



Full wwPDB EM Validation Report ⓘ

May 10, 2025 – 02:15 PM EDT

PDB ID : 9O38 / pdb_00009o38
EMDB ID : EMD-70072
Title : Transmembrane domains of the human sweet receptor (TAS1R2 + TAS1R3)
from Class 3 particles (rigidly fitted from PDB:9NOX and 9NOR)
Authors : Juen, Z.; Lu, Z.; Yu, R.; Chang, A.N.; Wang, B.; Fitzpatrick, A.W.P.; Zuker,
C.S.
Deposited on : 2025-04-06
Resolution : 3.00 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

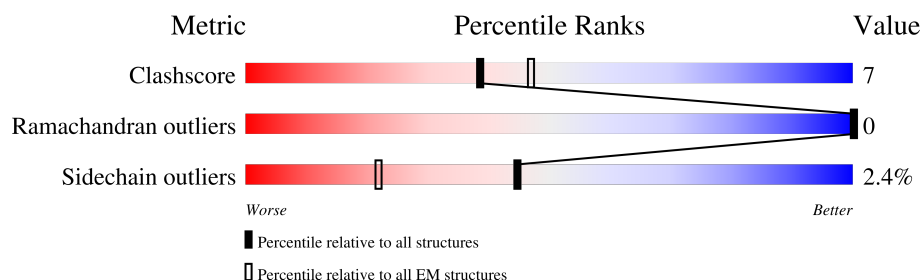
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	1128	
1	F	1128	
2	C	340	
3	D	71	
4	E	160	
5	A	848	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9824 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 Taste receptor type 1 member 3, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	238	Total	C	N	O	S	0	0
			1954	1236	346	366	6		
1	F	243	Total	C	N	O	S	0	0
			1859	1242	305	298	14		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-877	MET	-	expression tag	UNP Q7RTX0
B	-876	LYS	-	expression tag	UNP Q7RTX0
B	-875	THR	-	expression tag	UNP Q7RTX0
B	-874	ILE	-	expression tag	UNP Q7RTX0
B	-873	ILE	-	expression tag	UNP Q7RTX0
B	-872	ALA	-	expression tag	UNP Q7RTX0
B	-871	LEU	-	expression tag	UNP Q7RTX0
B	-870	SER	-	expression tag	UNP Q7RTX0
B	-869	TYR	-	expression tag	UNP Q7RTX0
B	-868	ILE	-	expression tag	UNP Q7RTX0
B	-867	PHE	-	expression tag	UNP Q7RTX0
B	-866	CYS	-	expression tag	UNP Q7RTX0
B	-865	LEU	-	expression tag	UNP Q7RTX0
B	-864	VAL	-	expression tag	UNP Q7RTX0
B	-863	PHE	-	expression tag	UNP Q7RTX0
B	-862	ALA	-	expression tag	UNP Q7RTX0
B	-861	ASP	-	expression tag	UNP Q7RTX0
B	-860	TYR	-	expression tag	UNP Q7RTX0
B	-859	LYS	-	expression tag	UNP Q7RTX0
B	-858	ASP	-	expression tag	UNP Q7RTX0
B	-857	ASP	-	expression tag	UNP Q7RTX0
B	-856	ASP	-	expression tag	UNP Q7RTX0
B	-855	ASP	-	expression tag	UNP Q7RTX0
B	-854	LYS	-	expression tag	UNP Q7RTX0
B	-853	ALA	-	expression tag	UNP Q7RTX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-852	ALA	-	expression tag	UNP Q7RTX0
B	-851	ALA	-	expression tag	UNP Q7RTX0
B	-114	ARG	CYS	conflict	UNP Q7RTX0
B	-18	GLY	-	linker	UNP Q7RTX0
B	-17	GLY	-	linker	UNP Q7RTX0
B	-16	GLY	-	linker	UNP Q7RTX0
B	-15	SER	-	linker	UNP Q7RTX0
B	-14	GLY	-	linker	UNP Q7RTX0
B	-13	GLY	-	linker	UNP Q7RTX0
B	-12	GLY	-	linker	UNP Q7RTX0
B	-11	SER	-	linker	UNP Q7RTX0
B	-10	GLY	-	linker	UNP Q7RTX0
B	-9	GLY	-	linker	UNP Q7RTX0
B	-8	GLY	-	linker	UNP Q7RTX0
B	-7	SER	-	linker	UNP Q7RTX0
B	-6	GLY	-	linker	UNP Q7RTX0
B	-5	GLY	-	linker	UNP Q7RTX0
B	-4	GLY	-	linker	UNP Q7RTX0
B	-3	SER	-	linker	UNP Q7RTX0
B	-2	GLY	-	linker	UNP Q7RTX0
B	-1	GLY	-	linker	UNP Q7RTX0
B	0	GLY	-	linker	UNP Q7RTX0
B	1	SER	-	linker	UNP Q7RTX0
B	46	ASP	GLY	conflict	UNP P63092
B	47	ASN	GLU	conflict	UNP P63092
B	62	GLY	-	linker	UNP P63092
B	63	GLY	-	linker	UNP P63092
B	64	SER	-	linker	UNP P63092
B	65	GLY	-	linker	UNP P63092
B	66	GLY	-	linker	UNP P63092
B	67	SER	-	linker	UNP P63092
B	68	GLY	-	linker	UNP P63092
B	69	GLY	-	linker	UNP P63092
B	115	ASP	ALA	conflict	UNP P63092
B	118	ASP	SER	conflict	UNP P63092
B	?	-	ASN	deletion	UNP P63092
B	?	-	MET	deletion	UNP P63092
B	?	-	VAL	deletion	UNP P63092
B	?	-	ILE	deletion	UNP P63092
B	?	-	ARG	deletion	UNP P63092
B	?	-	GLU	deletion	UNP P63092
B	?	-	ASP	deletion	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P63092
B	?	-	GLN	deletion	UNP P63092
B	?	-	THR	deletion	UNP P63092
B	128	ASP	LEU	conflict	UNP P63092
B	226	GLN	-	expression tag	UNP P63092
B	227	ASN	-	expression tag	UNP P63092
B	228	VAL	-	expression tag	UNP P63092
B	229	LYS	-	expression tag	UNP P63092
B	230	PHE	-	expression tag	UNP P63092
B	231	VAL	-	expression tag	UNP P63092
B	232	PHE	-	expression tag	UNP P63092
B	233	ASP	-	expression tag	UNP P63092
B	234	ALA	-	expression tag	UNP P63092
B	235	VAL	-	expression tag	UNP P63092
B	236	THR	-	expression tag	UNP P63092
B	237	ASP	-	expression tag	UNP P63092
B	238	ILE	-	expression tag	UNP P63092
B	239	ILE	-	expression tag	UNP P63092
B	240	ILE	-	expression tag	UNP P63092
B	241	LYS	-	expression tag	UNP P63092
B	242	GLU	-	expression tag	UNP P63092
B	243	ASN	-	expression tag	UNP P63092
B	244	LEU	-	expression tag	UNP P63092
B	245	LYS	-	expression tag	UNP P63092
B	246	ASP	-	expression tag	UNP P63092
B	247	CYS	-	expression tag	UNP P63092
B	248	GLY	-	expression tag	UNP P63092
B	249	LEU	-	expression tag	UNP P63092
B	250	PHE	-	expression tag	UNP P63092
F	-6	MET	-	expression tag	UNP Q7RTX0
F	-5	LYS	-	expression tag	UNP Q7RTX0
F	-4	THR	-	expression tag	UNP Q7RTX0
F	-3	ILE	-	expression tag	UNP Q7RTX0
F	-2	ILE	-	expression tag	UNP Q7RTX0
F	-1	ALA	-	expression tag	UNP Q7RTX0
F	0	LEU	-	expression tag	UNP Q7RTX0
F	1	SER	-	expression tag	UNP Q7RTX0
F	2	TYR	-	expression tag	UNP Q7RTX0
F	3	ILE	-	expression tag	UNP Q7RTX0
F	4	PHE	-	expression tag	UNP Q7RTX0
F	5	CYS	-	expression tag	UNP Q7RTX0
F	6	LEU	-	expression tag	UNP Q7RTX0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	VAL	-	expression tag	UNP Q7RTX0
F	8	PHE	-	expression tag	UNP Q7RTX0
F	9	ALA	-	expression tag	UNP Q7RTX0
F	10	ASP	-	expression tag	UNP Q7RTX0
F	11	TYR	-	expression tag	UNP Q7RTX0
F	12	LYS	-	expression tag	UNP Q7RTX0
F	13	ASP	-	expression tag	UNP Q7RTX0
F	14	ASP	-	expression tag	UNP Q7RTX0
F	15	ASP	-	expression tag	UNP Q7RTX0
F	16	ASP	-	expression tag	UNP Q7RTX0
F	17	LYS	-	expression tag	UNP Q7RTX0
F	18	ALA	-	expression tag	UNP Q7RTX0
F	19	ALA	-	expression tag	UNP Q7RTX0
F	20	ALA	-	expression tag	UNP Q7RTX0
F	757	ARG	CYS	conflict	UNP Q7RTX0
F	853	GLY	-	linker	UNP Q7RTX0
F	854	GLY	-	linker	UNP Q7RTX0
F	855	GLY	-	linker	UNP Q7RTX0
F	856	SER	-	linker	UNP Q7RTX0
F	857	GLY	-	linker	UNP Q7RTX0
F	858	GLY	-	linker	UNP Q7RTX0
F	859	GLY	-	linker	UNP Q7RTX0
F	860	SER	-	linker	UNP Q7RTX0
F	861	GLY	-	linker	UNP Q7RTX0
F	862	GLY	-	linker	UNP Q7RTX0
F	863	GLY	-	linker	UNP Q7RTX0
F	864	SER	-	linker	UNP Q7RTX0
F	865	GLY	-	linker	UNP Q7RTX0
F	866	GLY	-	linker	UNP Q7RTX0
F	867	GLY	-	linker	UNP Q7RTX0
F	868	SER	-	linker	UNP Q7RTX0
F	869	GLY	-	linker	UNP Q7RTX0
F	870	GLY	-	linker	UNP Q7RTX0
F	871	GLY	-	linker	UNP Q7RTX0
F	872	SER	-	linker	UNP Q7RTX0
F	917	ASP	GLY	conflict	UNP P63092
F	918	ASN	GLU	conflict	UNP P63092
F	933	GLY	-	linker	UNP P63092
F	934	GLY	-	linker	UNP P63092
F	935	SER	-	linker	UNP P63092
F	936	GLY	-	linker	UNP P63092
F	937	GLY	-	linker	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
F	938	SER	-	linker	UNP P63092
F	939	GLY	-	linker	UNP P63092
F	940	GLY	-	linker	UNP P63092
F	986	ASP	ALA	conflict	UNP P63092
F	989	ASP	SER	conflict	UNP P63092
F	?	-	ASN	deletion	UNP P63092
F	?	-	MET	deletion	UNP P63092
F	?	-	VAL	deletion	UNP P63092
F	?	-	ILE	deletion	UNP P63092
F	?	-	ARG	deletion	UNP P63092
F	?	-	GLU	deletion	UNP P63092
F	?	-	ASP	deletion	UNP P63092
F	?	-	ASN	deletion	UNP P63092
F	?	-	GLN	deletion	UNP P63092
F	?	-	THR	deletion	UNP P63092
F	999	ASP	LEU	conflict	UNP P63092
F	1097	GLN	-	expression tag	UNP P63092
F	1098	ASN	-	expression tag	UNP P63092
F	1099	VAL	-	expression tag	UNP P63092
F	1100	LYS	-	expression tag	UNP P63092
F	1101	PHE	-	expression tag	UNP P63092
F	1102	VAL	-	expression tag	UNP P63092
F	1103	PHE	-	expression tag	UNP P63092
F	1104	ASP	-	expression tag	UNP P63092
F	1105	ALA	-	expression tag	UNP P63092
F	1106	VAL	-	expression tag	UNP P63092
F	1107	THR	-	expression tag	UNP P63092
F	1108	ASP	-	expression tag	UNP P63092
F	1109	ILE	-	expression tag	UNP P63092
F	1110	ILE	-	expression tag	UNP P63092
F	1111	ILE	-	expression tag	UNP P63092
F	1112	LYS	-	expression tag	UNP P63092
F	1113	GLU	-	expression tag	UNP P63092
F	1114	ASN	-	expression tag	UNP P63092
F	1115	LEU	-	expression tag	UNP P63092
F	1116	LYS	-	expression tag	UNP P63092
F	1117	ASP	-	expression tag	UNP P63092
F	1118	CYS	-	expression tag	UNP P63092
F	1119	GLY	-	expression tag	UNP P63092
F	1120	LEU	-	expression tag	UNP P63092
F	1121	PHE	-	expression tag	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit

beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	339	Total	C	N	O	S	0	0
			2607	1607	468	511	21		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	53	Total	C	N	O	S	0	0
			400	249	70	78	3		

- Molecule 4 is a protein called Nanobody 35 (NB35).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 5 is a protein called Taste receptor type 1 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	257	Total	C	N	O	S	0	0
			2031	1355	315	339	22		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q8TE23
A	-7	LYS	-	expression tag	UNP Q8TE23
A	-6	THR	-	expression tag	UNP Q8TE23
A	-5	ILE	-	expression tag	UNP Q8TE23
A	-4	ILE	-	expression tag	UNP Q8TE23
A	-3	ALA	-	expression tag	UNP Q8TE23
A	-2	LEU	-	expression tag	UNP Q8TE23
A	-1	SER	-	expression tag	UNP Q8TE23
A	0	TYR	-	expression tag	UNP Q8TE23
A	1	ILE	-	expression tag	UNP Q8TE23
A	2	PHE	-	expression tag	UNP Q8TE23
A	3	CYS	-	expression tag	UNP Q8TE23
A	4	LEU	-	expression tag	UNP Q8TE23
A	5	VAL	-	expression tag	UNP Q8TE23
A	6	PHE	-	expression tag	UNP Q8TE23
A	7	ALA	-	expression tag	UNP Q8TE23

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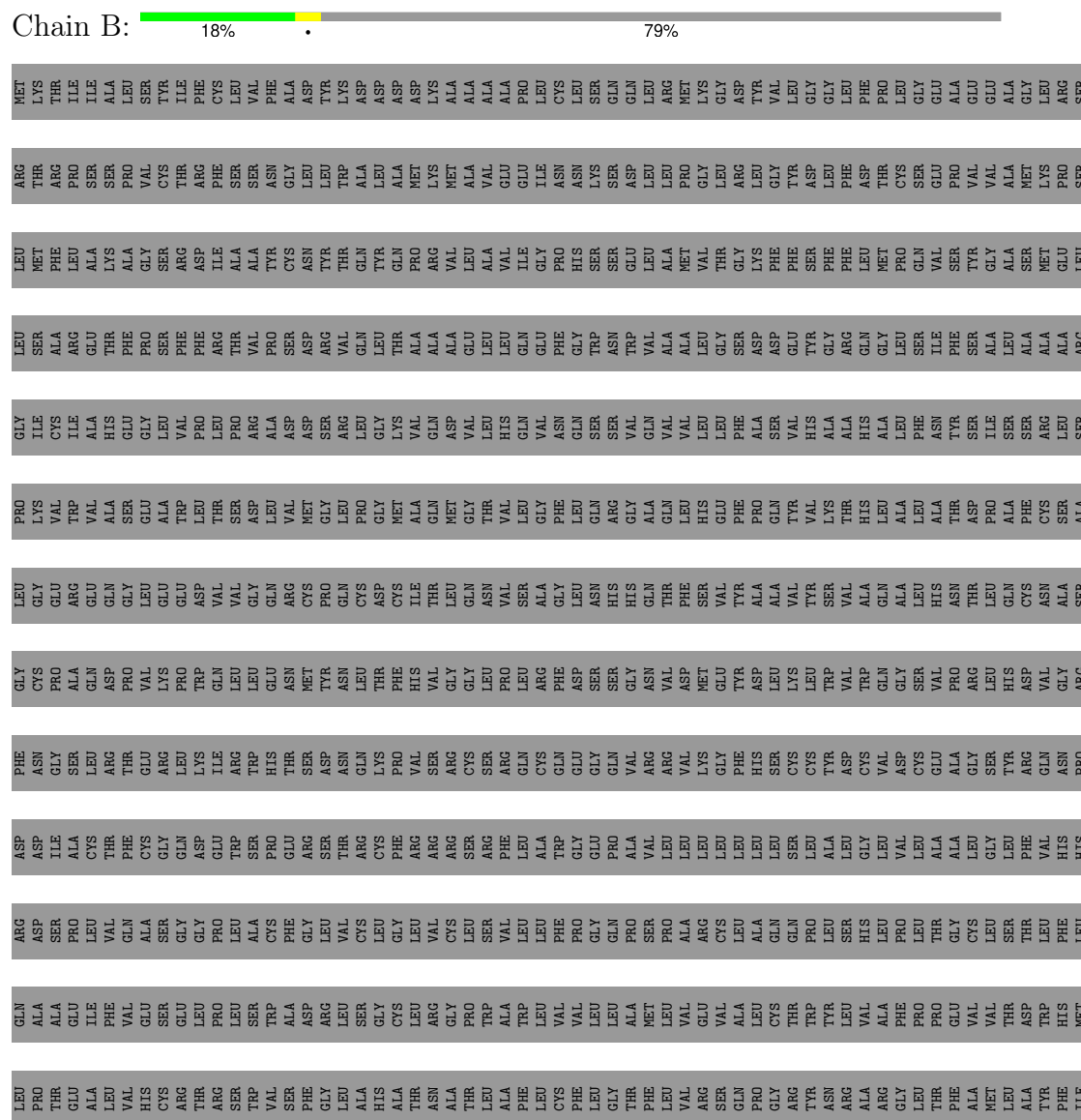
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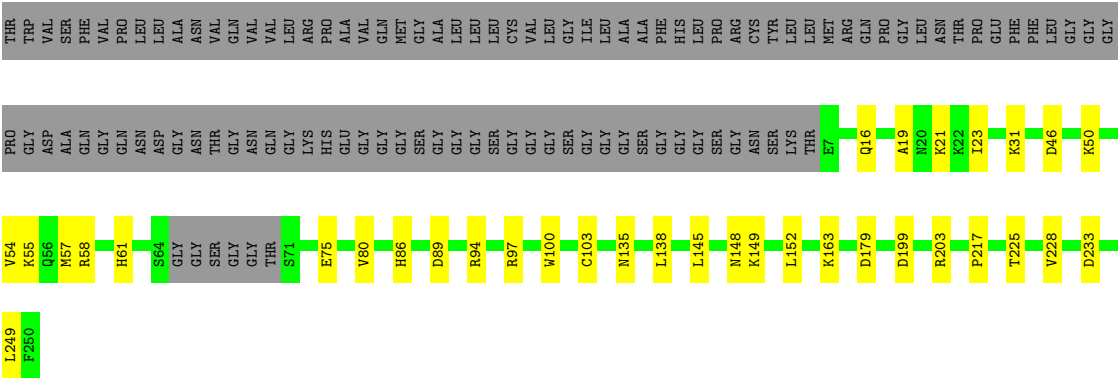
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	TYR	-	expression tag	UNP Q8TE23
A	9	PRO	-	expression tag	UNP Q8TE23
A	10	TYR	-	expression tag	UNP Q8TE23
A	11	ASP	-	expression tag	UNP Q8TE23
A	12	VAL	-	expression tag	UNP Q8TE23
A	13	PRO	-	expression tag	UNP Q8TE23
A	14	ASP	-	expression tag	UNP Q8TE23
A	15	TYR	-	expression tag	UNP Q8TE23
A	16	ALA	-	expression tag	UNP Q8TE23
A	17	ALA	-	expression tag	UNP Q8TE23
A	18	ALA	-	expression tag	UNP Q8TE23

3 Residue-property plots

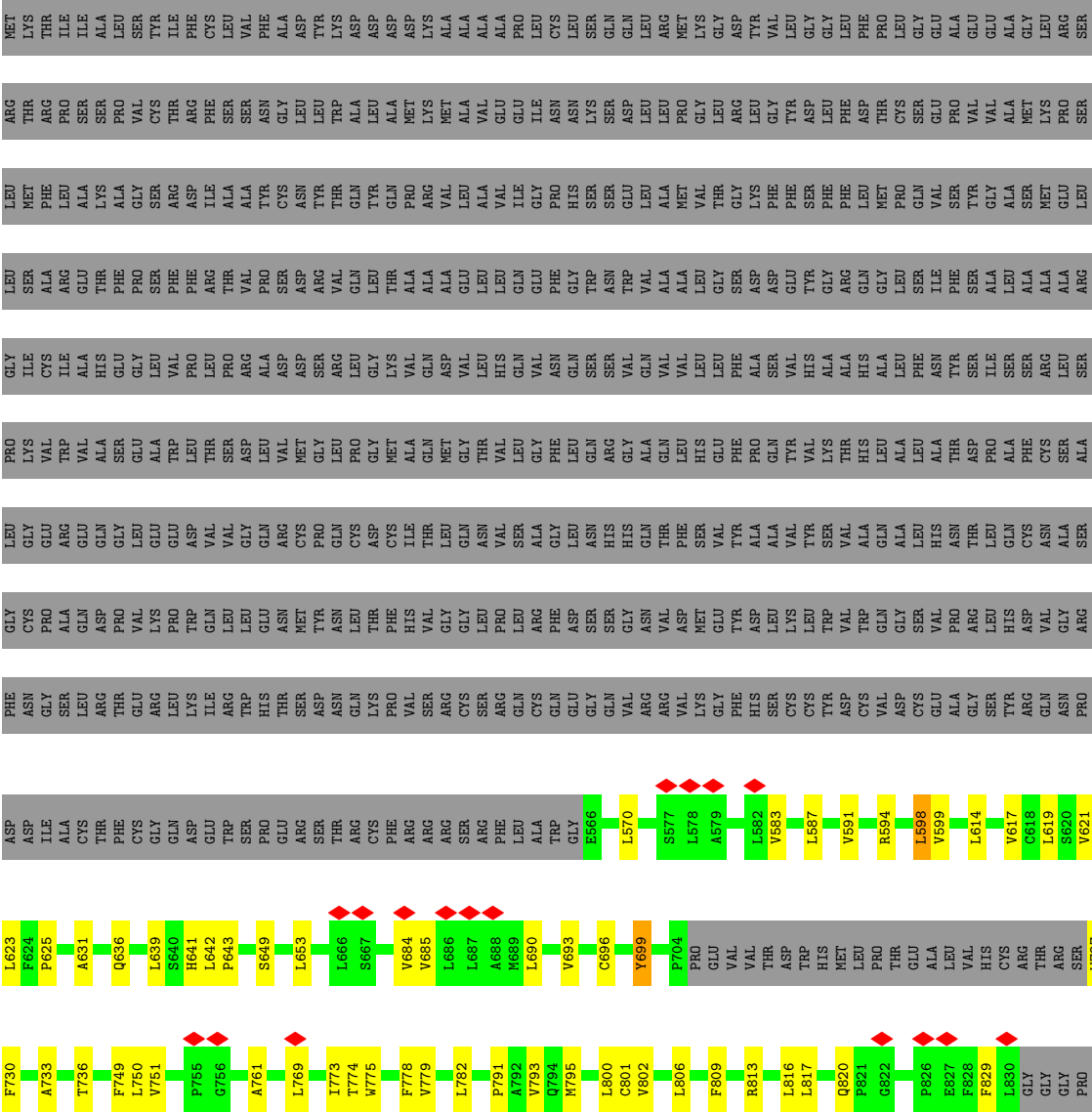
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

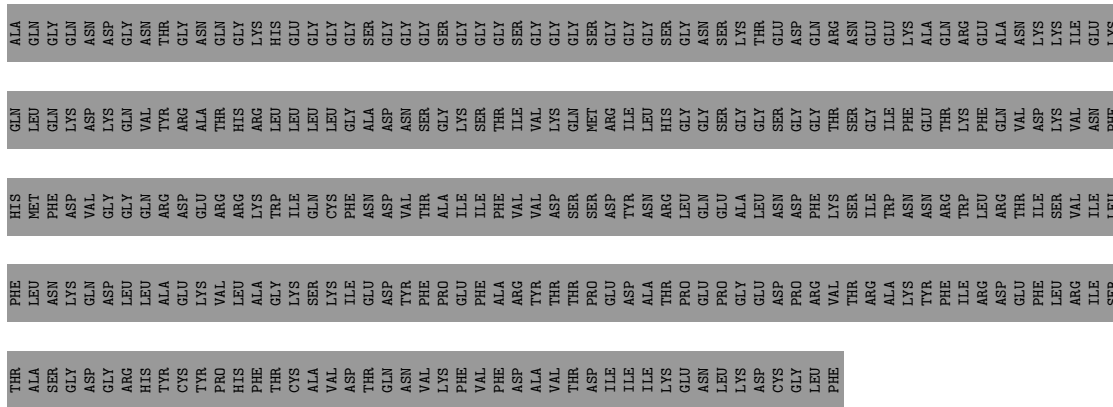
- Molecule 1: Taste receptor type 1 member 3, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



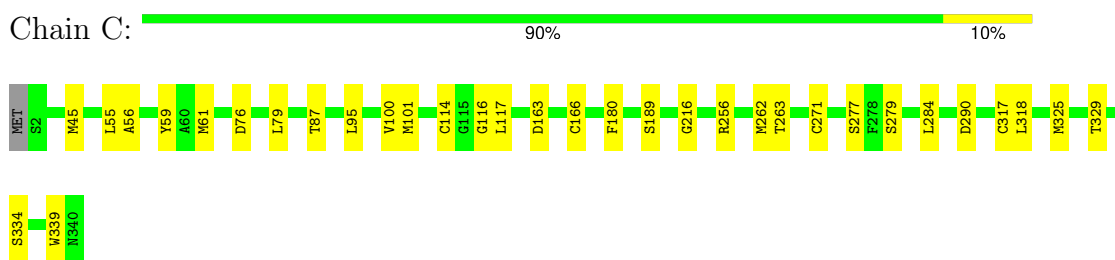


● Molecule 1: Taste receptor type 1 member 3, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

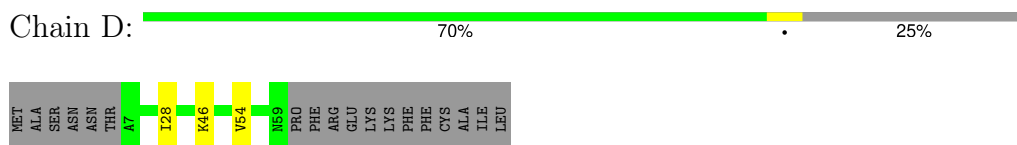




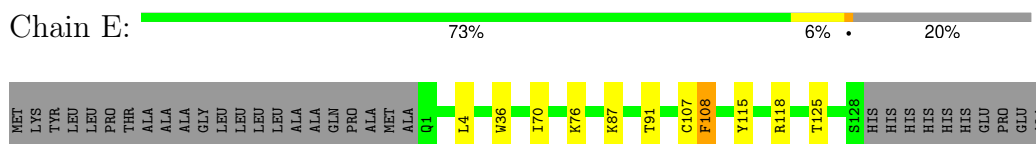
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



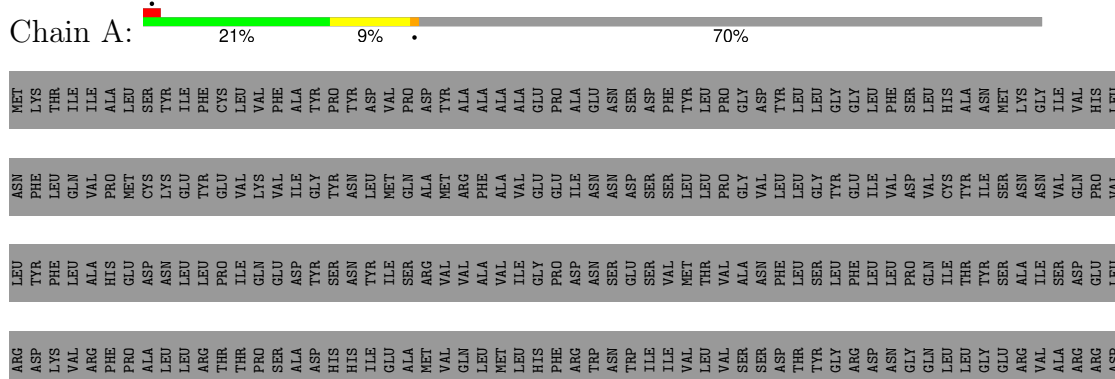
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

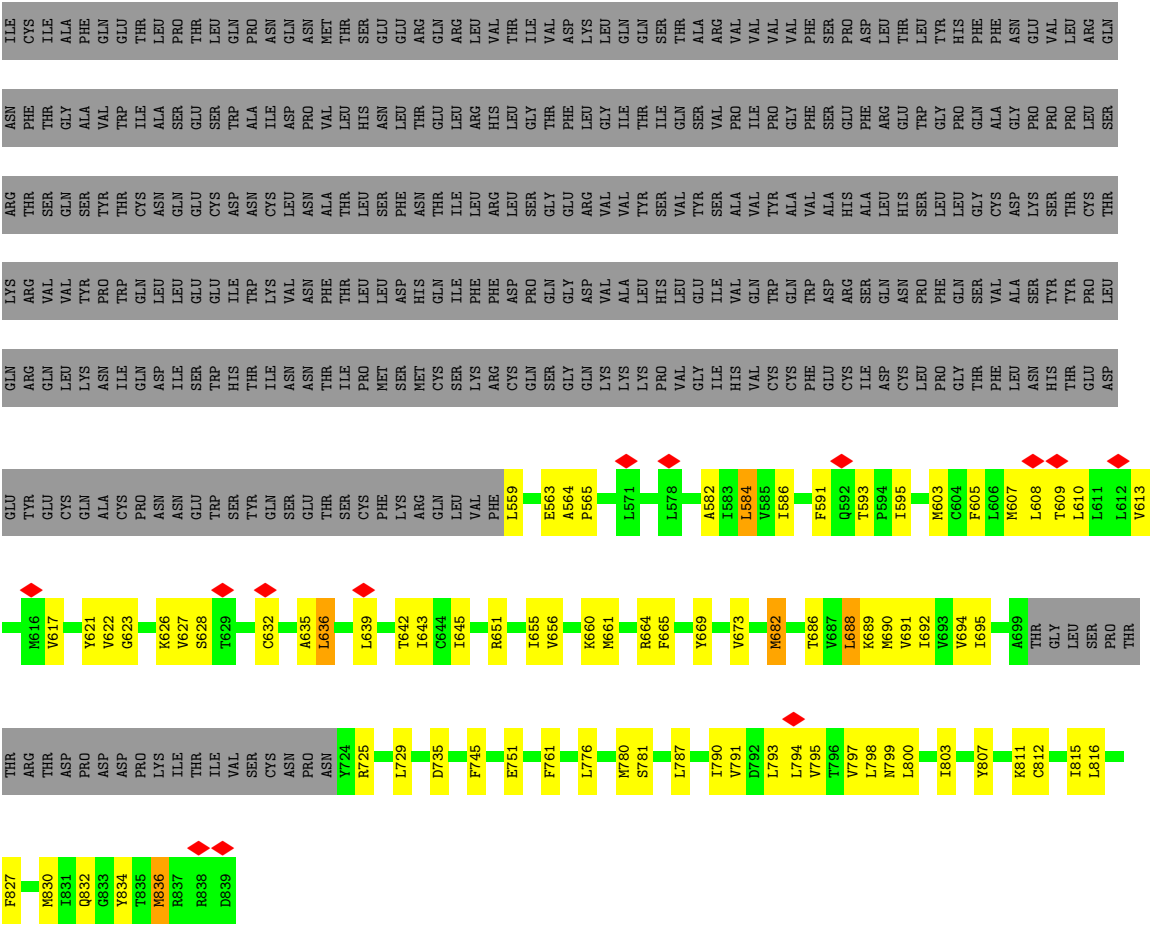


- Molecule 4: Nanobody 35 (NB35)



- Molecule 5: Taste receptor type 1 member 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	723893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.509	Depositor
Minimum map value	-0.213	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (\AA)	362.12, 362.12, 362.12	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.823, 0.823, 0.823	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.13	0/1992	0.23	0/2679
1	F	0.24	0/1911	0.38	0/2618
2	C	0.12	0/2654	0.27	0/3597
3	D	0.08	0/404	0.19	0/545
4	E	0.11	0/993	0.25	0/1345
5	A	0.14	0/2086	0.37	0/2839
All	All	0.15	0/10040	0.31	0/13623

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	B	1954	0	1925	23	0
1	F	1859	0	1944	37	0
2	C	2607	0	2510	23	0
3	D	400	0	412	3	0
4	E	973	0	938	6	0
5	A	2031	0	2094	63	0
All	All	9824	0	9823	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (139) 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:A:627:VAL:HG11	1:F:631:ALA:CB	1.32	1.59
5:A:627:VAL:CG1	1:F:631:ALA:HB2	1.27	1.57
5:A:627:VAL:CG1	1:F:631:ALA:CB	2.06	0.96
5:A:627:VAL:HG13	1:F:631:ALA:CB	2.12	0.78
1:F:621:VAL:HG13	1:F:795:MET:HB3	1.66	0.78
5:A:627:VAL:CG1	1:F:631:ALA:HB1	2.18	0.70
5:A:799:ASN:O	5:A:803:ILE:HD12	1.93	0.68
2:C:271:CYS:HB2	2:C:290:ASP:HB2	1.75	0.66
5:A:661:MET:HA	5:A:664:ARG:HB3	1.76	0.66
2:C:325:MET:HE1	3:D:54:VAL:HG11	1.76	0.66
5:A:586:ILE:HD13	5:A:816:LEU:HD21	1.77	0.66
5:A:617:VAL:HG21	5:A:636:LEU:HD13	1.78	0.65
1:B:249:LEU:HD13	5:A:655:ILE:HD12	1.78	0.64
1:B:55:LYS:HD2	1:B:58:ARG:HH12	1.63	0.64
1:F:623:LEU:HD11	1:F:636:GLN:HA	1.80	0.63
5:A:642:THR:HG23	5:A:643:ILE:HD13	1.81	0.62
1:F:617:VAL:HG23	1:F:643:PRO:HB2	1.80	0.62
1:B:75:GLU:HG2	1:B:86:HIS:HE1	1.63	0.62
5:A:793:LEU:O	5:A:797:VAL:HG22	2.02	0.60
5:A:776:LEU:O	5:A:780:MET:HG2	2.02	0.60
1:F:583:VAL:HG23	1:F:806:LEU:HD11	1.82	0.60
1:F:642:LEU:HD21	1:F:693:VAL:HG23	1.83	0.59
5:A:795:VAL:HA	5:A:798:LEU:HD12	1.85	0.59
1:B:233:ASP:HB3	5:A:836:MET:HB3	1.85	0.59
5:A:627:VAL:HG13	1:F:631:ALA:HB1	1.82	0.59
5:A:595:ILE:HD11	5:A:811:LYS:HG2	1.84	0.58
2:C:87:THR:HG22	2:C:87:THR:O	2.03	0.58
1:F:816:LEU:HA	1:F:820:GLN:HG3	1.85	0.58
1:F:774:THR:HG23	1:F:775:TRP:HD1	1.70	0.57
1:B:199:ASP:O	1:B:203:ARG:HG3	2.05	0.56
1:B:103:CYS:SG	2:C:101:MET:HE2	2.46	0.56
5:A:605:PHE:O	5:A:609:THR:HG23	2.05	0.56
5:A:827:PHE:HA	5:A:830:MET:HG2	1.88	0.56
5:A:559:LEU:HD11	5:A:622:VAL:HG13	1.86	0.56
5:A:794:LEU:HD23	5:A:798:LEU:HD11	1.89	0.55
1:F:625:PRO:HD3	1:F:795:MET:SD	2.47	0.55
1:F:791:PRO:O	1:F:795:MET:HG3	2.06	0.55
2:C:277:SER:HB3	2:C:318:LEU:HD23	1.89	0.55
1:B:100:TRP:HB2	2:C:117:LEU:HD21	1.89	0.54
2:C:101:MET:HG3	2:C:116:GLY:HA2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:594:ARG:HA	1:F:599:VAL:HG21	1.89	0.54
1:F:649:SER:OG	1:F:685:VAL:HG23	2.07	0.54
5:A:664:ARG:HG2	5:A:665:PHE:CD1	2.42	0.54
1:F:587:LEU:O	1:F:591:VAL:HG13	2.08	0.53
2:C:45:MET:HB3	2:C:339:TRP:HB3	1.90	0.53
5:A:595:ILE:HG21	5:A:815:ILE:HG21	1.92	0.52
5:A:690:MET:O	5:A:694:VAL:HG22	2.09	0.52
2:C:279:SER:HB2	2:C:284:LEU:HB2	1.92	0.51
5:A:691:VAL:O	5:A:695:ILE:HG23	2.10	0.51
5:A:761:PHE:HZ	5:A:803:ILE:HG23	1.75	0.51
1:F:769:LEU:O	1:F:773:ILE:HG23	2.11	0.51
1:F:778:PHE:CZ	1:F:782:LEU:HD22	2.45	0.51
5:A:632:CYS:HA	5:A:635:ALA:HB3	1.94	0.50
5:A:559:LEU:HD12	5:A:623:GLY:H	1.77	0.50
1:F:641:HIS:CD2	1:F:733:ALA:HB1	2.46	0.50
1:B:94:ARG:HD3	2:C:163:ASP:HA	1.92	0.50
5:A:584:LEU:HG	5:A:608:LEU:HB3	1.94	0.50
1:B:31:LYS:HB2	2:C:55:LEU:HD11	1.94	0.49
2:C:318:LEU:HD12	2:C:329:THR:HG22	1.93	0.49
5:A:603:MET:O	5:A:607:MET:HG2	2.13	0.48
4:E:36:TRP:HD1	4:E:70:ILE:HD12	1.78	0.48
2:C:262:MET:HG3	2:C:263:THR:N	2.28	0.48
1:F:775:TRP:O	1:F:779:VAL:HG23	2.13	0.48
5:A:563:GLU:CD	5:A:565:PRO:HD2	2.39	0.47
4:E:91:THR:HG23	4:E:125:THR:HA	1.96	0.47
5:A:812:CYS:O	5:A:816:LEU:HG	2.14	0.47
1:F:727:TRP:HA	1:F:730:PHE:CE2	2.49	0.47
5:A:689:LYS:HA	5:A:692:ILE:HG22	1.96	0.47
2:C:61:MET:HG3	2:C:317:CYS:HB2	1.96	0.47
5:A:669:TYR:O	5:A:673:VAL:HG12	2.15	0.47
1:F:598:LEU:HA	1:F:829:PHE:HE2	1.80	0.47
2:C:256:ARG:HD2	3:D:28:ILE:HD12	1.96	0.47
1:B:75:GLU:HG2	1:B:86:HIS:CE1	2.46	0.46
1:B:57:MET:HE3	1:B:228:VAL:HG13	1.98	0.46
1:B:61:HIS:HE1	1:B:228:VAL:HG11	1.79	0.46
5:A:682:MET:O	5:A:686:THR:HG22	2.16	0.46
1:F:775:TRP:HA	1:F:778:PHE:HB3	1.97	0.46
1:B:21:LYS:HB3	1:B:21:LYS:HE2	1.80	0.46
2:C:180:PHE:CE1	2:C:216:GLY:HA2	2.51	0.46
5:A:791:VAL:O	5:A:795:VAL:HG23	2.15	0.46
1:F:653:LEU:HD21	1:F:684:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:729:LEU:HD23	5:A:729:LEU:HA	1.80	0.46
1:F:598:LEU:HA	1:F:829:PHE:CE2	2.50	0.46
1:B:31:LYS:HA	2:C:55:LEU:HD21	1.97	0.46
5:A:645:ILE:HD12	5:A:735:ASP:OD1	2.16	0.45
1:B:50:LYS:HB2	1:B:50:LYS:HE3	1.63	0.45
1:F:598:LEU:HD12	1:F:817:LEU:HD13	1.97	0.45
5:A:639:LEU:O	5:A:643:ILE:HG12	2.17	0.45
5:A:656:VAL:HG21	5:A:745:PHE:O	2.17	0.45
5:A:642:THR:HG21	5:A:689:LYS:HD3	1.98	0.45
5:A:787:LEU:HA	5:A:790:ILE:HD12	1.99	0.45
2:C:166:CYS:HB2	2:C:180:PHE:HB2	1.99	0.44
1:B:135:ASN:HB3	1:B:138:LEU:HB2	1.99	0.44
5:A:811:LYS:O	5:A:815:ILE:HG23	2.18	0.44
5:A:751:GLU:HG2	5:A:834:TYR:HE1	1.83	0.44
1:F:619:LEU:HD23	1:F:619:LEU:HA	1.83	0.44
1:B:61:HIS:CD2	1:B:80:VAL:HG22	2.53	0.43
2:C:56:ALA:O	2:C:334:SER:HB3	2.18	0.43
5:A:832:GLN:O	5:A:836:MET:HG2	2.18	0.43
1:B:97:ARG:HH21	4:E:108:PHE:HE1	1.65	0.43
2:C:61:MET:HE2	2:C:61:MET:HB2	1.83	0.43
5:A:593:THR:HG23	5:A:595:ILE:HG22	2.00	0.43
1:F:642:LEU:HD23	1:F:642:LEU:HA	1.87	0.43
1:F:751:VAL:HG11	1:F:761:ALA:CB	2.47	0.43
1:F:809:PHE:HE1	1:F:813:ARG:HH21	1.66	0.43
2:C:95:LEU:HD13	2:C:100:VAL:HG21	2.00	0.43
5:A:800:LEU:HD23	5:A:800:LEU:HA	1.90	0.43
1:F:614:LEU:HD22	1:F:802:VAL:HG22	2.01	0.43
2:C:79:LEU:HD11	2:C:114:CYS:HB3	2.01	0.43
1:B:163:LYS:HB3	1:B:163:LYS:HE3	1.83	0.42
5:A:626:LYS:HG2	5:A:628:SER:H	1.84	0.42
4:E:115:TYR:HD2	4:E:118:ARG:HG3	1.84	0.42
4:E:76:LYS:HE3	4:E:76:LYS:HB3	1.87	0.42
5:A:582:ALA:O	5:A:586:ILE:HG13	2.20	0.42
1:B:149:LYS:HD3	1:B:152:LEU:HD12	2.02	0.42
1:B:145:LEU:HB3	1:B:217:PRO:HA	2.01	0.42
5:A:761:PHE:CE2	5:A:807:TYR:HB2	2.55	0.42
1:B:19:ALA:O	1:B:23:ILE:HG12	2.19	0.42
5:A:610:LEU:HA	5:A:613:VAL:HG12	2.02	0.42
5:A:610:LEU:O	5:A:613:VAL:HG12	2.19	0.42
5:A:690:MET:HE3	5:A:690:MET:HA	2.00	0.42
5:A:664:ARG:HG2	5:A:665:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:651:ARG:O	5:A:655:ILE:HD13	2.20	0.41
2:C:87:THR:O	2:C:87:THR:CG2	2.69	0.41
1:F:749:PHE:CE1	1:F:750:LEU:HD23	2.55	0.41
5:A:660:LYS:HB2	5:A:660:LYS:HE2	1.84	0.41
5:A:725:ARG:HH22	5:A:781:SER:HB3	1.85	0.41
1:F:696:CYS:HA	1:F:699:TYR:HD1	1.84	0.41
1:B:50:LYS:O	1:B:54:VAL:HG23	2.21	0.41
5:A:591:PHE:HD1	5:A:591:PHE:HA	1.77	0.41
5:A:682:MET:HE2	5:A:682:MET:HB2	1.81	0.41
5:A:688:LEU:O	5:A:692:ILE:HG22	2.21	0.41
5:A:812:CYS:HA	5:A:815:ILE:HG12	2.01	0.41
3:D:46:LYS:HB3	3:D:46:LYS:HE3	1.69	0.40
4:E:87:LYS:HE3	4:E:87:LYS:HB2	1.70	0.40
1:F:570:LEU:HD23	1:F:570:LEU:HA	1.81	0.40
5:A:761:PHE:CD1	5:A:761:PHE:C	2.98	0.40
5:A:564:ALA:HB3	5:A:565:PRO:HD3	2.04	0.40
1:F:769:LEU:HD12	1:F:769:LEU:HA	1.84	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	B	234/1128 (21%)	228 (97%)	6 (3%)	0	100	100
1	F	239/1128 (21%)	229 (96%)	10 (4%)	0	100	100
2	C	337/340 (99%)	329 (98%)	8 (2%)	0	100	100
3	D	51/71 (72%)	50 (98%)	1 (2%)	0	100	100
4	E	126/160 (79%)	125 (99%)	1 (1%)	0	100	100
5	A	253/848 (30%)	248 (98%)	5 (2%)	0	100	100
All	All	1240/3675 (34%)	1209 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	212/935 (23%)	206 (97%)	6 (3%)	38	70
1	F	199/935 (21%)	191 (96%)	8 (4%)	27	61
2	C	282/283 (100%)	279 (99%)	3 (1%)	70	87
3	D	42/58 (72%)	42 (100%)	0	100	100
4	E	106/129 (82%)	103 (97%)	3 (3%)	38	70
5	A	225/760 (30%)	219 (97%)	6 (3%)	40	71
All	All	1066/3100 (34%)	1040 (98%)	26 (2%)	45	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	46	ASP
1	B	89	ASP
1	B	148	ASN
1	B	179	ASP
1	B	225	THR
2	C	59	TYR
2	C	76	ASP
2	C	189	SER
4	E	4	LEU
4	E	107	CYS
4	E	108	PHE
5	A	584	LEU
5	A	621	TYR
5	A	636	LEU
5	A	682	MET
5	A	688	LEU
5	A	836	MET
1	F	598	LEU

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Mol	Chain	Res	Type
1	F	639	LEU
1	F	690	LEU
1	F	699	TYR
1	F	736	THR
1	F	793	VAL
1	F	800	LEU
1	F	801	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	GLN
1	B	61	HIS
1	B	105	ASN
2	C	44	GLN
4	E	3	GLN
4	E	120	GLN
1	F	637	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

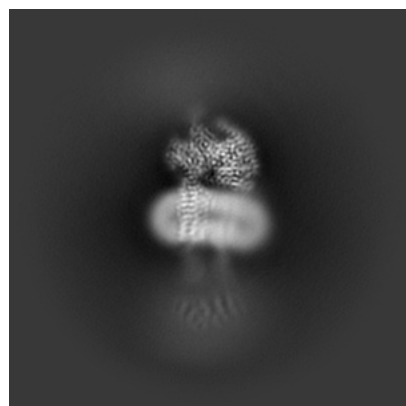
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70072. These allow visual inspection of the internal detail of the map and identification of artifacts.

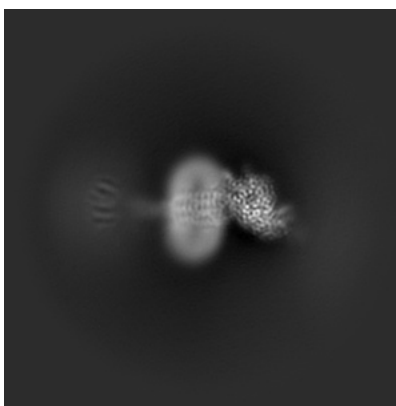
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

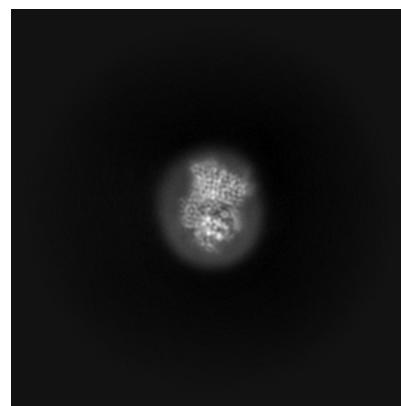
6.1.1 Primary map



X

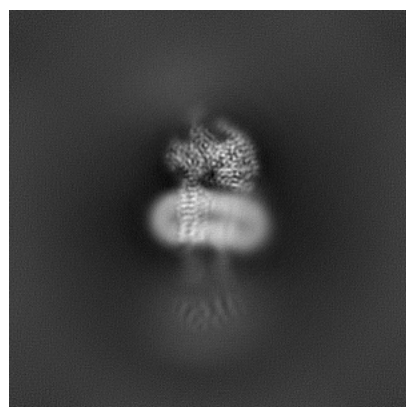


Y

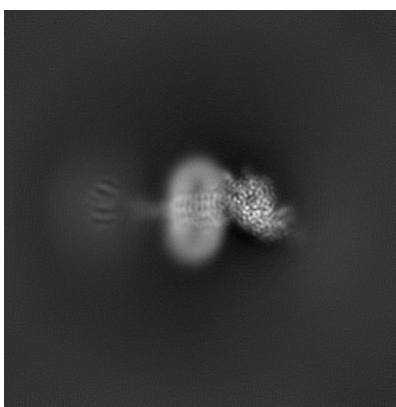


Z

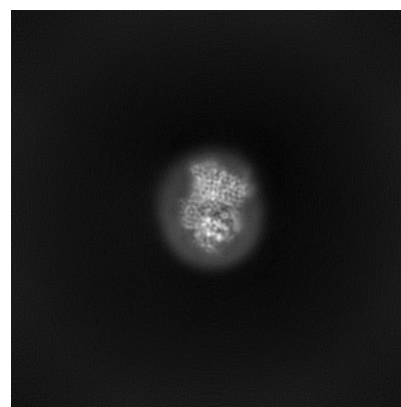
6.1.2 Raw map



X



Y



Z

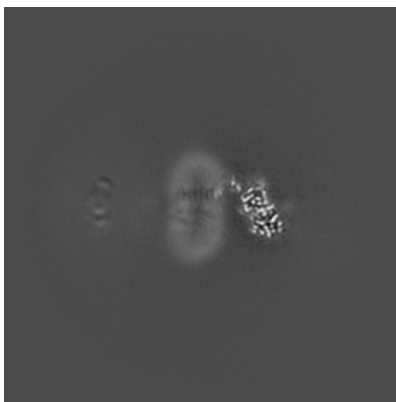
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

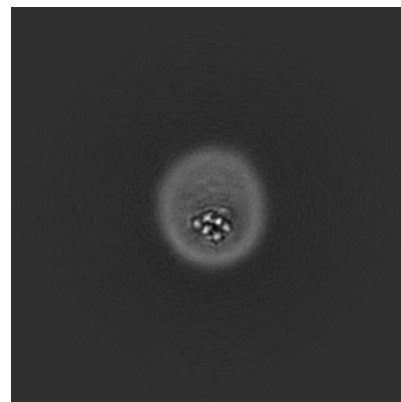
6.2.1 Primary map



X Index: 220



Y Index: 220

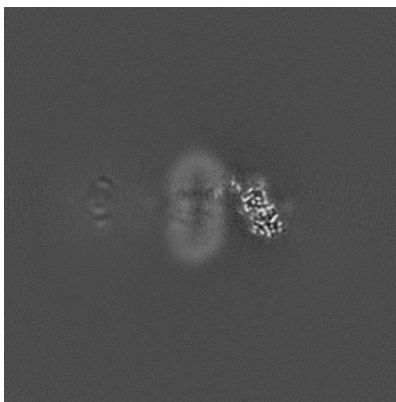


Z Index: 220

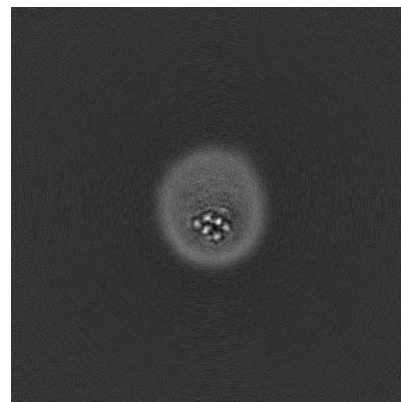
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

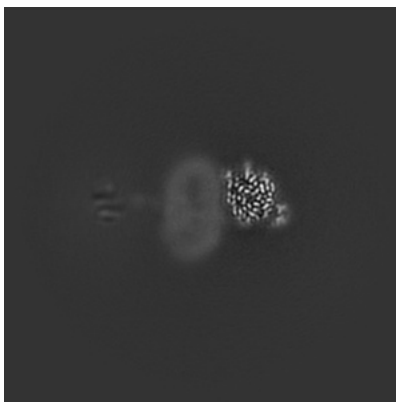
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

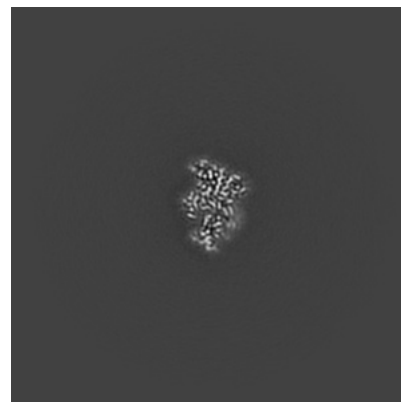
6.3.1 Primary map



X Index: 217

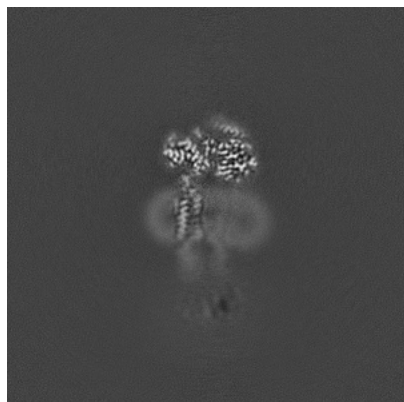


Y Index: 246

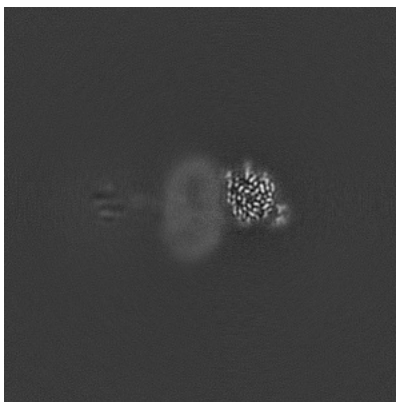


Z Index: 279

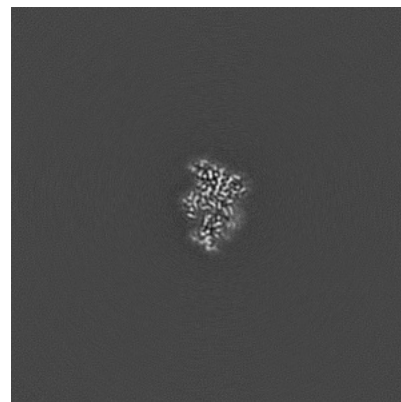
6.3.2 Raw map



X Index: 217



Y Index: 246

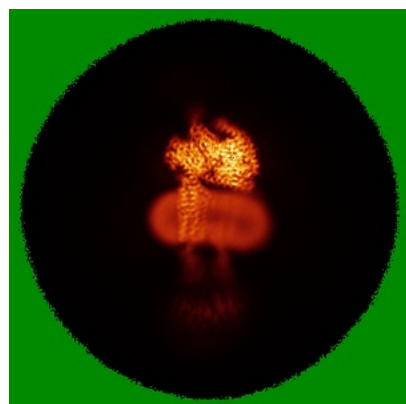


Z Index: 279

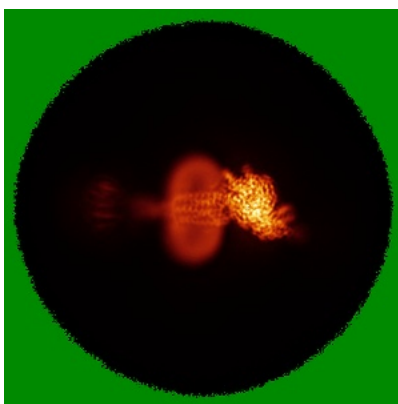
The images above show the largest variance slices of the map in three orthogonal directions.

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

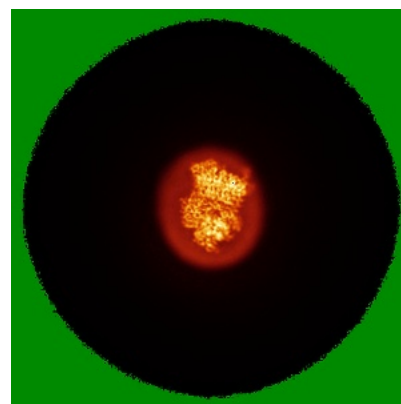
6.4.1 Primary map



X

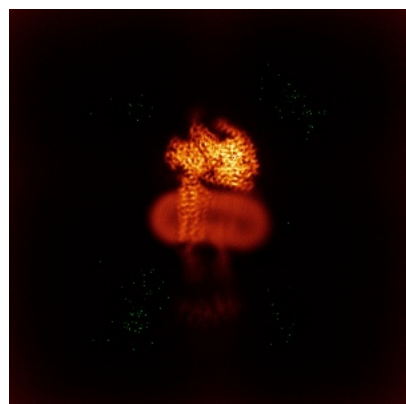


Y

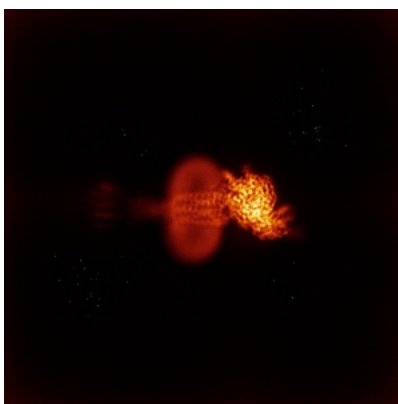


Z

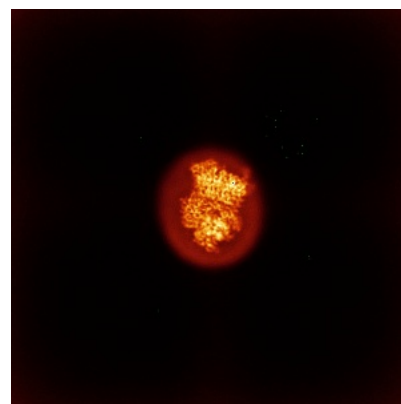
6.4.2 Raw map



X



Y

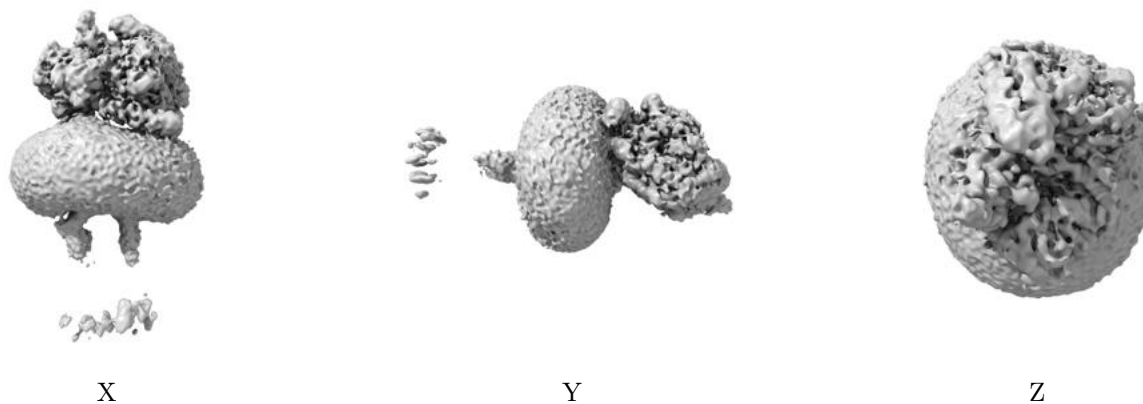


Z

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.

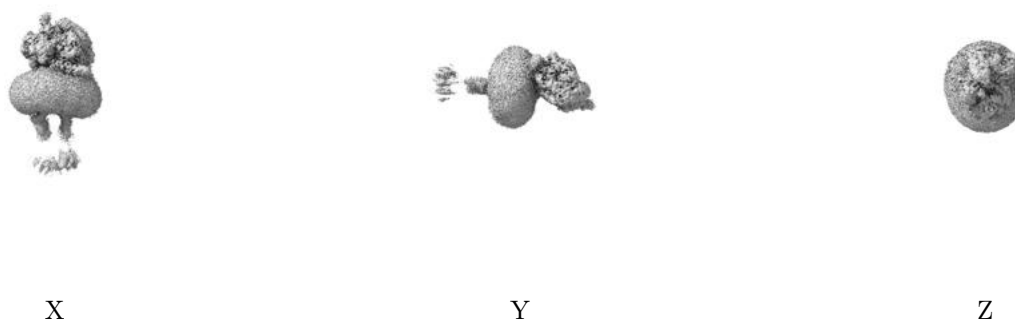
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

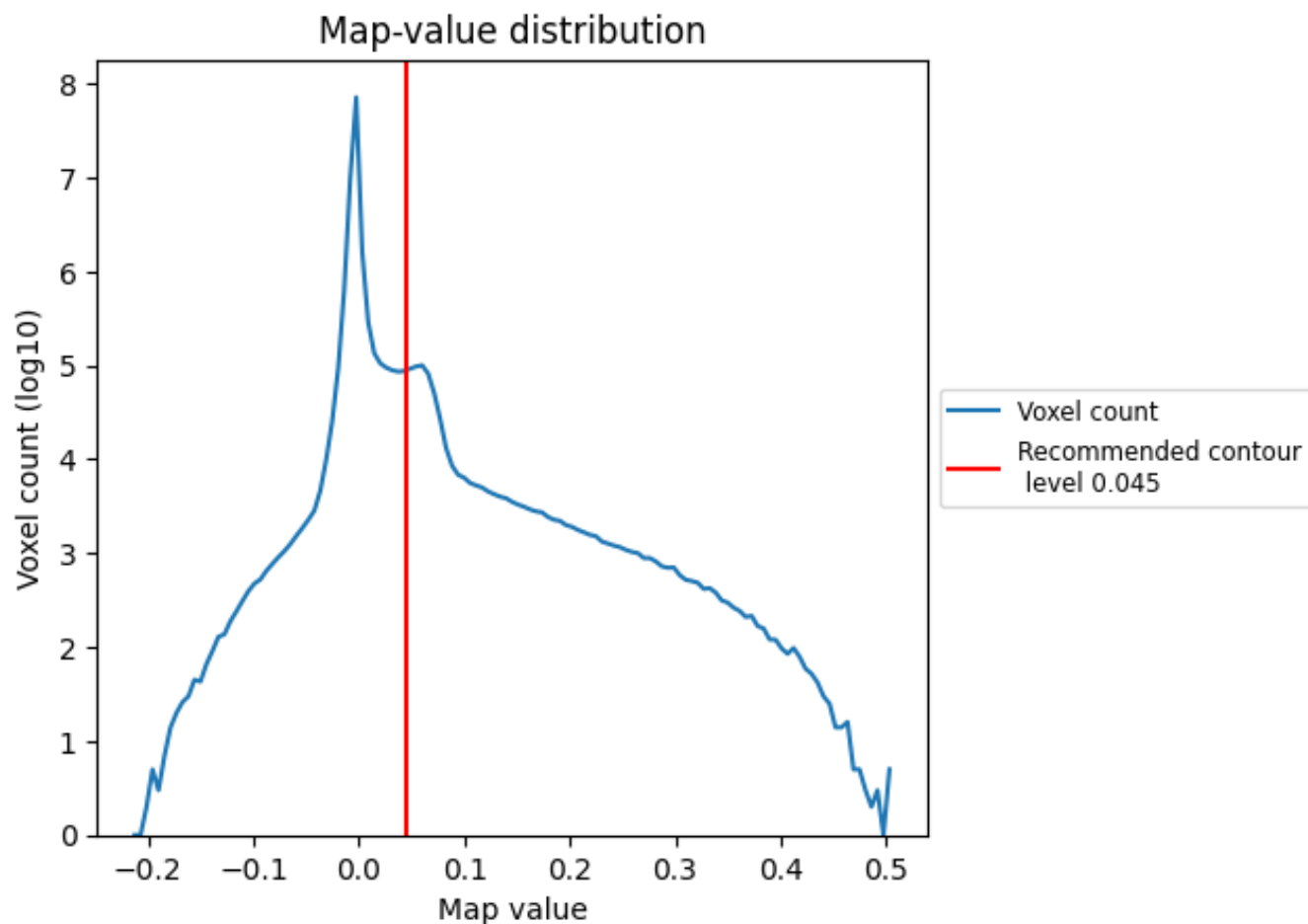
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

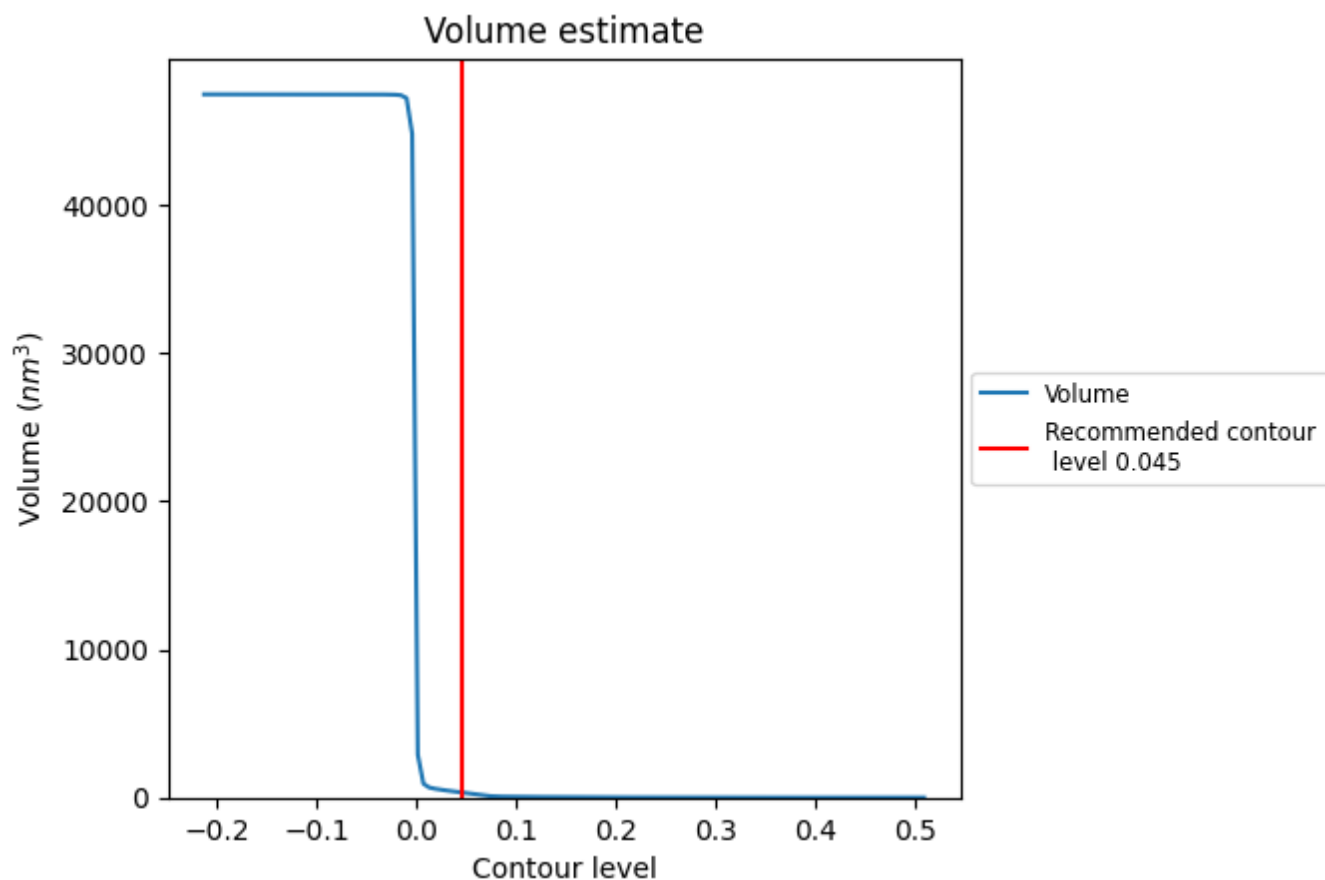
This section contains the results of statistical analysis of the map.

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.

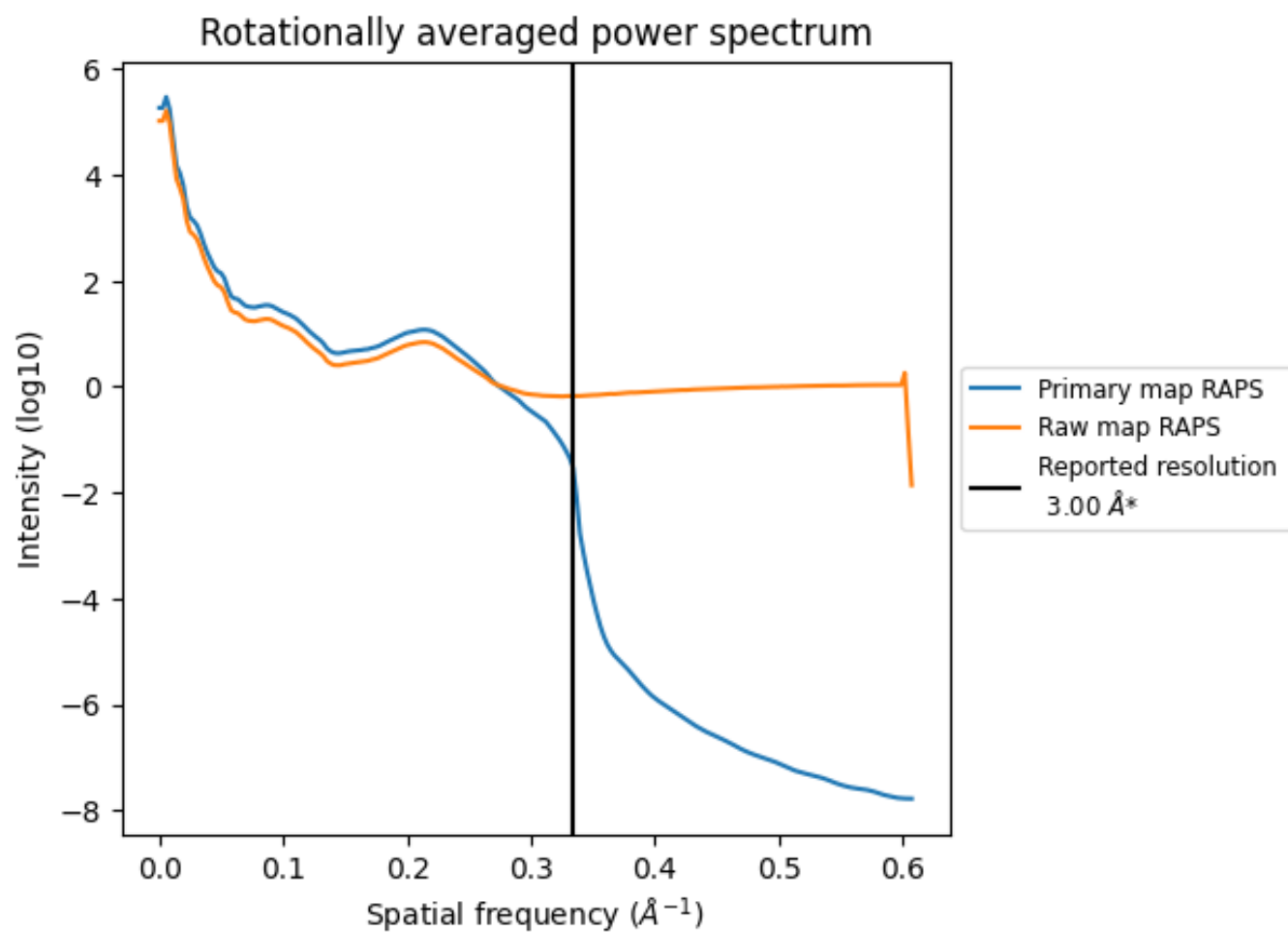
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm^3 ; this corresponds to an approximate mass of 315 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 ⓘ

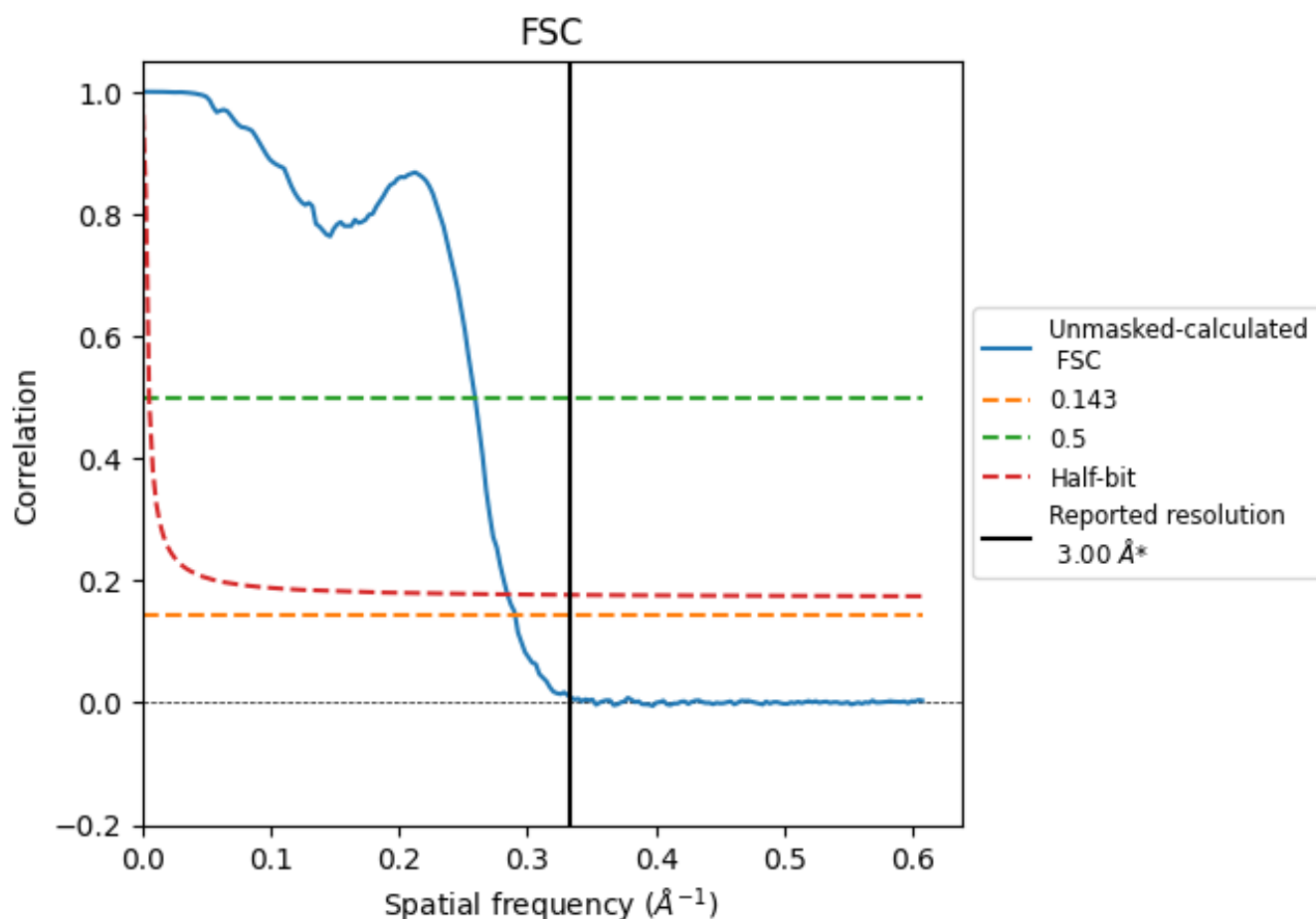


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

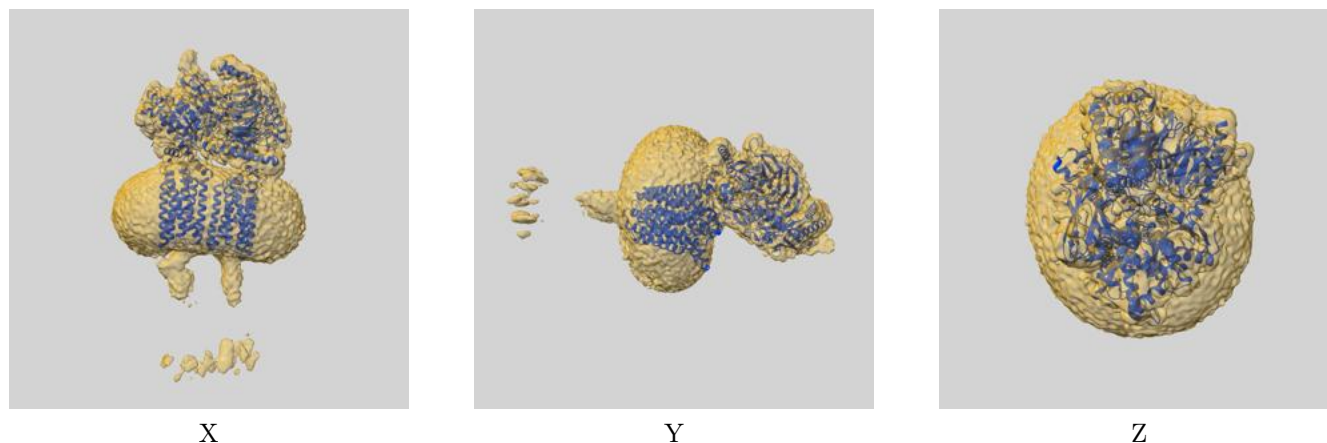
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.86	3.51

*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 3.44 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

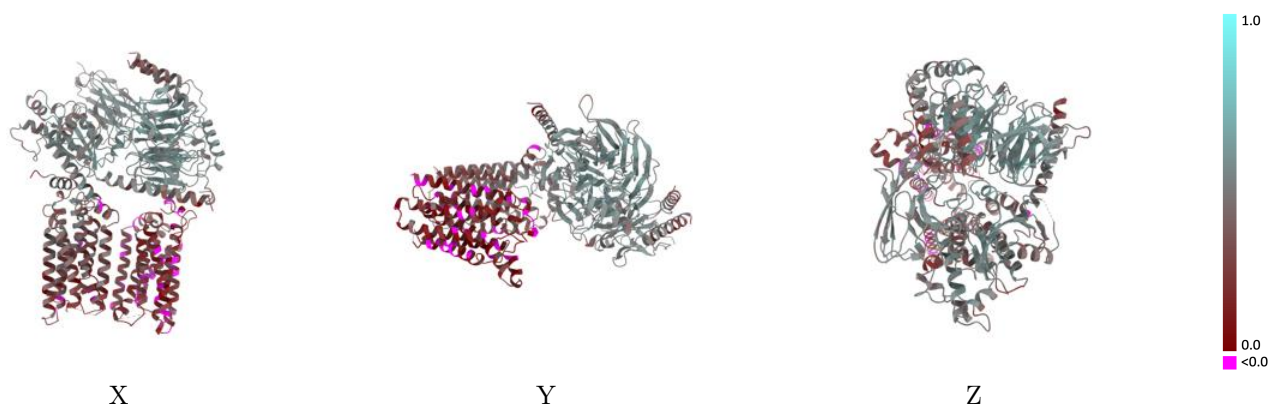
This section contains information regarding the fit between EMDB map EMD-70072 and PDB model 9O38. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



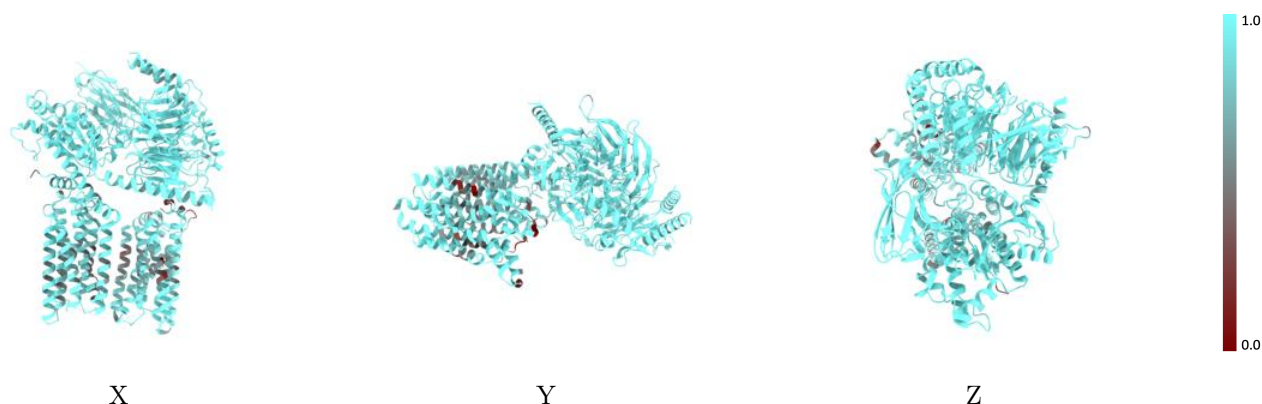
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



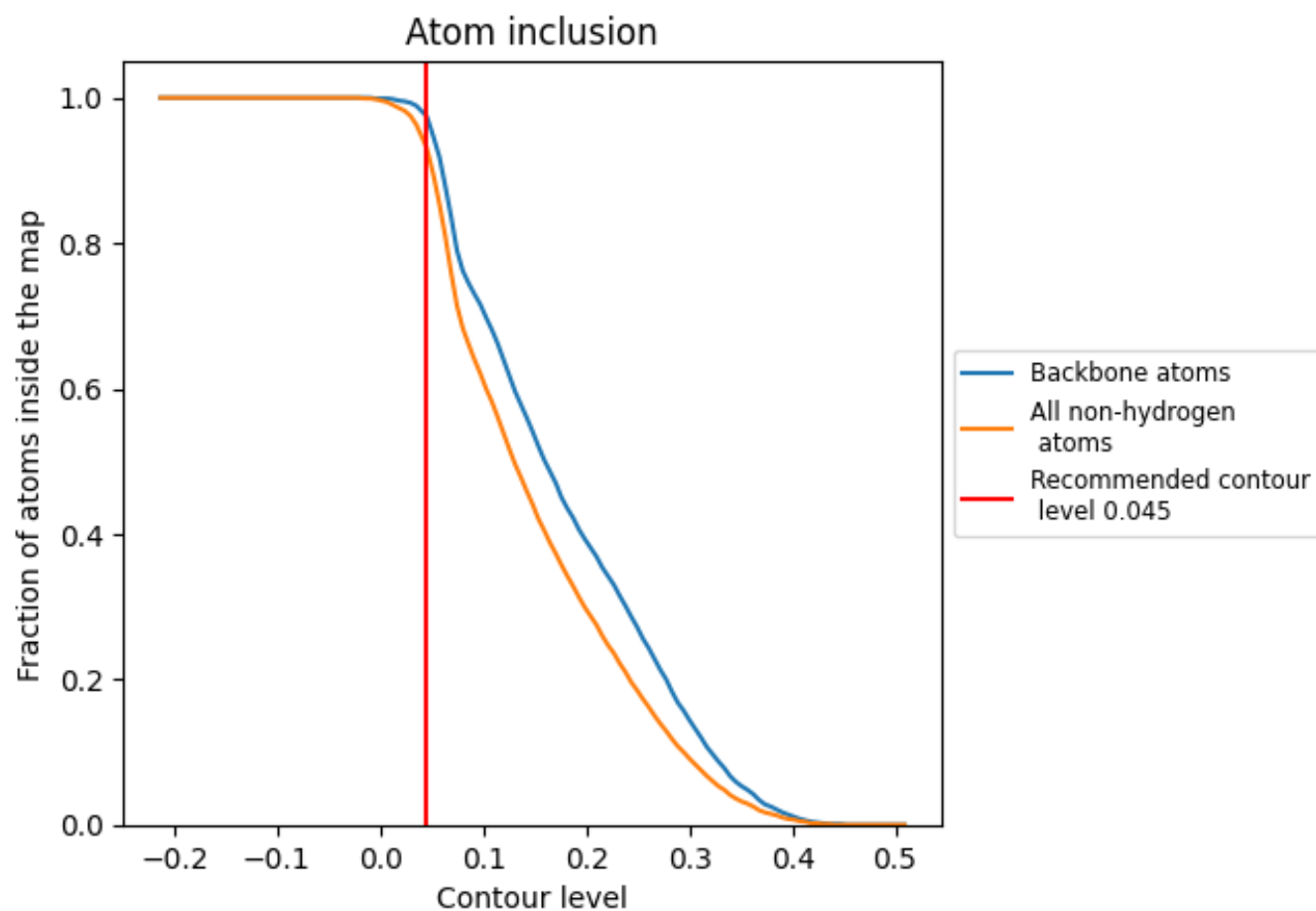
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9320</div>	<div><div></div>0.3830</div>
A	<div><div></div>0.8700</div>	<div><div></div>0.2780</div>
B	<div><div></div>0.9650</div>	<div><div></div>0.4850</div>
C	<div><div></div>0.9810</div>	<div><div></div>0.5230</div>
D	<div><div></div>0.9570</div>	<div><div></div>0.4540</div>
E	<div><div></div>0.9790</div>	<div><div></div>0.5050</div>
F	<div><div></div>0.8670</div>	<div><div></div>0.1150</div>

1.0

0.0

<0.0