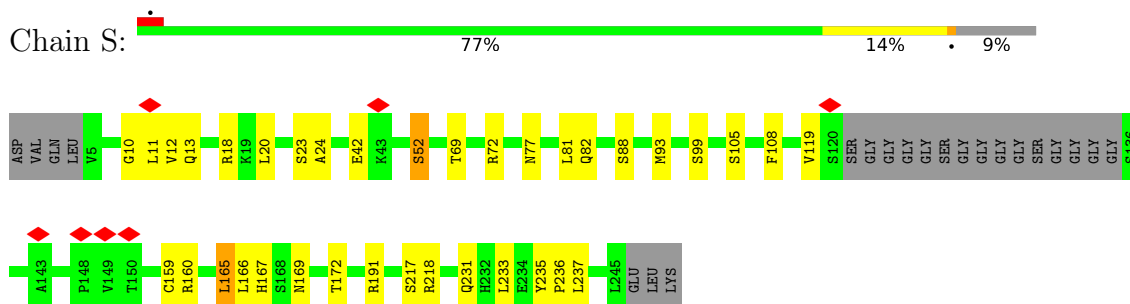
### 3 Residue-property plots [i](#)

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.

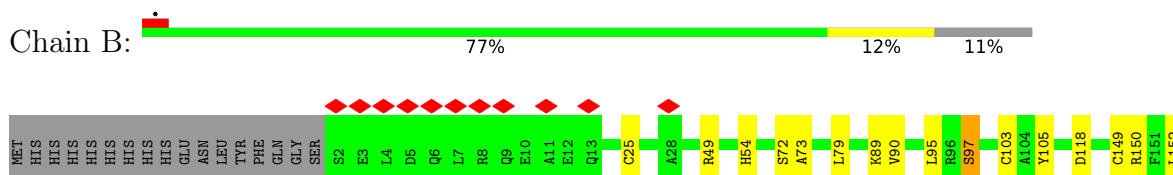
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



- Molecule 2: scFv16



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.884	Depositor
Minimum map value	-1.177	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.188	Depositor
Map size ( $\text{\AA}$ )	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: FI7, NAG

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	0.24	0/1734	0.43	0/2332
2	S	0.27	0/1734	0.51	0/2359
3	B	0.29	0/2532	0.51	0/3450
4	C	0.24	0/389	0.39	0/534
5	R	0.25	0/2455	0.48	0/3330
All	All	0.26	0/8844	0.48	0/12005

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	1706	0	1638	21	0
2	S	1690	0	1588	23	0
3	B	2485	0	2307	27	0
4	C	383	0	339	1	0
5	R	2385	0	2440	29	0
6	R	14	0	13	1	0
7	R	28	0	0	3	0
All	All	8691	0	8325	94	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 6.

The worst 5 of 94 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)
5:R:18:CYS:HA	5:R:183:CYS:HB3	1.53	0.90
1:A:15:ARG:NH1	3:B:90:VAL:O	2.22	0.73
2:S:231:GLN:HE21	2:S:237:LEU:HA	1.52	0.73
5:R:170:GLN:NE2	5:R:172:GLY:O	2.23	0.71
3:B:25:CYS:SG	3:B:259:GLN:NE2	2.67	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/354 (60%)	211 (100%)	1 (0%)	0	100	100
2	S	222/248 (90%)	202 (91%)	20 (9%)	0	100	100
3	B	337/382 (88%)	327 (97%)	10 (3%)	0	100	100
4	C	54/70 (77%)	54 (100%)	0	0	100	100
5	R	290/658 (44%)	279 (96%)	11 (4%)	0	100	100
All	All	1115/1712 (65%)	1073 (96%)	42 (4%)	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	A	178/305 (58%)	173 (97%)	5 (3%)	38	69
2	S	180/201 (90%)	176 (98%)	4 (2%)	47	74
3	B	249/313 (80%)	244 (98%)	5 (2%)	50	76
4	C	33/57 (58%)	33 (100%)	0	100	100
5	R	263/580 (45%)	258 (98%)	5 (2%)	52	77
All	All	903/1456 (62%)	884 (98%)	19 (2%)	49	75

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	23	ASP
5	R	59	TRP
5	R	189	HIS
5	R	55	HIS
2	S	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	231	GLN
3	B	259	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
7	FI7	R	602	-	25,30,30	1.01	2 (8%)	30,43,43	0.69	1 (3%)
6	NAG	R	601	5	14,14,15	0.23	0	17,19,21	0.48	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
7	FI7	R	602	-	-	8/21/34/34	0/3/3/3
6	NAG	R	601	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	602	FI7	O23-C22	3.19	1.31	1.22
7	R	602	FI7	O24-C22	-2.78	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	602	FI7	O23-C22-C21	-2.54	115.17	122.46

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	602	FI7	C20-C21-C22-O24
7	R	602	FI7	C25-C21-C22-O23
7	R	602	FI7	C25-C21-C22-O24

*Continued on next page...*

*Continued from previous page...*

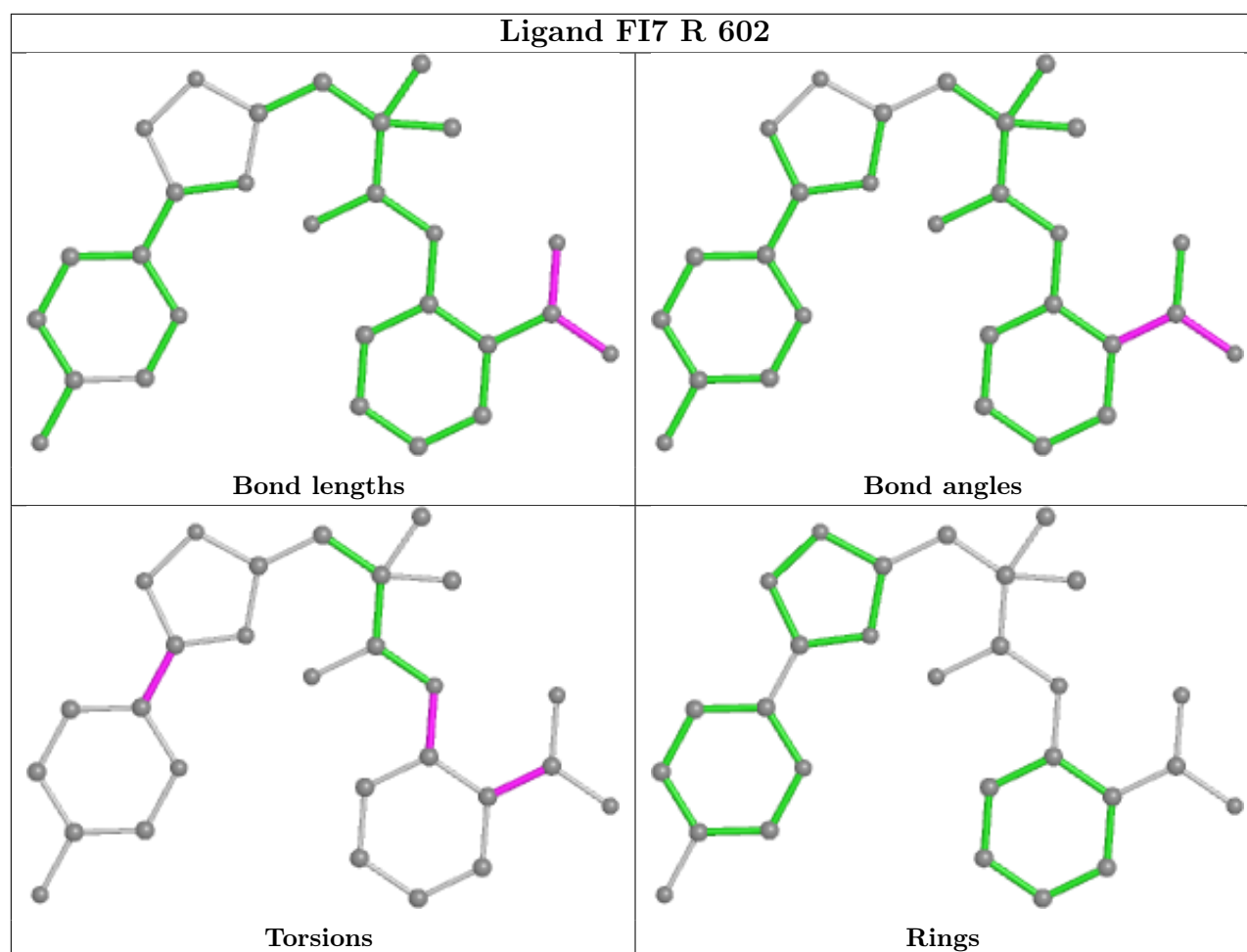
Mol	Chain	Res	Type	Atoms
7	R	602	FI7	C28-C20-N19-C17
7	R	602	FI7	C21-C20-N19-C17

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	602	FI7	3	0
6	R	601	NAG	1	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.

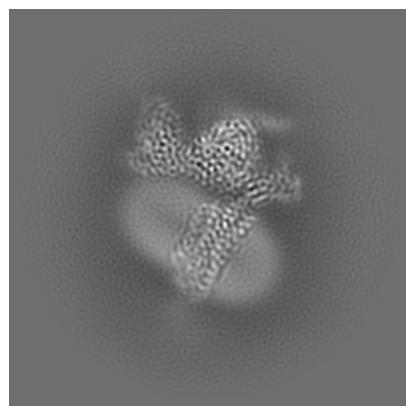
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35443. These allow visual inspection of the internal detail of the map and identification of artifacts.

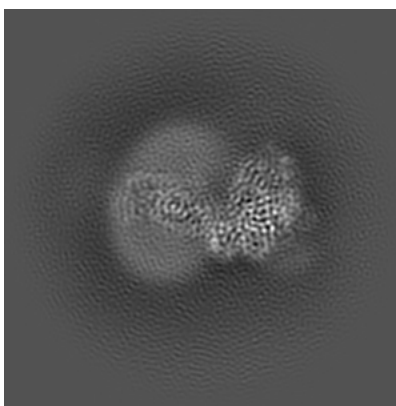
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

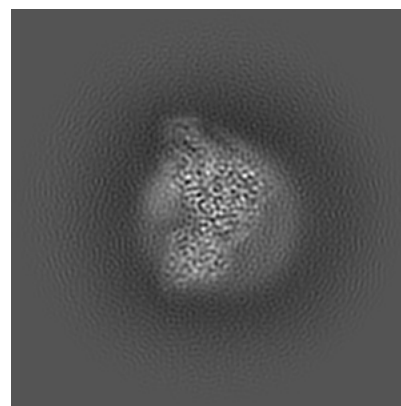
#### 6.1.1 Primary map



X

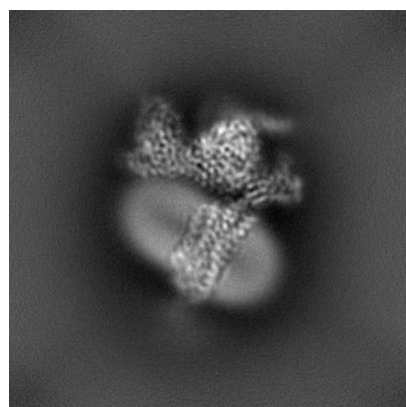


Y

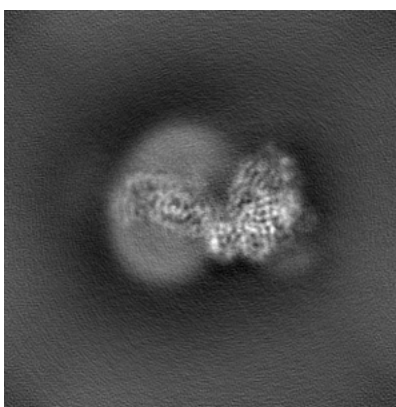


Z

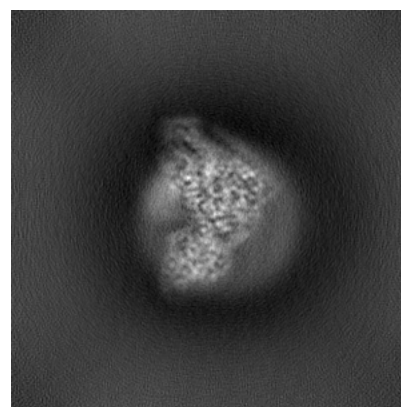
#### 6.1.2 Raw map



X



Y

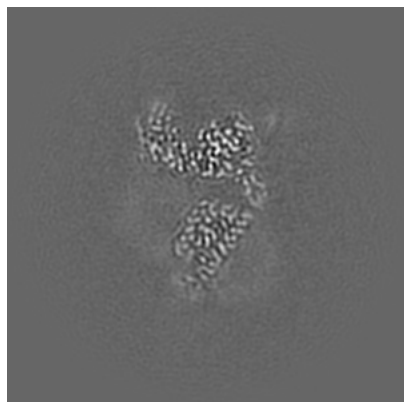


Z

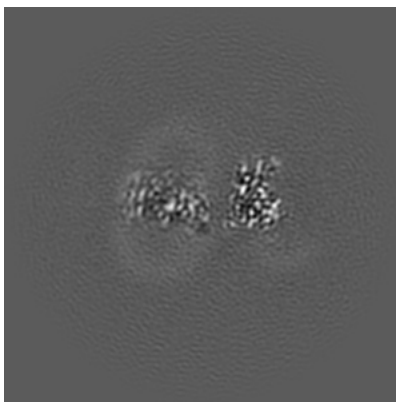
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

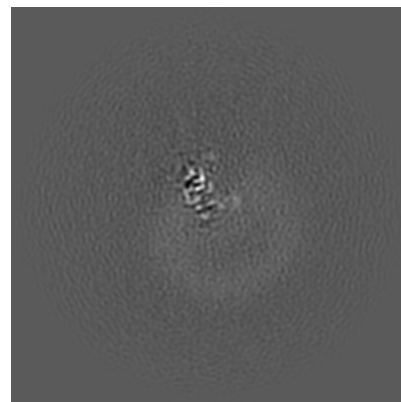
### 6.2.1 Primary map



X Index: 144

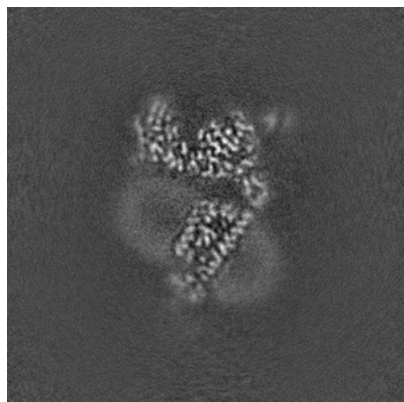


Y Index: 144

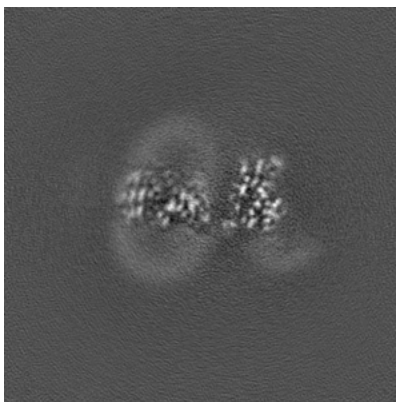


Z Index: 144

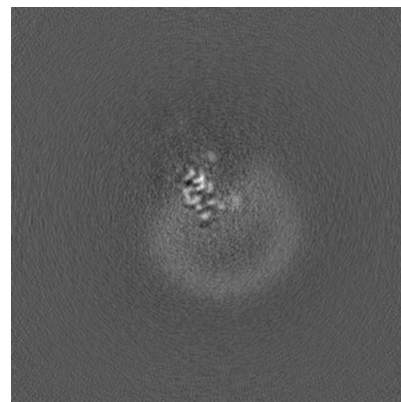
### 6.2.2 Raw map



X Index: 144



Y Index: 144

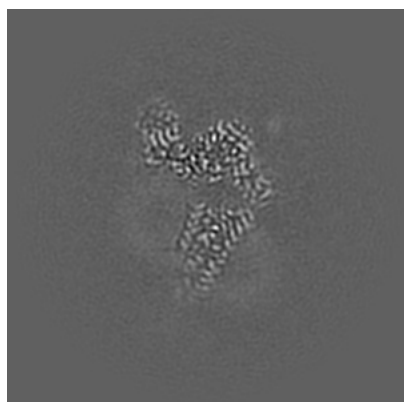


Z Index: 144

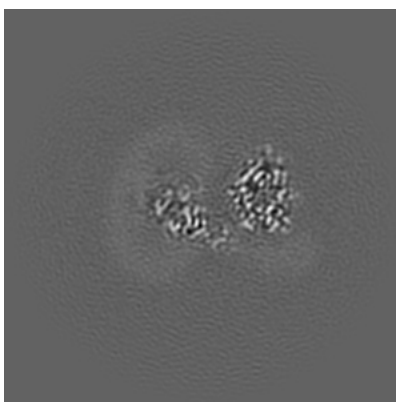
The images above show central slices of the map in three orthogonal directions.

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

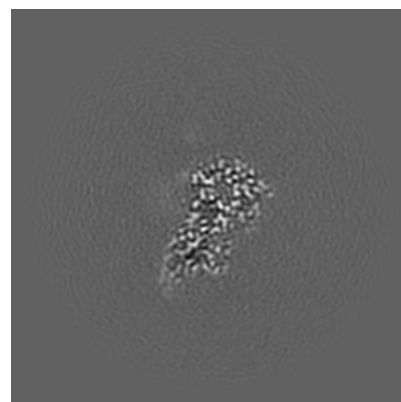
### 6.3.1 Primary map



X Index: 141

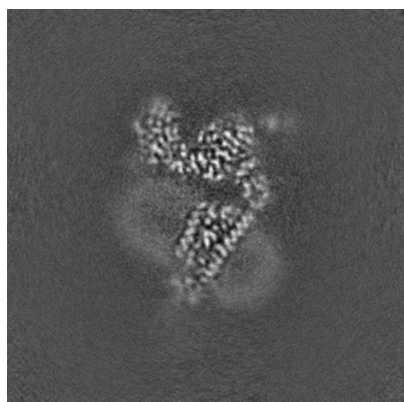


Y Index: 156

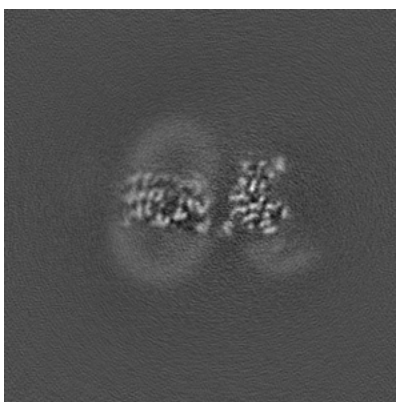


Z Index: 185

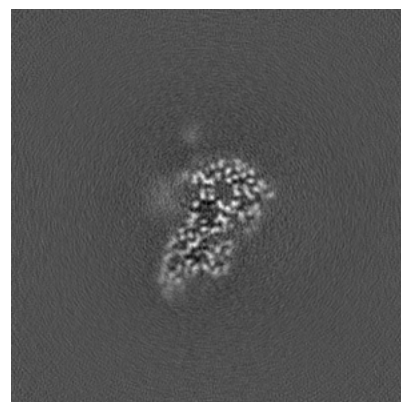
### 6.3.2 Raw map



X Index: 143



Y Index: 146



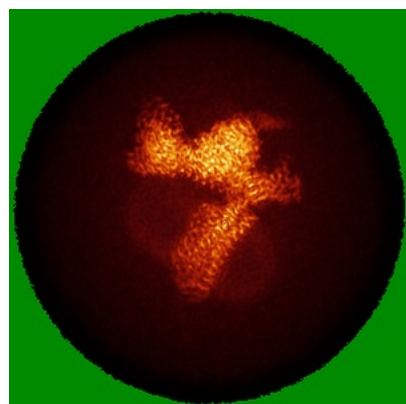
Z Index: 185

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

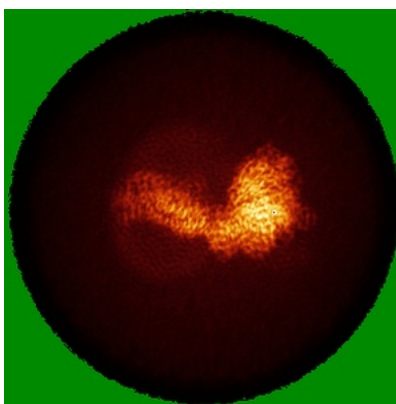


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

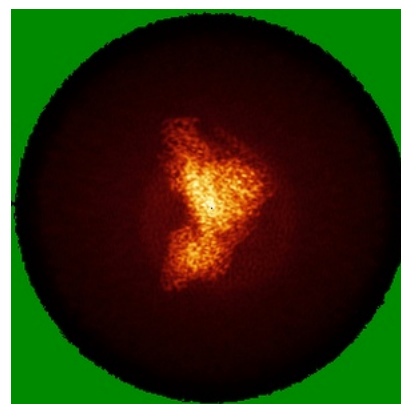
### 6.4.1 Primary map



X

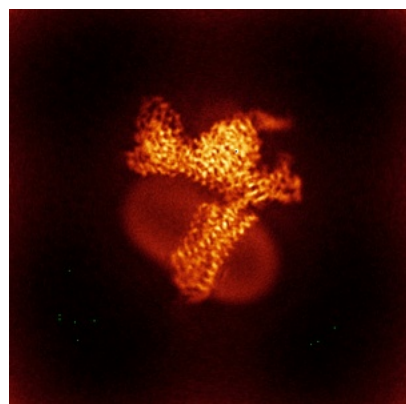


Y

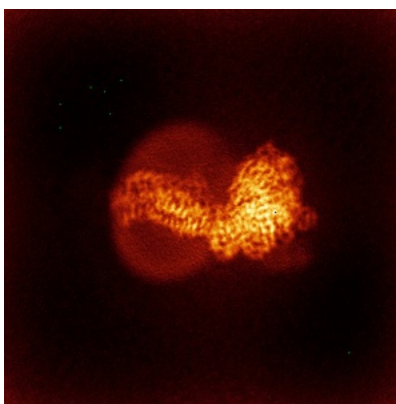


Z

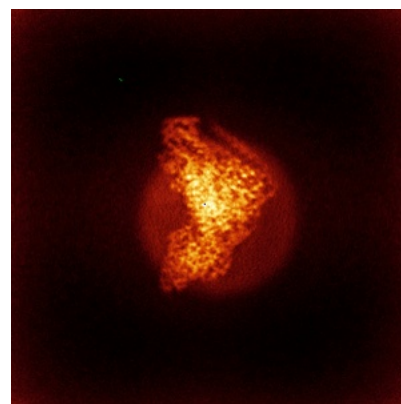
### 6.4.2 Raw map



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 0.188. 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.

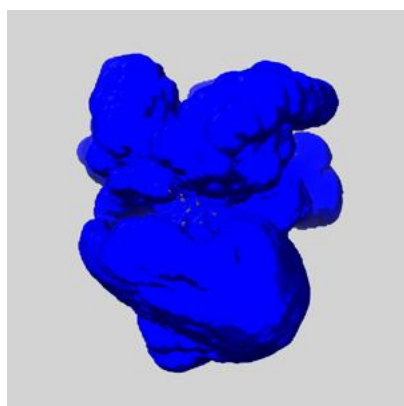
## 6.6 Mask visualisation [i](#)

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

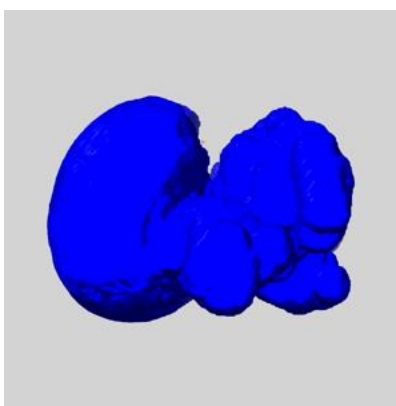
A mask typically either:

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

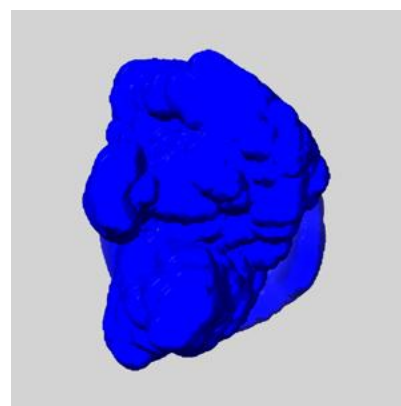
### 6.6.1 emd\_35443\_msk\_1.map [i](#)



X



Y

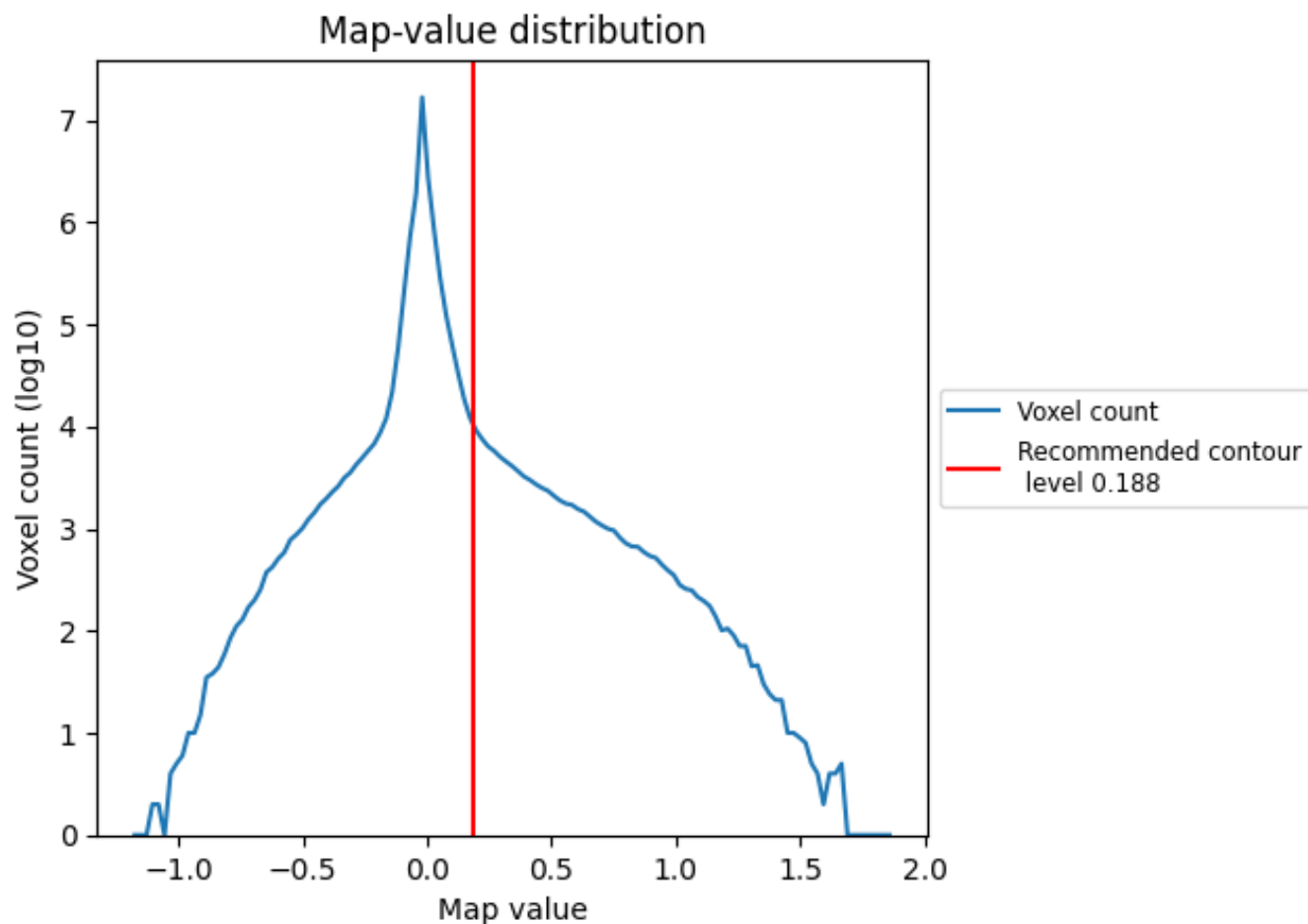


Z

## 7 Map analysis [i](#)

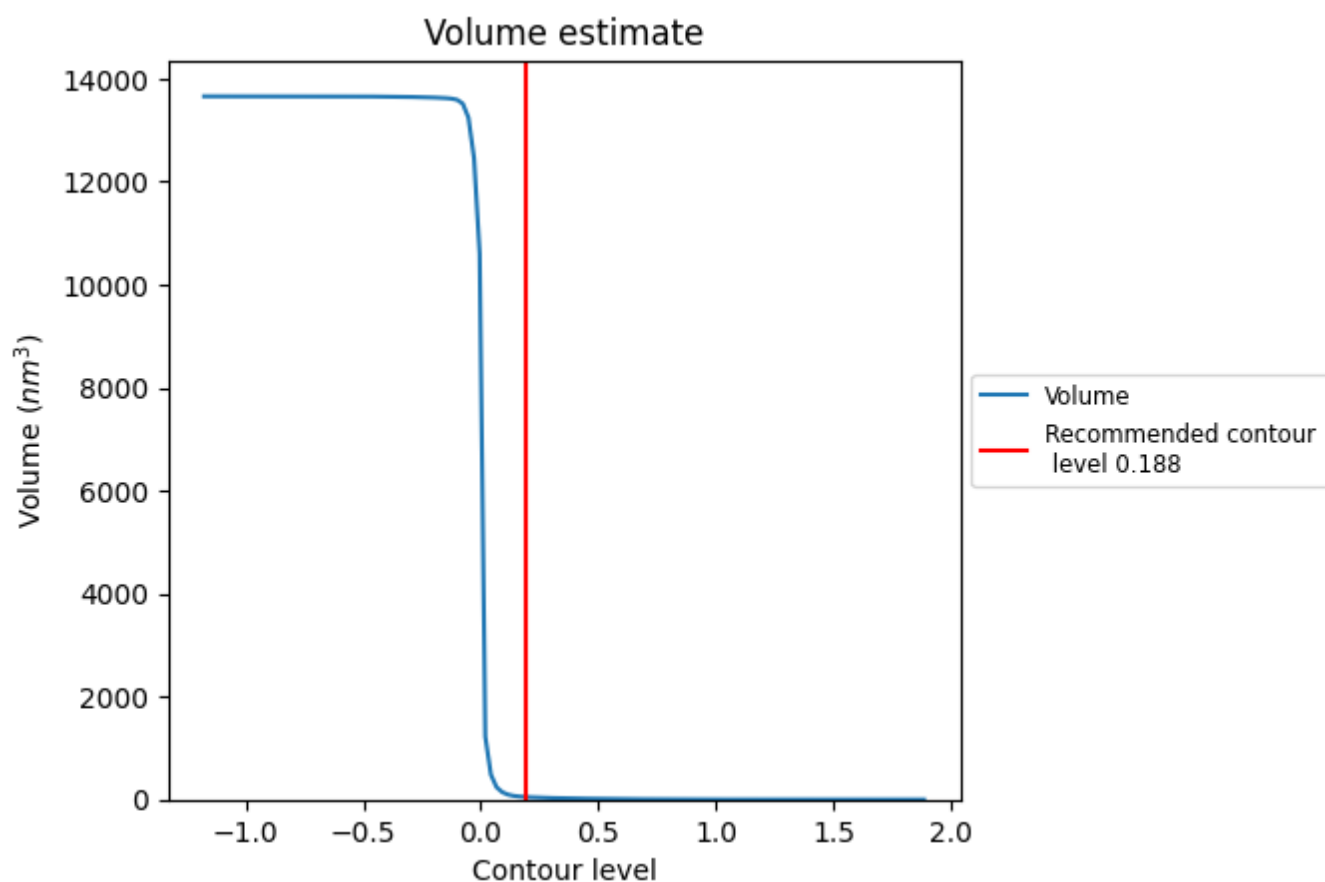
This section contains the results of statistical analysis of the map.

### 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.

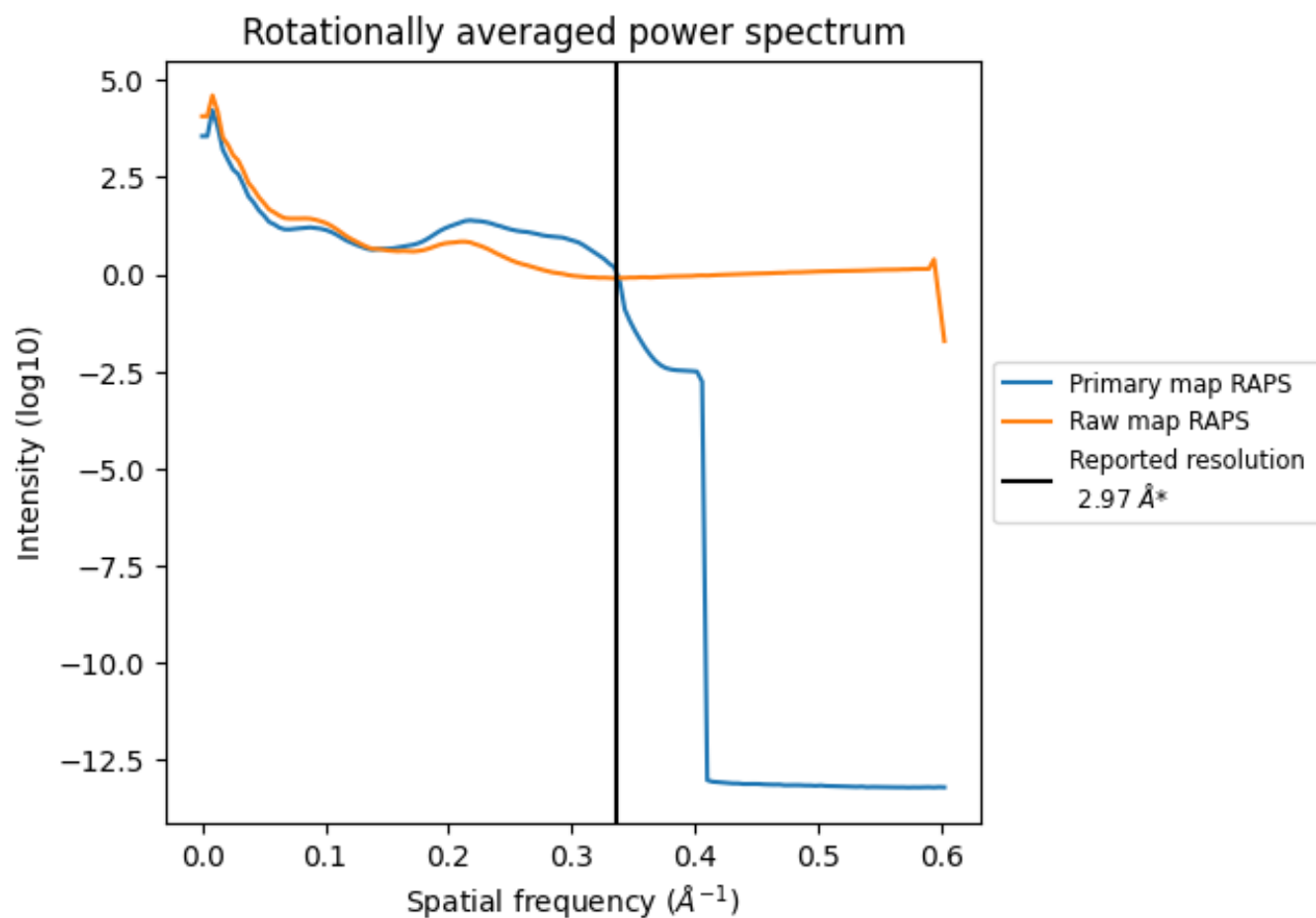
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm<sup>3</sup>; 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 ⓘ

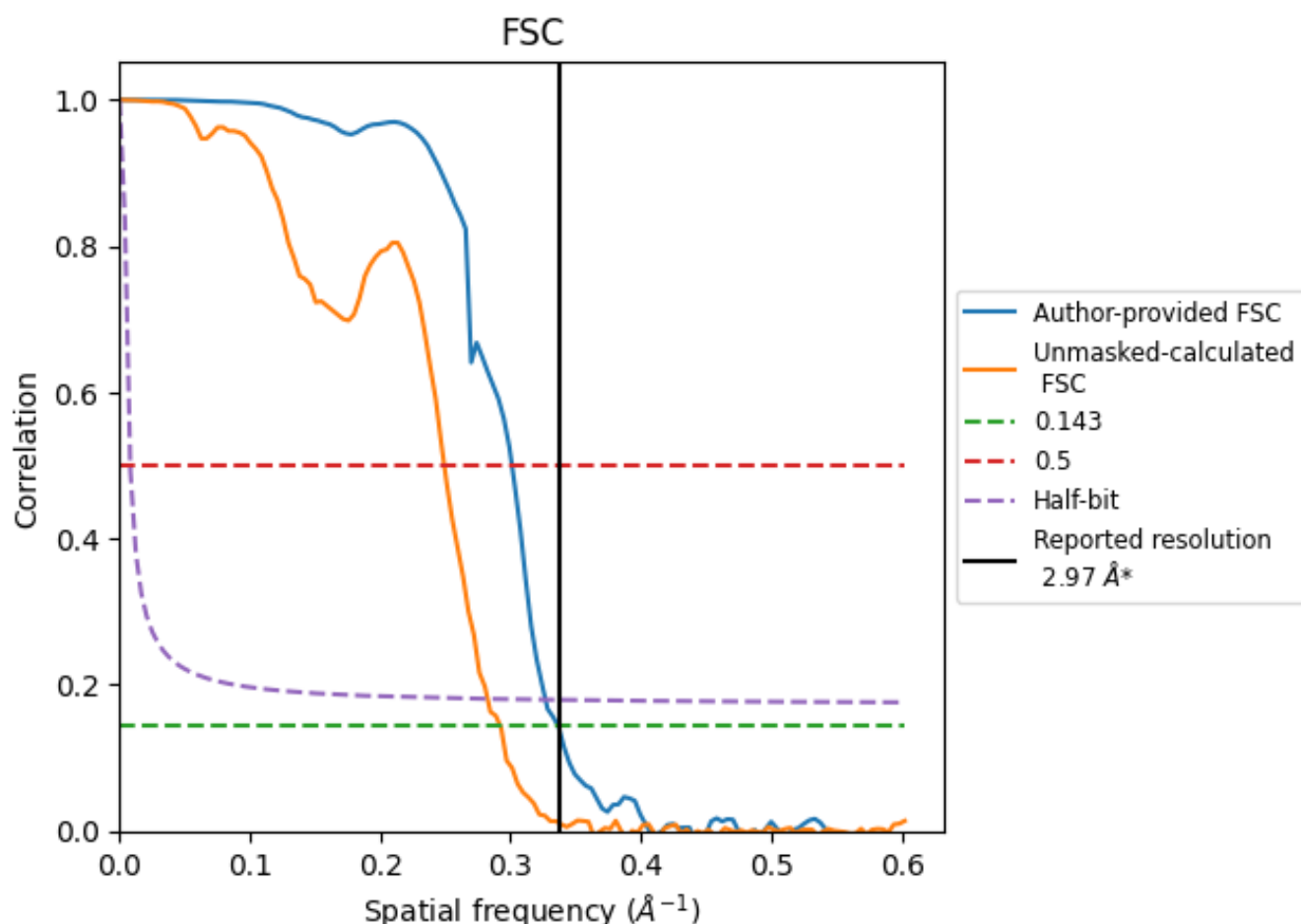


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 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 0.337 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

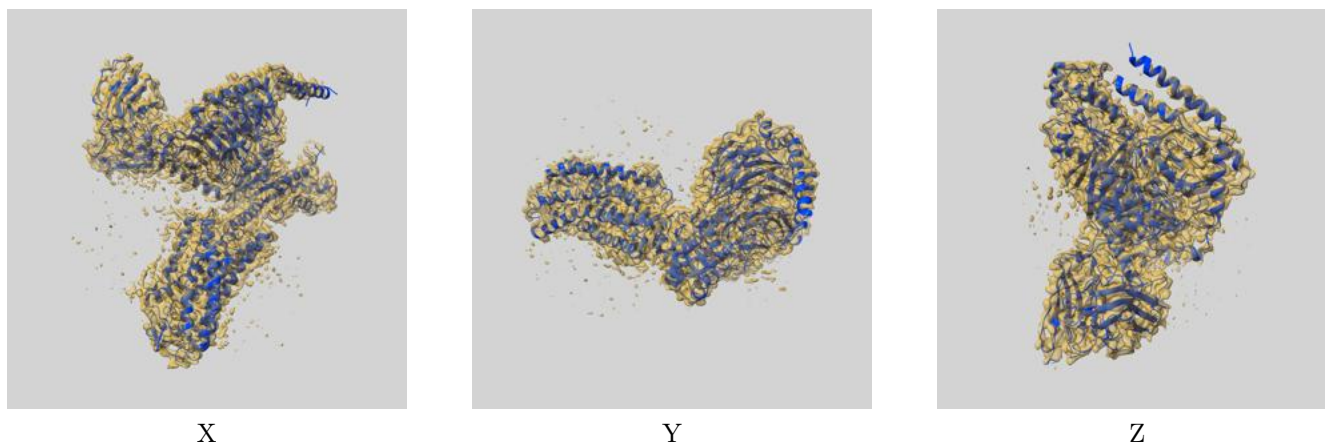
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.32	3.06
Unmasked-calculated*	3.42	4.01	3.54

\*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 3.42 differs from the reported value 2.97 by more than 10 %

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

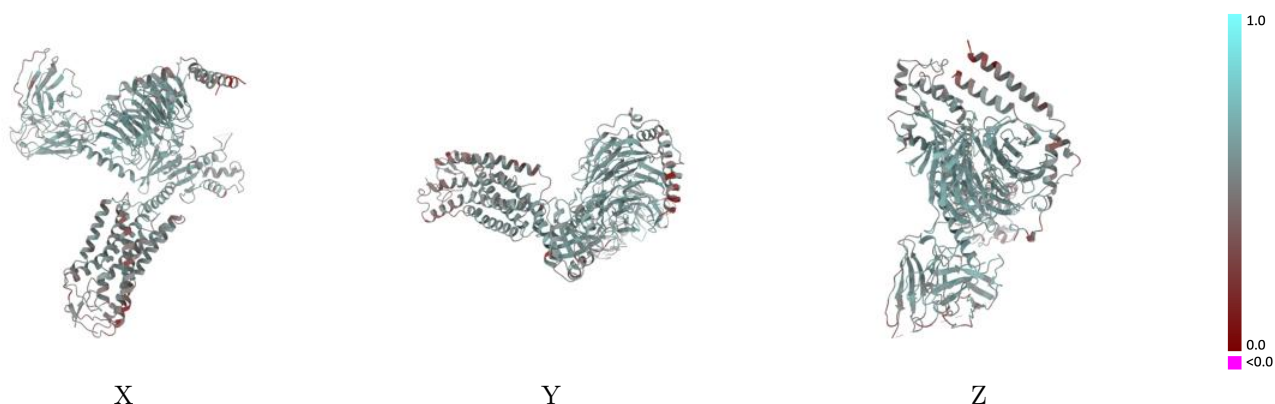
This section contains information regarding the fit between EMDB map EMD-35443 and PDB model 8IHF. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



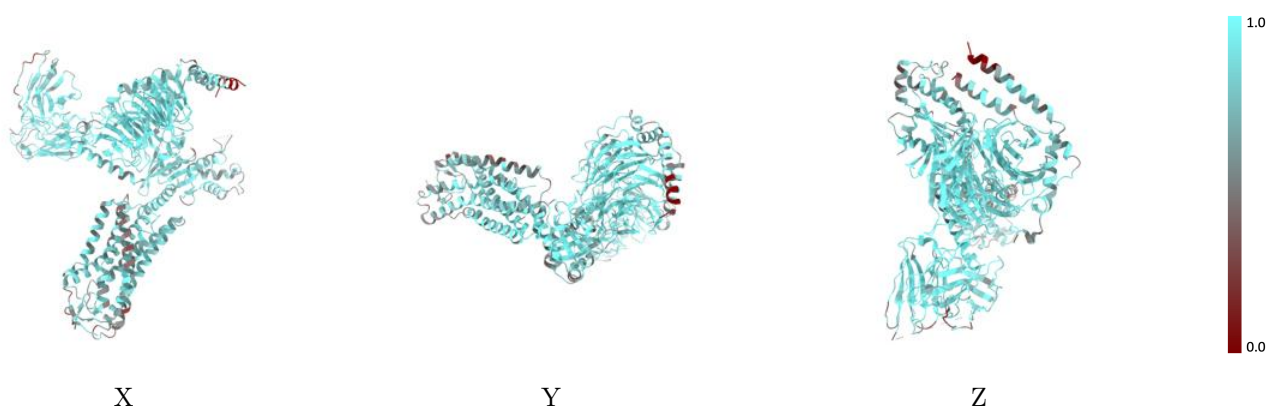
The images above show the 3D surface view of the map at the recommended contour level 0.188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



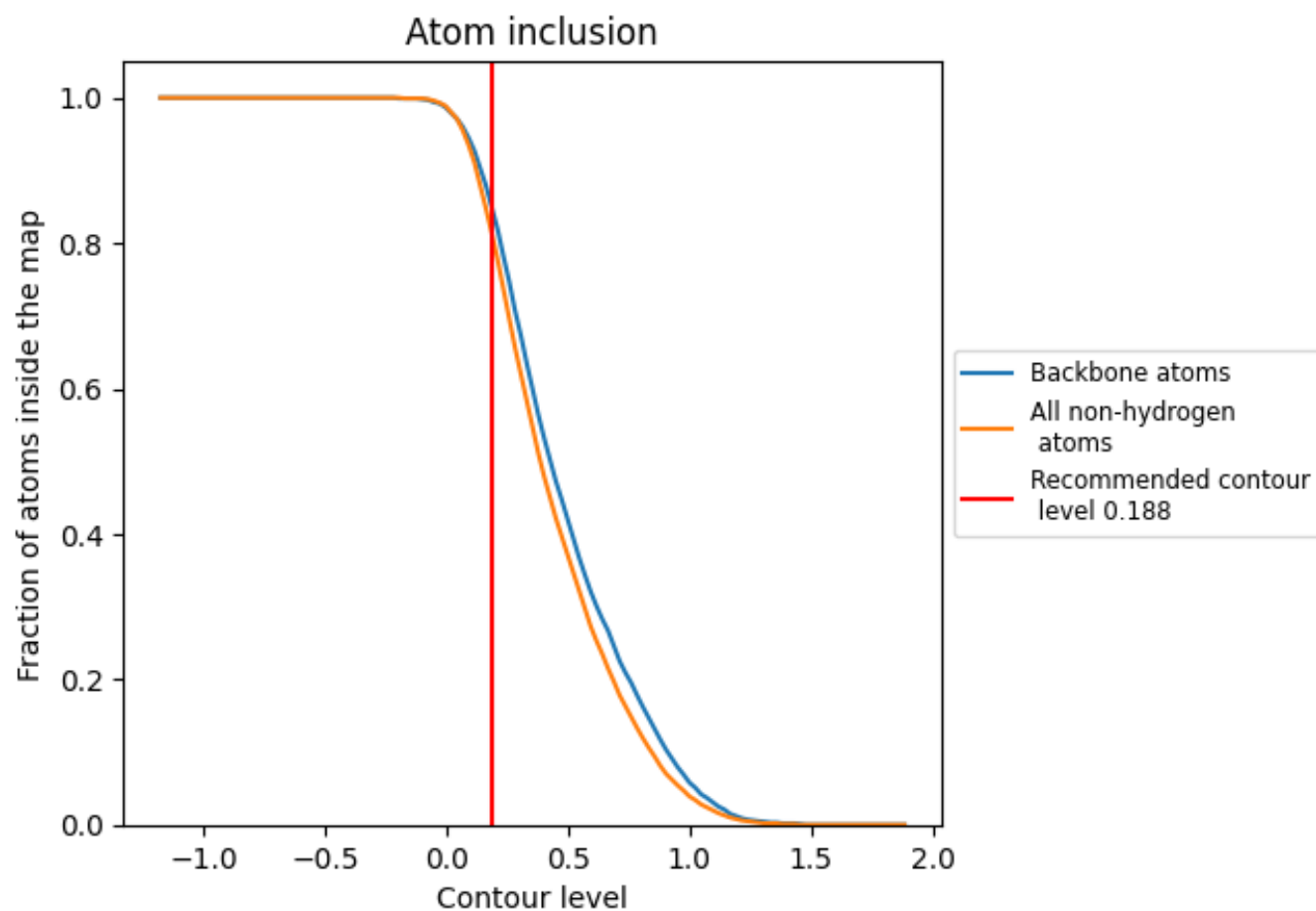
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.188).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8110	<div></div> 0.5370
A	<div></div> 0.8060	<div></div> 0.5460
B	<div></div> 0.8920	<div></div> 0.5800
C	<div></div> 0.6970	<div></div> 0.4880
R	<div></div> 0.7330	<div></div> 0.4900
S	<div></div> 0.8360	<div></div> 0.5430

