Full wwPDB EM Validation Report ⓘ

Apr 28, 2024 – 02:01 AM JST

PDB ID	:	7YFD
EMDB ID	:	EMD-33786
Title	:	Cryo-EM structure of the imetit-bound histamine H4 receptor and Gq complex
Authors	:	Im, D.; Iwata, S.; Asada, H.
Deposited on	:	2022-07-08
Resolution	:	3.10 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:

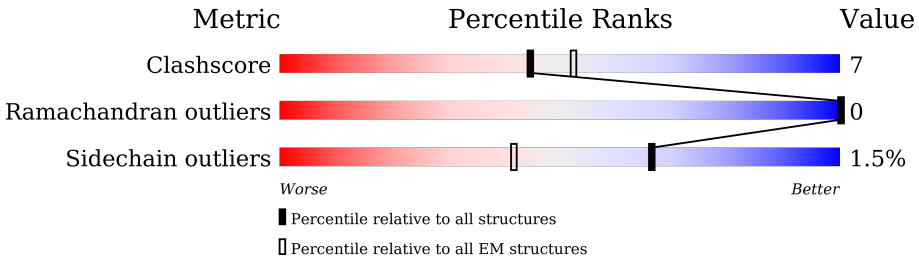
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	361	55% 11% 34%
2	B	388	73% 14% 12%
3	C	259	75% 15% 9%
4	R	548	7% 38% 10% 52%
5	G	71	61% 18% 21%
6	N	129	84% 16%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9934 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 Engineered G-alpha-q.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	238	Total	C	N	O	S	0	0
			1912	1210	338	355	9		

- 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	B	342	Total	C	N	O	S	0	0
			2622	1615	471	515	21		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P62873
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 3 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1799	1139	298	352	10		

- Molecule 4 is a protein called Histamine H4 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	261	Total	C	N	O	S	0	0
			2132	1450	329	343	10		

There are 158 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	391	VAL	-	expression tag	UNP Q9H3N8
R	392	PHE	-	expression tag	UNP Q9H3N8
R	393	THR	-	expression tag	UNP Q9H3N8
R	394	LEU	-	expression tag	UNP Q9H3N8
R	395	GLU	-	expression tag	UNP Q9H3N8
R	396	ASP	-	expression tag	UNP Q9H3N8
R	397	PHE	-	expression tag	UNP Q9H3N8
R	398	VAL	-	expression tag	UNP Q9H3N8
R	399	GLY	-	expression tag	UNP Q9H3N8
R	400	ASP	-	expression tag	UNP Q9H3N8
R	401	TRP	-	expression tag	UNP Q9H3N8
R	402	GLU	-	expression tag	UNP Q9H3N8
R	403	GLN	-	expression tag	UNP Q9H3N8
R	404	THR	-	expression tag	UNP Q9H3N8
R	405	ALA	-	expression tag	UNP Q9H3N8
R	406	ALA	-	expression tag	UNP Q9H3N8
R	407	TYR	-	expression tag	UNP Q9H3N8
R	408	ASN	-	expression tag	UNP Q9H3N8
R	409	LEU	-	expression tag	UNP Q9H3N8
R	410	ASP	-	expression tag	UNP Q9H3N8
R	411	GLN	-	expression tag	UNP Q9H3N8
R	412	VAL	-	expression tag	UNP Q9H3N8
R	413	LEU	-	expression tag	UNP Q9H3N8
R	414	GLU	-	expression tag	UNP Q9H3N8
R	415	GLN	-	expression tag	UNP Q9H3N8
R	416	GLY	-	expression tag	UNP Q9H3N8
R	417	GLY	-	expression tag	UNP Q9H3N8
R	418	VAL	-	expression tag	UNP Q9H3N8
R	419	SER	-	expression tag	UNP Q9H3N8
R	420	SER	-	expression tag	UNP Q9H3N8
R	421	LEU	-	expression tag	UNP Q9H3N8
R	422	LEU	-	expression tag	UNP Q9H3N8
R	423	GLN	-	expression tag	UNP Q9H3N8
R	424	ASN	-	expression tag	UNP Q9H3N8
R	425	LEU	-	expression tag	UNP Q9H3N8
R	426	ALA	-	expression tag	UNP Q9H3N8
R	427	VAL	-	expression tag	UNP Q9H3N8
R	428	SER	-	expression tag	UNP Q9H3N8
R	429	VAL	-	expression tag	UNP Q9H3N8
R	430	THR	-	expression tag	UNP Q9H3N8
R	431	PRO	-	expression tag	UNP Q9H3N8
R	432	ILE	-	expression tag	UNP Q9H3N8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	433	GLN	-	expression tag	UNP Q9H3N8
R	434	ARG	-	expression tag	UNP Q9H3N8
R	435	ILE	-	expression tag	UNP Q9H3N8
R	436	VAL	-	expression tag	UNP Q9H3N8
R	437	ARG	-	expression tag	UNP Q9H3N8
R	438	SER	-	expression tag	UNP Q9H3N8
R	439	GLY	-	expression tag	UNP Q9H3N8
R	440	GLU	-	expression tag	UNP Q9H3N8
R	441	ASN	-	expression tag	UNP Q9H3N8
R	442	ALA	-	expression tag	UNP Q9H3N8
R	443	LEU	-	expression tag	UNP Q9H3N8
R	444	LYS	-	expression tag	UNP Q9H3N8
R	445	ILE	-	expression tag	UNP Q9H3N8
R	446	ASP	-	expression tag	UNP Q9H3N8
R	447	ILE	-	expression tag	UNP Q9H3N8
R	448	HIS	-	expression tag	UNP Q9H3N8
R	449	VAL	-	expression tag	UNP Q9H3N8
R	450	ILE	-	expression tag	UNP Q9H3N8
R	451	ILE	-	expression tag	UNP Q9H3N8
R	452	PRO	-	expression tag	UNP Q9H3N8
R	453	TYR	-	expression tag	UNP Q9H3N8
R	454	GLU	-	expression tag	UNP Q9H3N8
R	455	GLY	-	expression tag	UNP Q9H3N8
R	456	LEU	-	expression tag	UNP Q9H3N8
R	457	SER	-	expression tag	UNP Q9H3N8
R	458	ALA	-	expression tag	UNP Q9H3N8
R	459	ASP	-	expression tag	UNP Q9H3N8
R	460	GLN	-	expression tag	UNP Q9H3N8
R	461	MET	-	expression tag	UNP Q9H3N8
R	462	ALA	-	expression tag	UNP Q9H3N8
R	463	GLN	-	expression tag	UNP Q9H3N8
R	464	ILE	-	expression tag	UNP Q9H3N8
R	465	GLU	-	expression tag	UNP Q9H3N8
R	466	GLU	-	expression tag	UNP Q9H3N8
R	467	VAL	-	expression tag	UNP Q9H3N8
R	468	PHE	-	expression tag	UNP Q9H3N8
R	469	LYS	-	expression tag	UNP Q9H3N8
R	470	VAL	-	expression tag	UNP Q9H3N8
R	471	VAL	-	expression tag	UNP Q9H3N8
R	472	TYR	-	expression tag	UNP Q9H3N8
R	473	PRO	-	expression tag	UNP Q9H3N8
R	474	VAL	-	expression tag	UNP Q9H3N8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	475	ASP	-	expression tag	UNP Q9H3N8
R	476	ASP	-	expression tag	UNP Q9H3N8
R	477	HIS	-	expression tag	UNP Q9H3N8
R	478	HIS	-	expression tag	UNP Q9H3N8
R	479	PHE	-	expression tag	UNP Q9H3N8
R	480	LYS	-	expression tag	UNP Q9H3N8
R	481	VAL	-	expression tag	UNP Q9H3N8
R	482	ILE	-	expression tag	UNP Q9H3N8
R	483	LEU	-	expression tag	UNP Q9H3N8
R	484	PRO	-	expression tag	UNP Q9H3N8
R	485	TYR	-	expression tag	UNP Q9H3N8
R	486	GLY	-	expression tag	UNP Q9H3N8
R	487	THR	-	expression tag	UNP Q9H3N8
R	488	LEU	-	expression tag	UNP Q9H3N8
R	489	VAL	-	expression tag	UNP Q9H3N8
R	490	ILE	-	expression tag	UNP Q9H3N8
R	491	ASP	-	expression tag	UNP Q9H3N8
R	492	GLY	-	expression tag	UNP Q9H3N8
R	493	VAL	-	expression tag	UNP Q9H3N8
R	494	THR	-	expression tag	UNP Q9H3N8
R	495	PRO	-	expression tag	UNP Q9H3N8
R	496	ASN	-	expression tag	UNP Q9H3N8
R	497	MET	-	expression tag	UNP Q9H3N8
R	498	LEU	-	expression tag	UNP Q9H3N8
R	499	ASN	-	expression tag	UNP Q9H3N8
R	500	TYR	-	expression tag	UNP Q9H3N8
R	501	PHE	-	expression tag	UNP Q9H3N8
R	502	GLY	-	expression tag	UNP Q9H3N8
R	503	ARG	-	expression tag	UNP Q9H3N8
R	504	PRO	-	expression tag	UNP Q9H3N8
R	505	TYR	-	expression tag	UNP Q9H3N8
R	506	GLU	-	expression tag	UNP Q9H3N8
R	507	GLY	-	expression tag	UNP Q9H3N8
R	508	ILE	-	expression tag	UNP Q9H3N8
R	509	ALA	-	expression tag	UNP Q9H3N8
R	510	VAL	-	expression tag	UNP Q9H3N8
R	511	PHE	-	expression tag	UNP Q9H3N8
R	512	ASP	-	expression tag	UNP Q9H3N8
R	513	GLY	-	expression tag	UNP Q9H3N8
R	514	LYS	-	expression tag	UNP Q9H3N8
R	515	LYS	-	expression tag	UNP Q9H3N8
R	516	ILE	-	expression tag	UNP Q9H3N8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	517	THR	-	expression tag	UNP Q9H3N8
R	518	VAL	-	expression tag	UNP Q9H3N8
R	519	THR	-	expression tag	UNP Q9H3N8
R	520	GLY	-	expression tag	UNP Q9H3N8
R	521	THR	-	expression tag	UNP Q9H3N8
R	522	LEU	-	expression tag	UNP Q9H3N8
R	523	TRP	-	expression tag	UNP Q9H3N8
R	524	ASN	-	expression tag	UNP Q9H3N8
R	525	GLY	-	expression tag	UNP Q9H3N8
R	526	ASN	-	expression tag	UNP Q9H3N8
R	527	LYS	-	expression tag	UNP Q9H3N8
R	528	ILE	-	expression tag	UNP Q9H3N8
R	529	ILE	-	expression tag	UNP Q9H3N8
R	530	ASP	-	expression tag	UNP Q9H3N8
R	531	GLU	-	expression tag	UNP Q9H3N8
R	532	ARG	-	expression tag	UNP Q9H3N8
R	533	LEU	-	expression tag	UNP Q9H3N8
R	534	ILE	-	expression tag	UNP Q9H3N8
R	535	THR	-	expression tag	UNP Q9H3N8
R	536	PRO	-	expression tag	UNP Q9H3N8
R	537	ASP	-	expression tag	UNP Q9H3N8
R	538	GLY	-	expression tag	UNP Q9H3N8
R	539	SER	-	expression tag	UNP Q9H3N8
R	540	MET	-	expression tag	UNP Q9H3N8
R	541	LEU	-	expression tag	UNP Q9H3N8
R	542	PHE	-	expression tag	UNP Q9H3N8
R	543	ARG	-	expression tag	UNP Q9H3N8
R	544	VAL	-	expression tag	UNP Q9H3N8
R	545	THR	-	expression tag	UNP Q9H3N8
R	546	ILE	-	expression tag	UNP Q9H3N8
R	547	ASN	-	expression tag	UNP Q9H3N8
R	548	SER	-	expression tag	UNP Q9H3N8

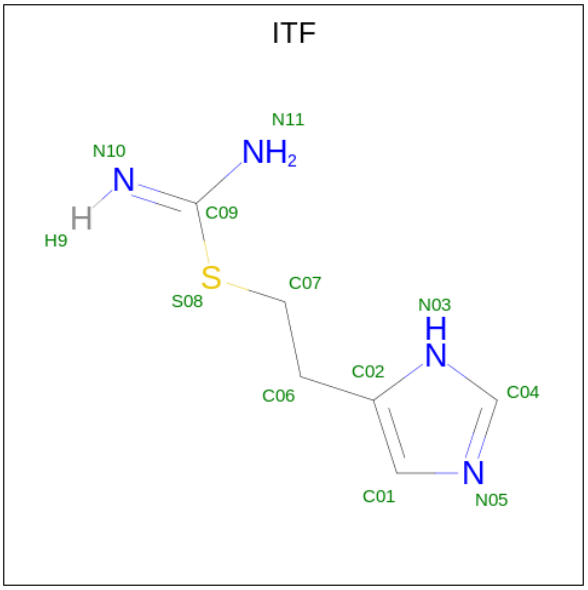
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 6 is a protein called Nb35.

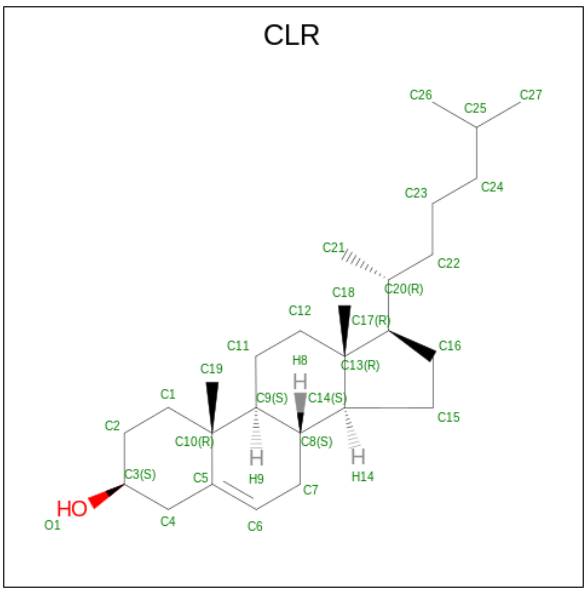
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 7 is 2-(1 {H}-imidazol-5-yl)ethyl carbamimidothioate (three-letter code: ITF) (formula: $C_6H_{10}N_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	S	0
			11	6	4	1	

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



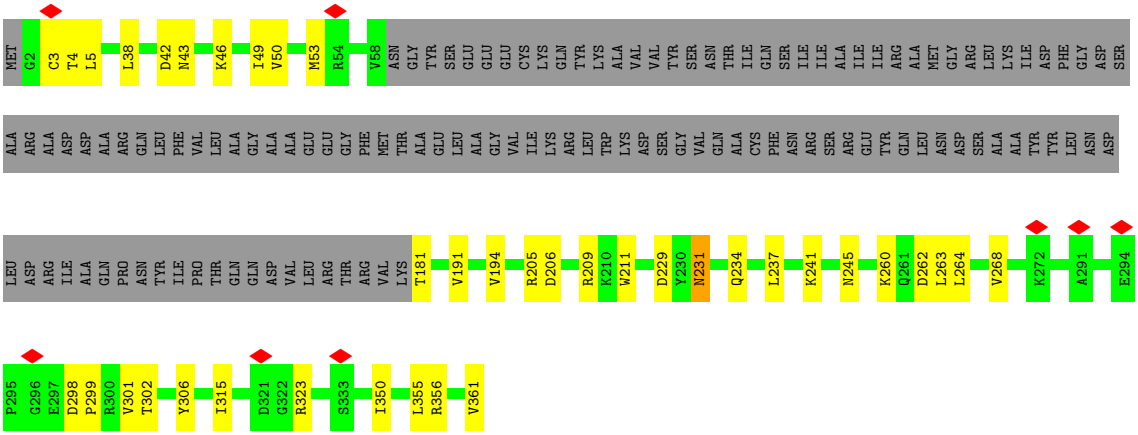
Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			28	27	1	
8	R	1	Total	C	O	0
			28	27	1	

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.

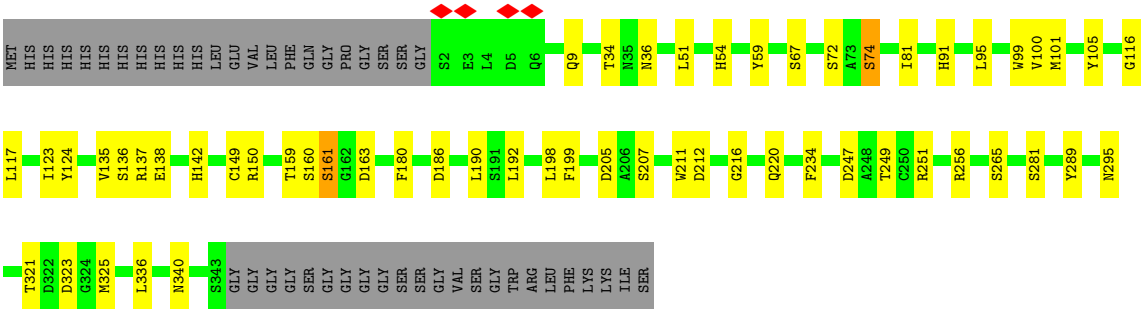
• Molecule 1: Engineered G-alpha-q

Chain A:



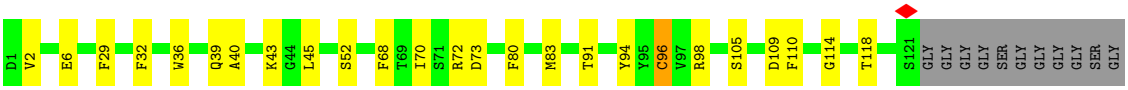
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

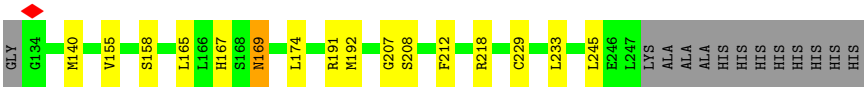
Chain B:



• Molecule 3: scFv16

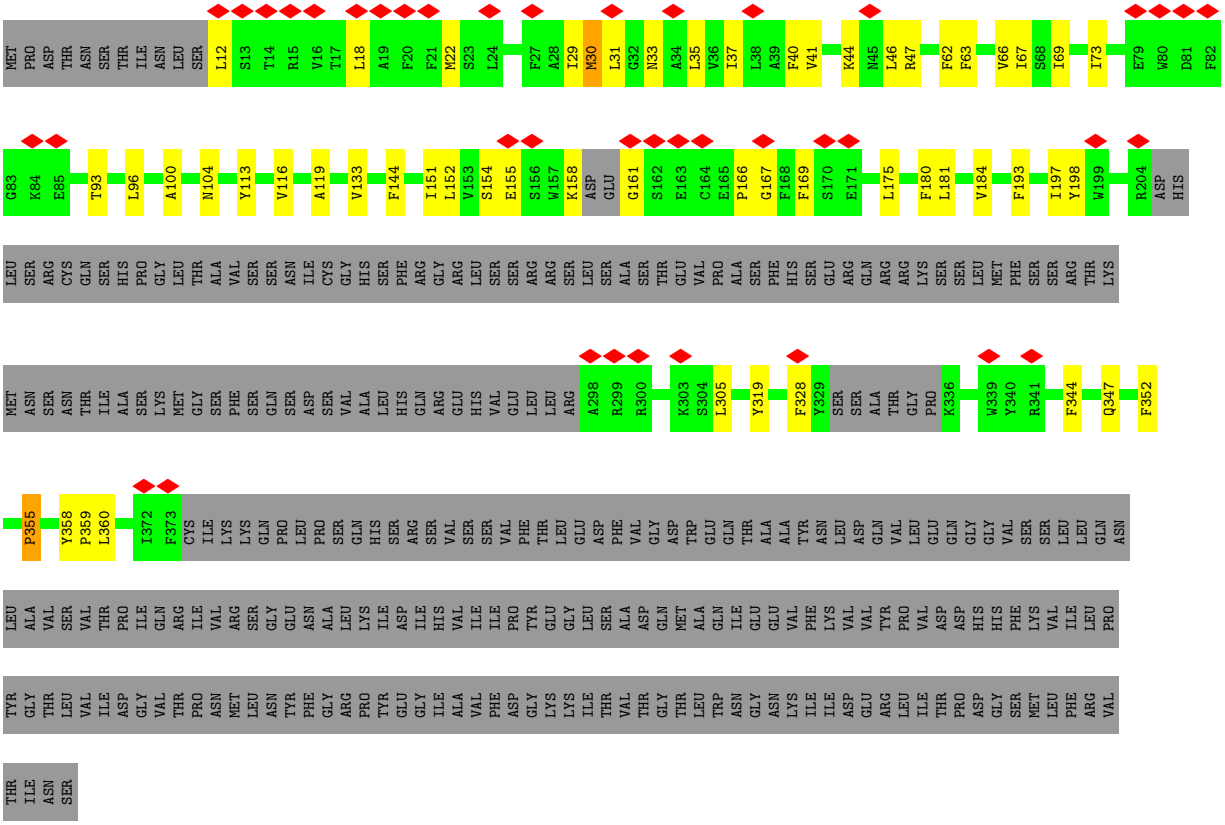
Chain C:





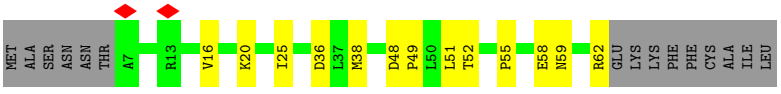
• Molecule 4: Histamine H4 receptor

Chain R:



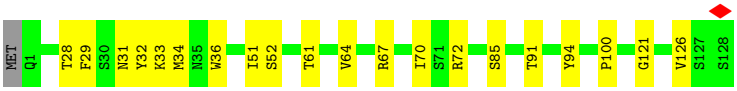
• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



• Molecule 6: Nb35

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	628467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	59.883	Depositor
Minimum map value	-47.621	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, ITF

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	0.25	0/1947	0.48	0/2626
2	B	0.25	0/2669	0.54	0/3618
3	C	0.26	0/1843	0.50	0/2498
4	R	0.26	0/2199	0.44	1/2998 (0.0%)
5	G	0.30	0/435	0.49	0/587
6	N	0.26	0/993	0.50	0/1345
All	All	0.26	0/10086	0.49	1/13672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	355	PRO	CA-N-CD	-5.79	103.39	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1912	0	1875	26	0
2	B	2622	0	2523	36	0
3	C	1799	0	1730	26	0
4	R	2132	0	2159	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	429	0	441	10	0
6	N	973	0	938	12	0
7	R	11	0	0	1	0
8	R	56	0	92	3	0
All	All	9934	0	9758	134	0

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

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:113:TYR:HA	4:R:197:ILE:HD11	1.65	0.78
3:C:98:ARG:HD3	3:C:110:PHE:HB3	1.68	0.76
3:C:94:TYR:O	3:C:114:GLY:HA2	1.89	0.72
2:B:51:LEU:HD12	2:B:336:LEU:HD22	1.76	0.66
4:R:344:PHE:O	7:R:601:ITF:N11	2.29	0.65
1:A:264:LEU:O	1:A:268:VAL:HG12	1.97	0.65
3:C:32:PHE:O	3:C:72:ARG:NH2	2.33	0.61
3:C:36:TRP:HD1	3:C:70:ILE:HD12	1.64	0.61
2:B:256:ARG:NH2	5:G:36:ASP:OD2	2.29	0.60
3:C:52:SER:O	3:C:72:ARG:NH1	2.34	0.60
3:C:105:SER:O	3:C:191:ARG:NH2	2.34	0.60
1:A:350:ILE:HG22	4:R:119:ALA:HB1	1.84	0.60
6:N:61:THR:HG22	6:N:64:VAL:HG22	1.84	0.60
1:A:46:LYS:O	1:A:50:VAL:HG13	2.02	0.59
4:R:358:TYR:HB2	4:R:359:PRO:HD3	1.84	0.59
1:A:205:ARG:NH2	2:B:186:ASP:OD1	2.36	0.59
4:R:40:PHE:HA	4:R:46:LEU:HD12	1.85	0.58
2:B:205:ASP:OD2	2:B:207:SER:OG	2.20	0.58
1:A:209:ARG:HD3	6:N:100:PRO:HG3	1.86	0.57
2:B:340:ASN:ND2	5:G:59:ASN:OD1	2.38	0.57
1:A:355:LEU:HD23	1:A:361:VAL:HB	1.87	0.57
6:N:67:ARG:NH1	6:N:85:SER:O	2.37	0.57
4:R:100:ALA:O	4:R:104:ASN:ND2	2.38	0.56
3:C:29:PHE:O	3:C:72:ARG:NH2	2.37	0.56
3:C:39:GLN:HB2	3:C:45:LEU:HD23	1.88	0.55
2:B:289:TYR:HE1	2:B:295:ASN:HB2	1.73	0.54
2:B:321:THR:HG22	2:B:323:ASP:H	1.73	0.53
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.89	0.53
2:B:198:LEU:HD23	2:B:212:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:HA	1:A:302:THR:HG22	1.91	0.52
4:R:355:PRO:O	4:R:359:PRO:HD2	2.10	0.52
1:A:205:ARG:HG2	1:A:206:ASP:H	1.76	0.51
2:B:149:CYS:O	2:B:150:ARG:NH1	2.42	0.51
4:R:152:LEU:O	4:R:155:GLU:HG3	2.10	0.51
2:B:161:SER:HB3	2:B:163:ASP:OD1	2.11	0.51
6:N:94:TYR:O	6:N:121:GLY:HA2	2.11	0.51
2:B:180:PHE:CE2	2:B:216:GLY:HA2	2.46	0.51
2:B:142:HIS:NE2	2:B:159:THR:OG1	2.37	0.50
4:R:69:ILE:O	4:R:73:ILE:HG12	2.11	0.50
3:C:68:PHE:CE1	3:C:83:MET:HB3	2.45	0.50
2:B:67:SER:HB3	2:B:321:THR:HG23	1.94	0.50
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.93	0.50
1:A:298:ASP:OD1	1:A:299:PRO:HD2	2.12	0.50
3:C:207:GLY:HA3	3:C:212:PHE:HD1	1.77	0.49
6:N:29:PHE:O	6:N:72:ARG:NH2	2.45	0.49
4:R:31:LEU:O	4:R:35:LEU:HD13	2.12	0.49
4:R:37:ILE:O	4:R:41:VAL:HG23	2.13	0.49
4:R:319:TYR:HB3	4:R:347:GLN:HE21	1.78	0.49
1:A:241:LYS:HG2	1:A:315:ILE:HG21	1.95	0.49
4:R:29:ILE:HG12	4:R:352:PHE:HB2	1.95	0.48
3:C:73:ASP:HB2	3:C:80:PHE:HE2	1.76	0.48
3:C:165:LEU:HA	3:C:233:LEU:HD22	1.96	0.48
4:R:133:VAL:HG12	8:R:602:CLR:H6	1.96	0.48
4:R:96:LEU:HD13	4:R:144:PHE:HB2	1.96	0.48
2:B:81:ILE:HD13	2:B:91:HIS:HB2	1.95	0.48
4:R:169:PHE:HD1	4:R:175:LEU:HD11	1.78	0.48
1:A:191:VAL:O	1:A:194:VAL:HG12	2.14	0.47
1:A:260:LYS:HD3	1:A:263:LEU:HD12	1.95	0.47
3:C:91:THR:OG1	3:C:118:THR:HA	2.14	0.47
4:R:180:PHE:O	4:R:184:VAL:HB	2.14	0.47
2:B:325:MET:HA	5:G:49:PRO:HB2	1.95	0.47
3:C:2:VAL:HG11	3:C:98:ARG:NH1	2.29	0.47
2:B:249:THR:OG1	2:B:251:ARG:NH1	2.47	0.47
3:C:174:LEU:HD11	3:C:229:CYS:SG	2.54	0.47
5:G:59:ASN:O	5:G:62:ARG:NH2	2.48	0.47
2:B:101:MET:HG3	2:B:116:GLY:HA2	1.95	0.47
6:N:91:THR:HB	6:N:126:VAL:H	1.79	0.47
3:C:192:MET:HG2	3:C:192:MET:O	2.13	0.47
4:R:67:ILE:HG21	4:R:93:THR:HG21	1.97	0.47
5:G:16:VAL:HG12	5:G:20:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:32:TYR:O	6:N:72:ARG:NH2	2.37	0.47
2:B:99:TRP:HB3	2:B:117:LEU:HD12	1.95	0.47
1:A:241:LYS:O	1:A:245:ASN:ND2	2.44	0.46
4:R:154:SER:OG	4:R:166:PRO:O	2.23	0.46
5:G:55:PRO:HD2	5:G:58:GLU:OE2	2.14	0.46
3:C:174:LEU:HB3	3:C:192:MET:HB2	1.98	0.46
3:C:6:GLU:OE2	3:C:96:CYS:HB3	2.16	0.46
1:A:211:TRP:HB2	2:B:117:LEU:HD21	1.97	0.46
2:B:249:THR:HG22	2:B:265:SER:HB3	1.98	0.46
2:B:54:HIS:ND1	2:B:74:SER:HB3	2.31	0.46
4:R:18:LEU:O	4:R:22:MET:HG3	2.16	0.46
4:R:158:LYS:HD2	4:R:167:GLY:HA3	1.97	0.46
4:R:193:PHE:O	4:R:197:ILE:HG12	2.15	0.45
1:A:234:GLN:HA	1:A:237:LEU:HD12	1.98	0.45
4:R:63:PHE:HA	4:R:66:VAL:HG12	1.98	0.45
4:R:151:ILE:HD12	4:R:166:PRO:HB3	1.98	0.45
3:C:6:GLU:OE1	3:C:114:GLY:N	2.29	0.45
6:N:28:THR:OG1	6:N:31:ASN:OD1	2.25	0.45
2:B:281:SER:OG	5:G:48:ASP:OD2	2.34	0.45
3:C:155:VAL:HG11	3:C:245:LEU:HD21	1.98	0.44
4:R:360:LEU:HD23	4:R:360:LEU:HA	1.83	0.44
4:R:44:LYS:HA	4:R:47:ARG:NH1	2.33	0.44
3:C:207:GLY:HA3	3:C:212:PHE:CD1	2.53	0.44
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.52	0.44
1:A:298:ASP:HB3	1:A:301:VAL:HG23	2.00	0.44
1:A:38:LEU:HD21	1:A:46:LYS:HB2	1.98	0.43
4:R:158:LYS:HE3	4:R:161:GLY:HA2	2.00	0.43
1:A:181:THR:O	1:A:181:THR:OG1	2.35	0.43
4:R:30:MET:HG3	4:R:62:PHE:CE1	2.54	0.43
4:R:33:ASN:HB3	4:R:62:PHE:HB2	2.00	0.43
1:A:43:ASN:ND2	1:A:229:ASP:OD2	2.52	0.43
6:N:33:LYS:HG3	6:N:51:ILE:O	2.19	0.43
2:B:150:ARG:HB3	2:B:192:LEU:HD12	1.99	0.43
5:G:51:LEU:O	5:G:52:THR:OG1	2.32	0.43
3:C:208:SER:O	3:C:208:SER:OG	2.32	0.42
2:B:321:THR:HG22	2:B:323:ASP:N	2.32	0.42
6:N:36:TRP:HD1	6:N:70:ILE:HD12	1.85	0.42
1:A:3:CYS:SG	1:A:4:THR:N	2.93	0.42
8:R:602:CLR:H262	8:R:602:CLR:H231	1.81	0.42
2:B:220:GLN:HG2	5:G:25:ILE:HD13	2.00	0.42
2:B:95:LEU:HD13	2:B:100:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.93	0.41
4:R:116:VAL:HB	4:R:197:ILE:HD12	2.02	0.41
1:A:49:ILE:HG13	1:A:50:VAL:N	2.35	0.41
3:C:109:ASP:OD1	3:C:109:ASP:N	2.52	0.41
4:R:181:LEU:HD22	8:R:603:CLR:H261	2.03	0.41
1:A:231:ASN:OD1	1:A:231:ASN:N	2.52	0.41
2:B:247:ASP:N	2:B:247:ASP:OD1	2.53	0.41
2:B:34:THR:HG22	5:G:38:MET:SD	2.60	0.41
2:B:199:PHE:CE1	2:B:211:TRP:HB2	2.56	0.41
6:N:52:SER:O	6:N:72:ARG:NH1	2.54	0.41
1:A:262:ASP:OD1	1:A:263:LEU:N	2.52	0.41
4:R:12:LEU:HD12	4:R:12:LEU:HA	1.91	0.41
3:C:167:HIS:ND1	3:C:169:ASN:OD1	2.53	0.40
6:N:34:MET:HE2	6:N:34:MET:HB3	2.00	0.40
2:B:36:ASN:OD1	2:B:36:ASN:N	2.54	0.40
3:C:140:MET:HE1	3:C:229:CYS:SG	2.61	0.40
2:B:123:ILE:O	2:B:136:SER:N	2.55	0.40
2:B:150:ARG:HD3	2:B:150:ARG:HA	1.74	0.40
4:R:198:TYR:HB2	4:R:305:LEU:HD12	2.04	0.40
1:A:302:THR:OG1	1:A:306:TYR:HE2	2.04	0.40
1:A:323:ARG:HA	1:A:356:ARG:NH1	2.37	0.40
2:B:137:ARG:HG3	2:B:138:GLU:N	2.36	0.40
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.55	0.40

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	234/361 (65%)	231 (99%)	3 (1%)	0	100	100
2	B	340/388 (88%)	331 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	231/259 (89%)	218 (94%)	13 (6%)	0	100	100
4	R	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
5	G	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
6	N	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
All	All	1238/1756 (70%)	1201 (97%)	37 (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	A	205/316 (65%)	202 (98%)	3 (2%)	65	85
2	B	284/317 (90%)	277 (98%)	7 (2%)	47	75
3	C	198/209 (95%)	194 (98%)	4 (2%)	55	80
4	R	230/490 (47%)	228 (99%)	2 (1%)	78	91
5	G	45/58 (78%)	45 (100%)	0	100	100
6	N	106/107 (99%)	106 (100%)	0	100	100
All	All	1068/1497 (71%)	1052 (98%)	16 (2%)	66	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	53	MET
1	A	231	ASN
2	B	9	GLN
2	B	59	TYR
2	B	72	SER
2	B	74	SER
2	B	105	TYR
2	B	161	SER

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Mol	Chain	Res	Type
2	B	234	PHE
3	C	96	CYS
3	C	158	SER
3	C	169	ASN
3	C	218	ARG
4	R	30	MET
4	R	328	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

3 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	ITF	R	601	-	6,11,11	1.21	1 (16%)	6,13,13	1.77	1 (16%)
8	CLR	R	603	-	31,31,31	0.30	0	48,48,48	0.42	0
8	CLR	R	602	-	31,31,31	0.29	0	48,48,48	0.46	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	ITF	R	601	-	-	3/5/6/6	0/1/1/1
8	CLR	R	603	-	-	0/10/68/68	0/4/4/4
8	CLR	R	602	-	-	7/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	601	ITF	C09-N11	2.06	1.38	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	601	ITF	C07-S08-C09	3.47	111.62	102.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	601	ITF	C06-C07-S08-C09
7	R	601	ITF	N10-C09-S08-C07
7	R	601	ITF	N11-C09-S08-C07
8	R	602	CLR	C22-C23-C24-C25
8	R	602	CLR	C23-C24-C25-C26
8	R	602	CLR	C16-C17-C20-C22
8	R	602	CLR	C20-C22-C23-C24
8	R	602	CLR	C23-C24-C25-C27
8	R	602	CLR	C17-C20-C22-C23
8	R	602	CLR	C13-C17-C20-C22

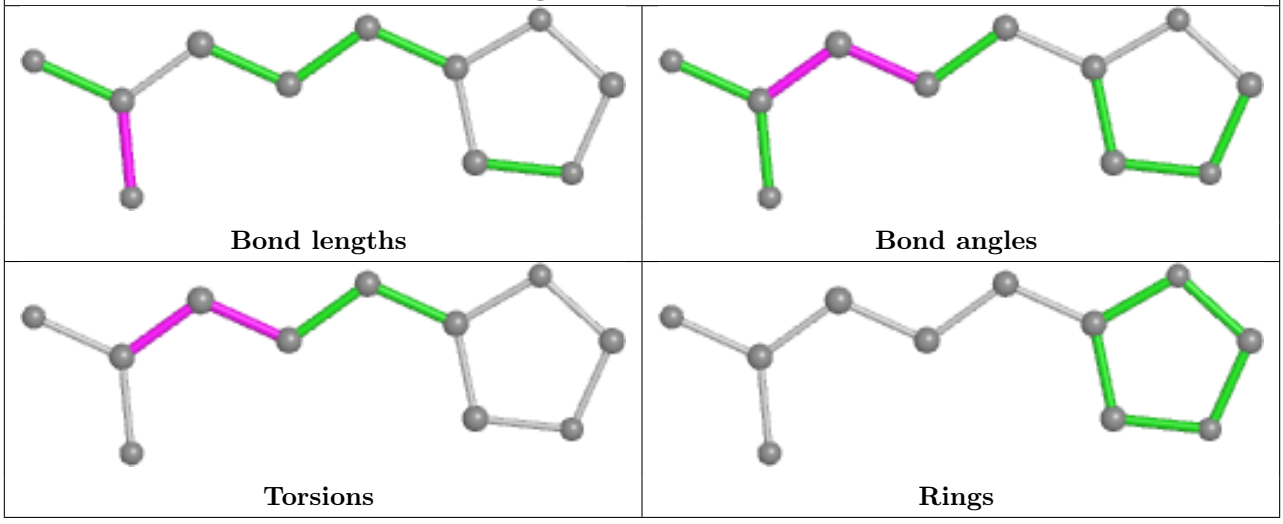
There are no ring outliers.

3 monomers are involved in 4 short contacts:

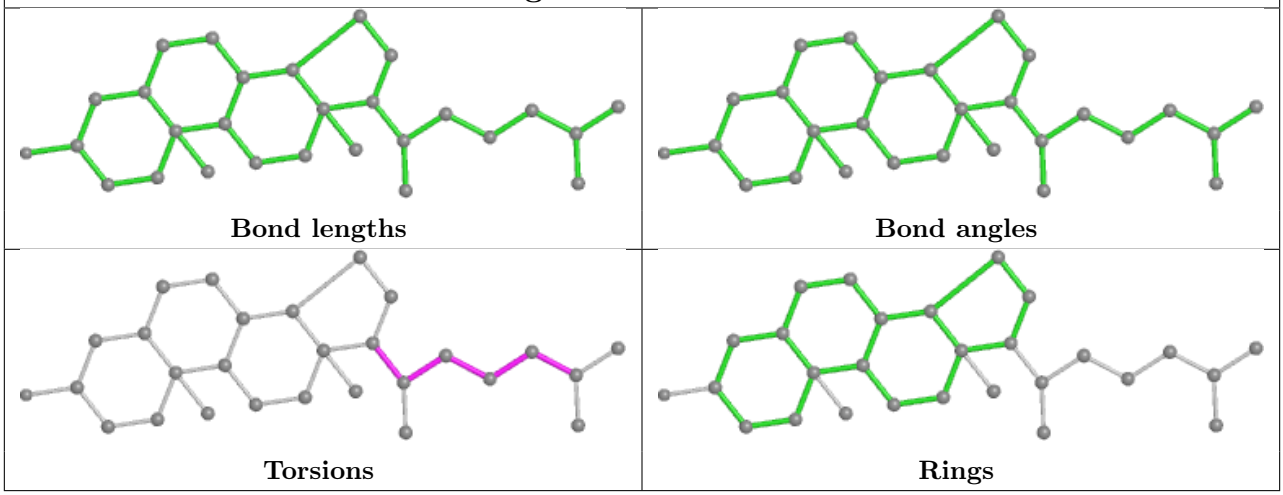
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	601	ITF	1	0
8	R	603	CLR	1	0
8	R	602	CLR	2	0

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 then 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.

Ligand ITF R 601



Ligand CLR R 602



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.

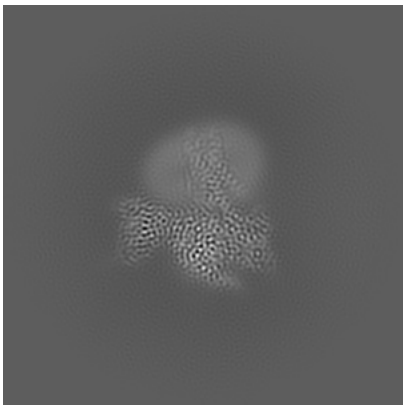
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33786. These allow visual inspection of the internal detail of the map and identification of artifacts.

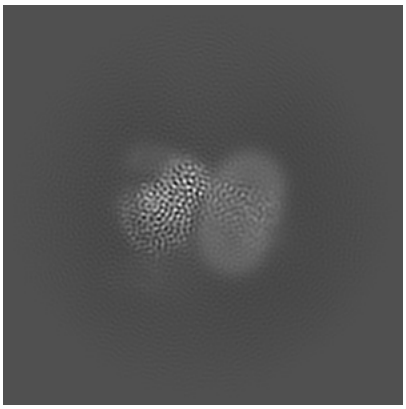
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

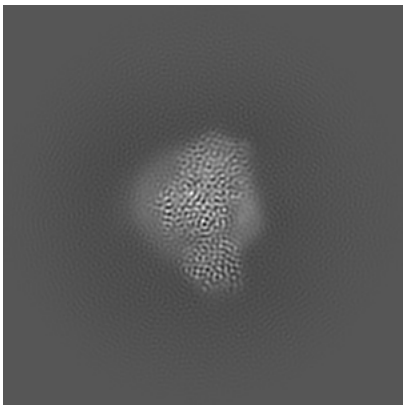
6.1.1 Primary map



X

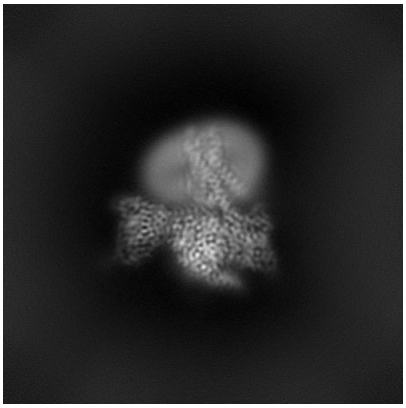


Y

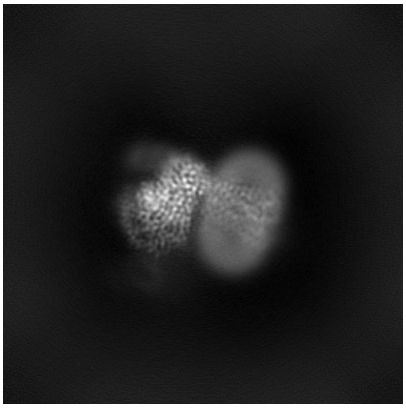


Z

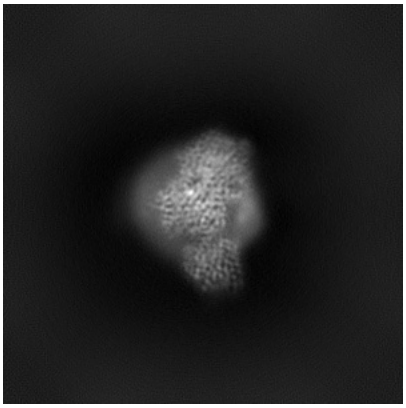
6.1.2 Raw map



X



Y

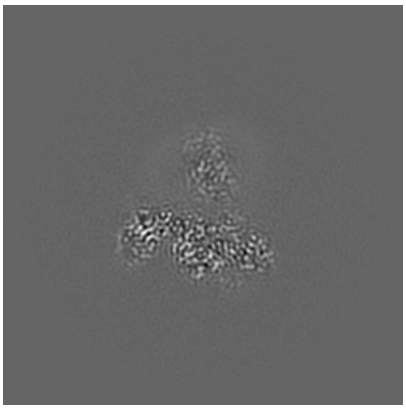


Z

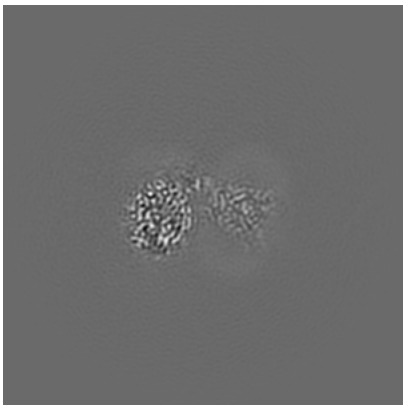
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

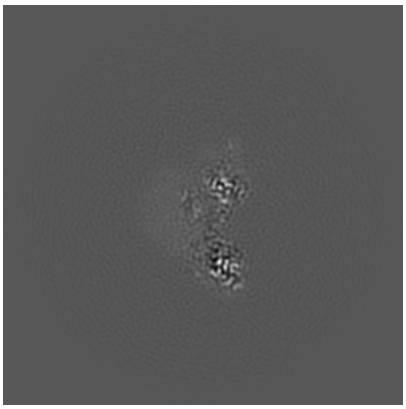
6.2.1 Primary map



X Index: 160

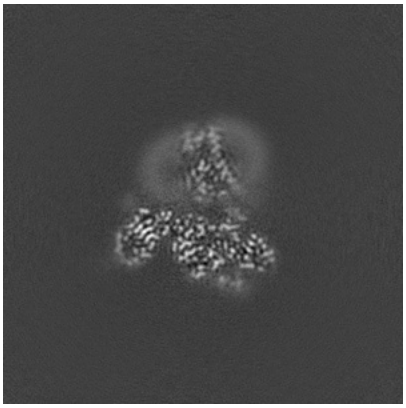


Y Index: 160

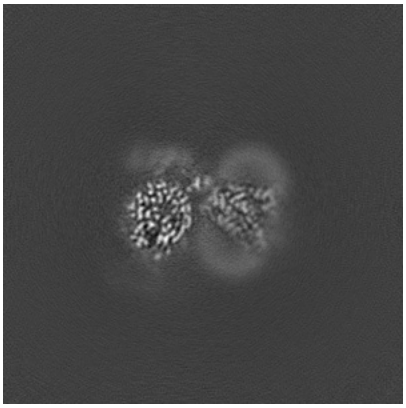


Z Index: 160

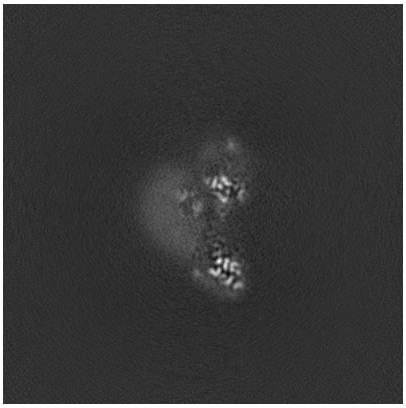
6.2.2 Raw map



X Index: 160



Y Index: 160

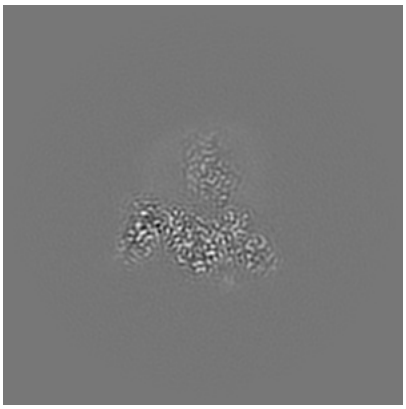


Z Index: 160

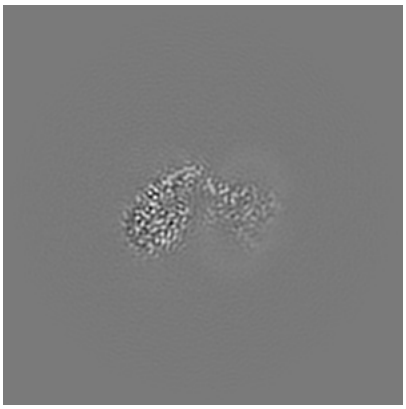
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

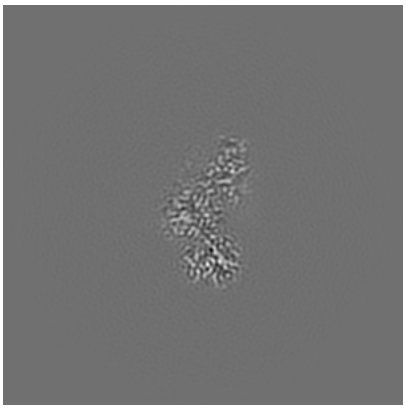
6.3.1 Primary map



X Index: 166

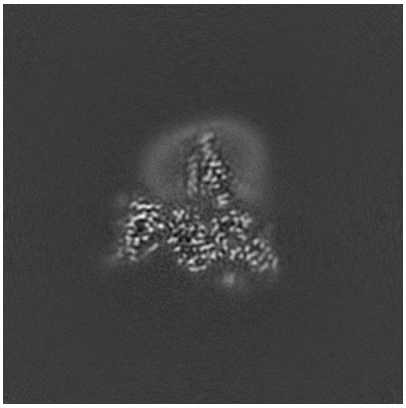


Y Index: 166

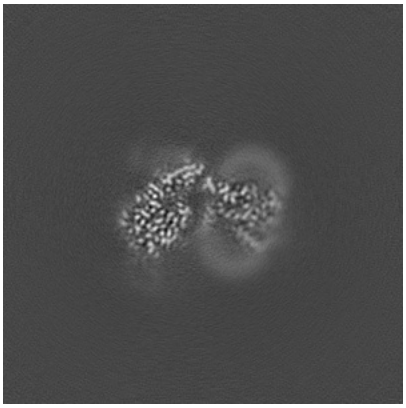


Z Index: 143

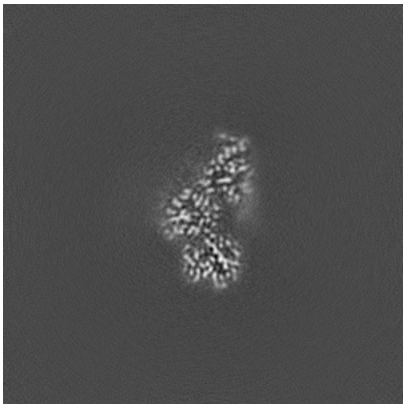
6.3.2 Raw map



X Index: 168



Y Index: 166

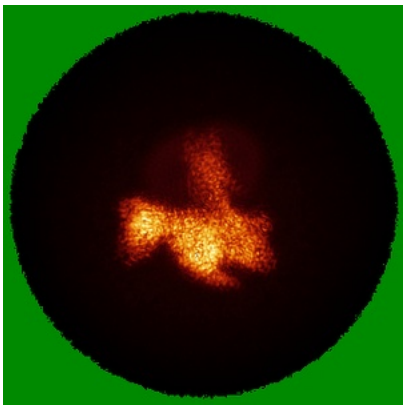


Z Index: 143

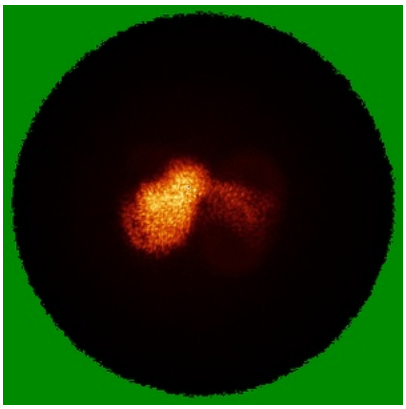
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

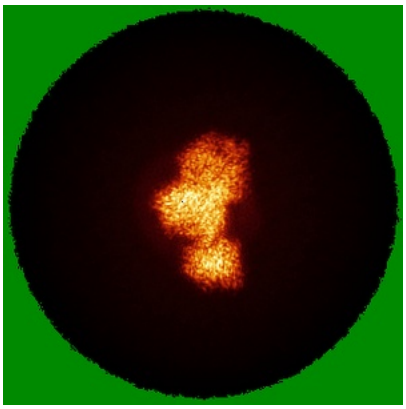
6.4.1 Primary map



X

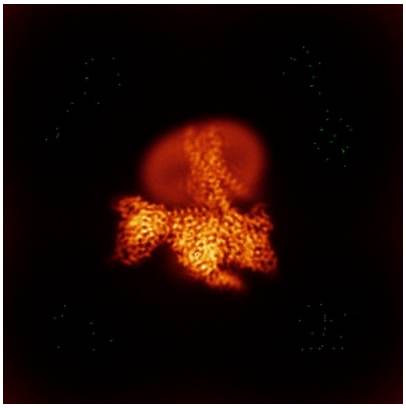


Y

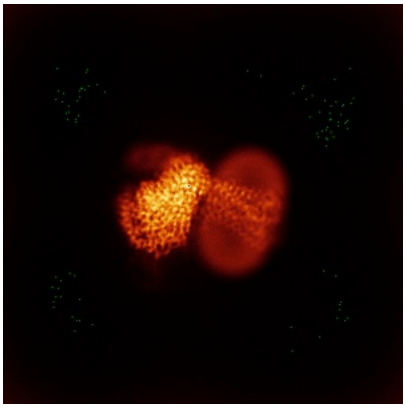


Z

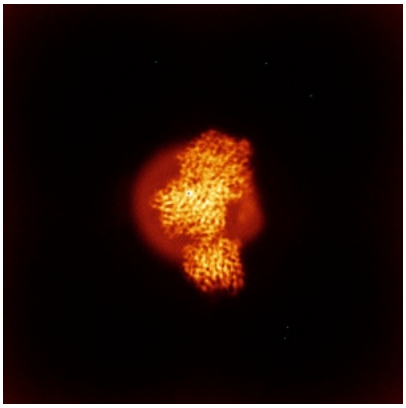
6.4.2 Raw map



X



Y

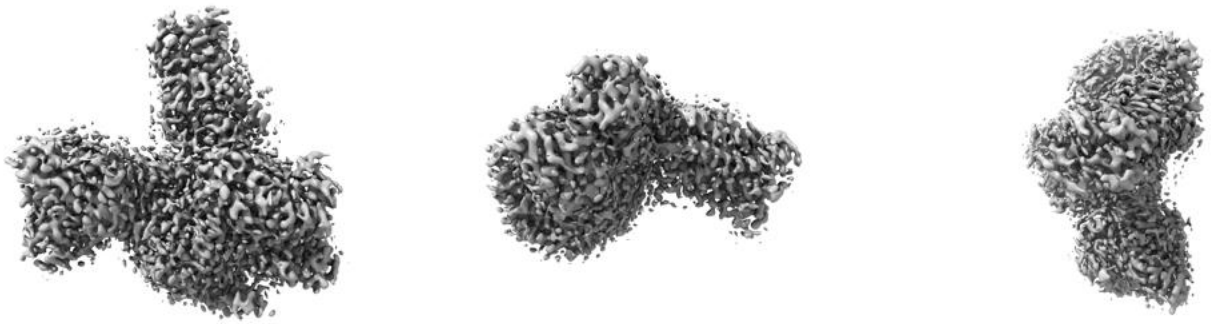


Z

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)

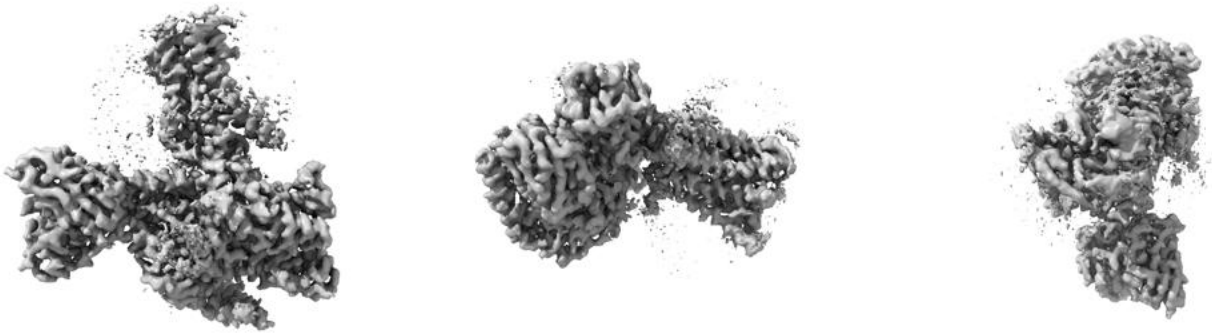
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. 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.

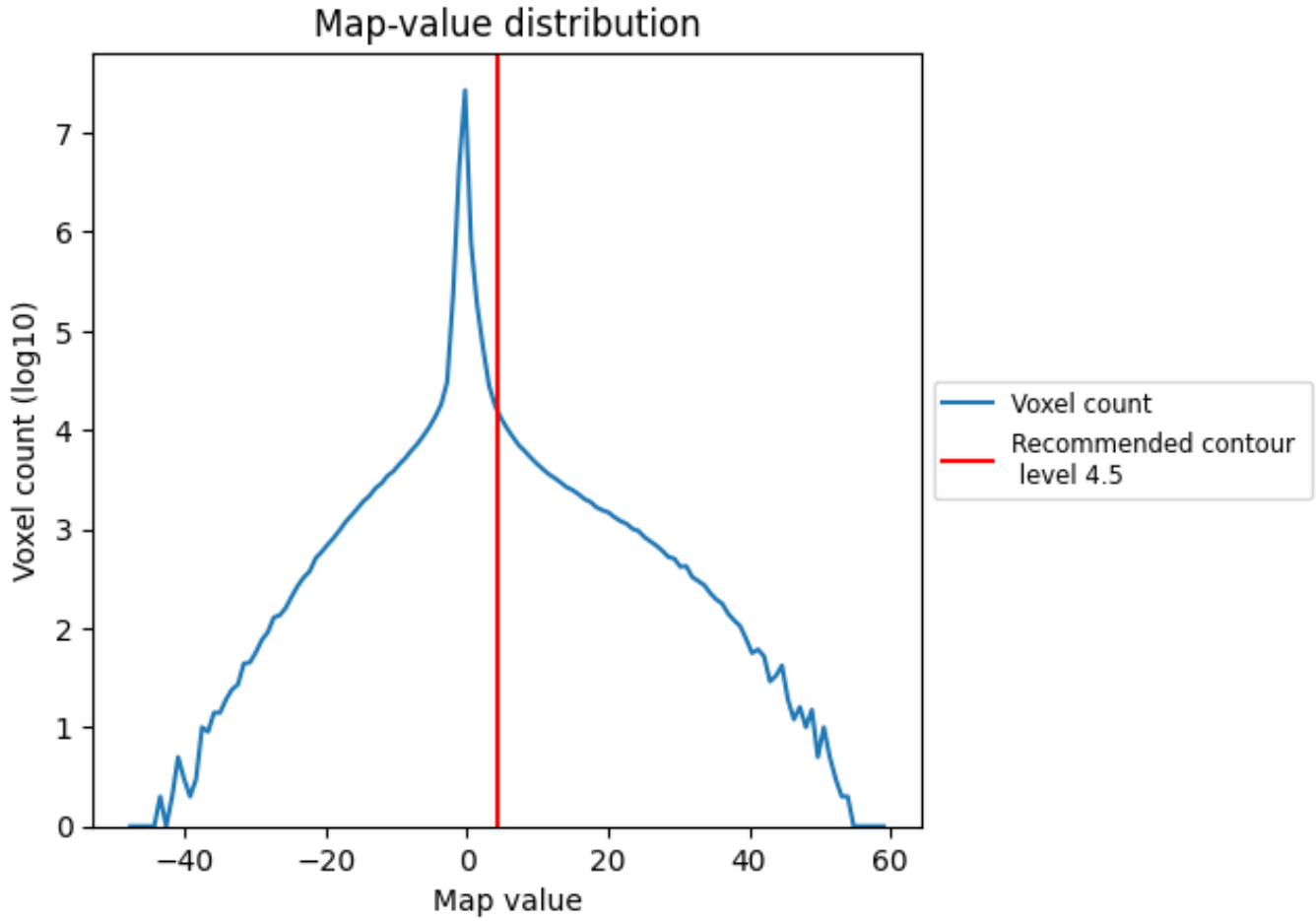
6.6 Mask visualisation (i)

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

7 Map analysis

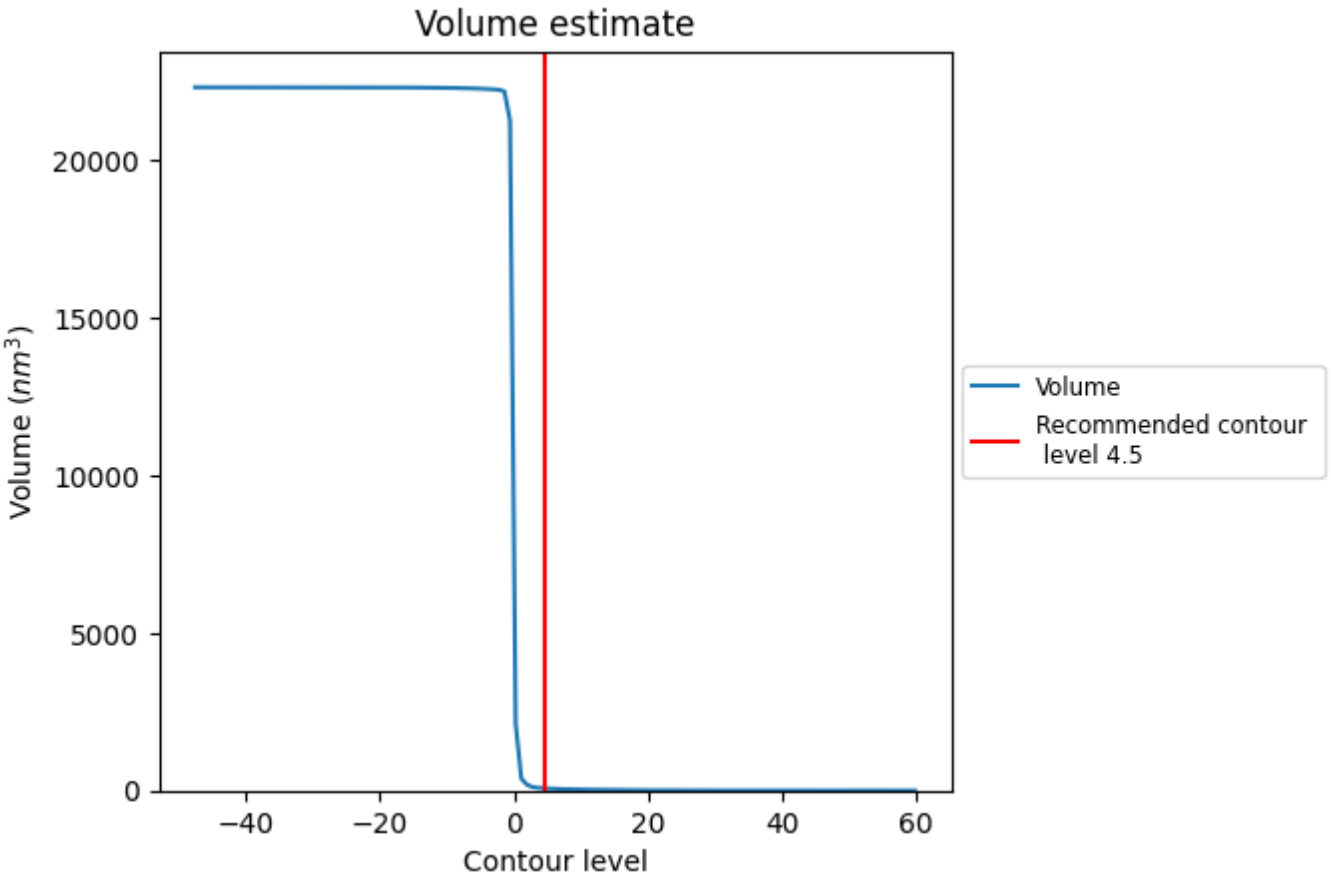
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

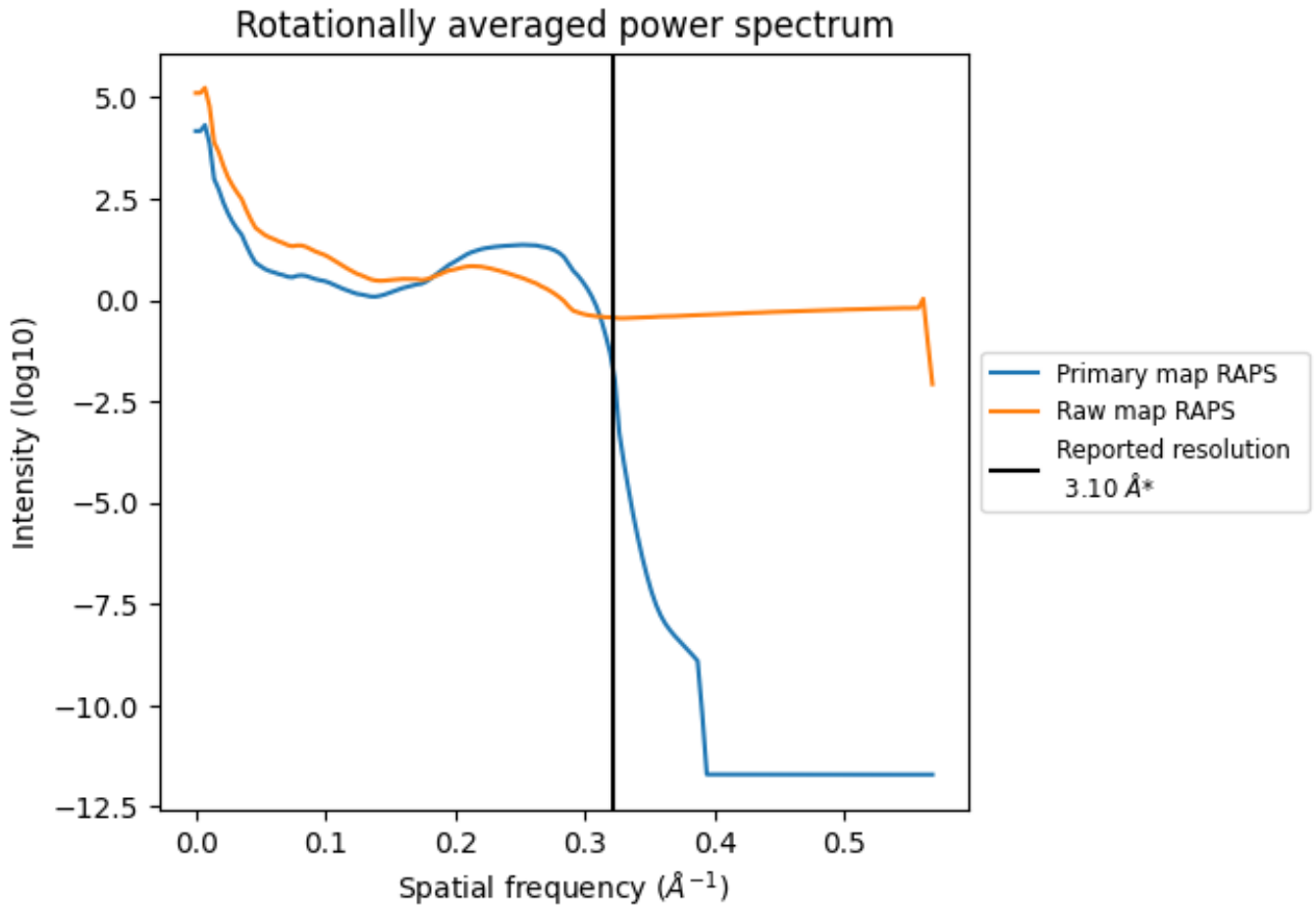
7.2 Volume estimate



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 64 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 (i)

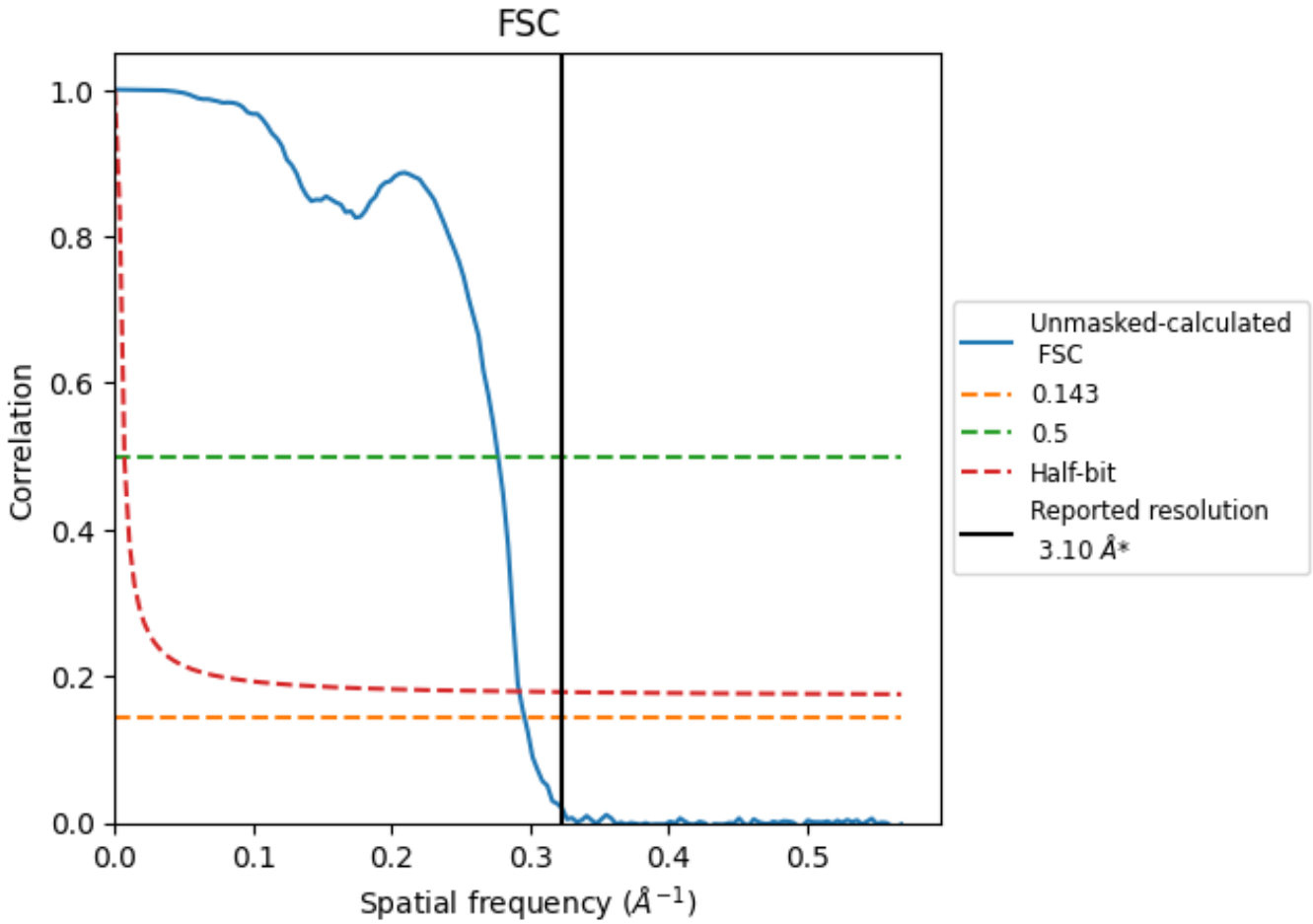


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

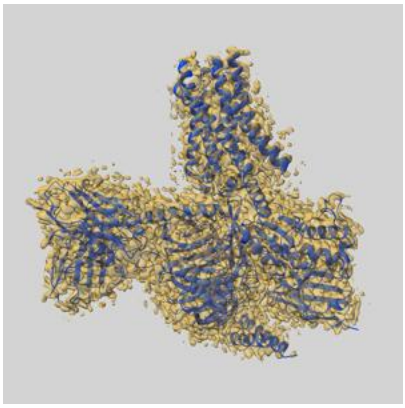
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.61	3.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

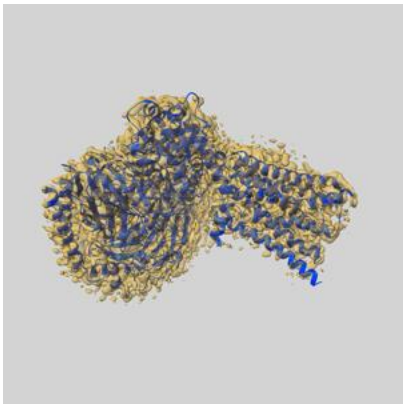
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33786 and PDB model 7YFD. Per-residue inclusion information can be found in section 3 on page 11.

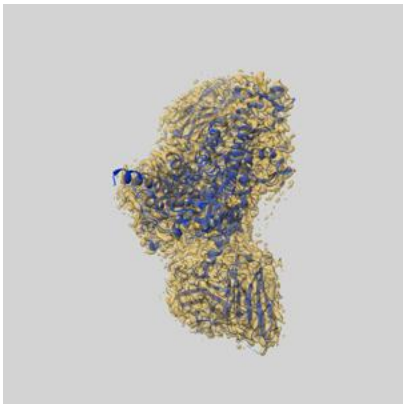
9.1 Map-model overlay



X



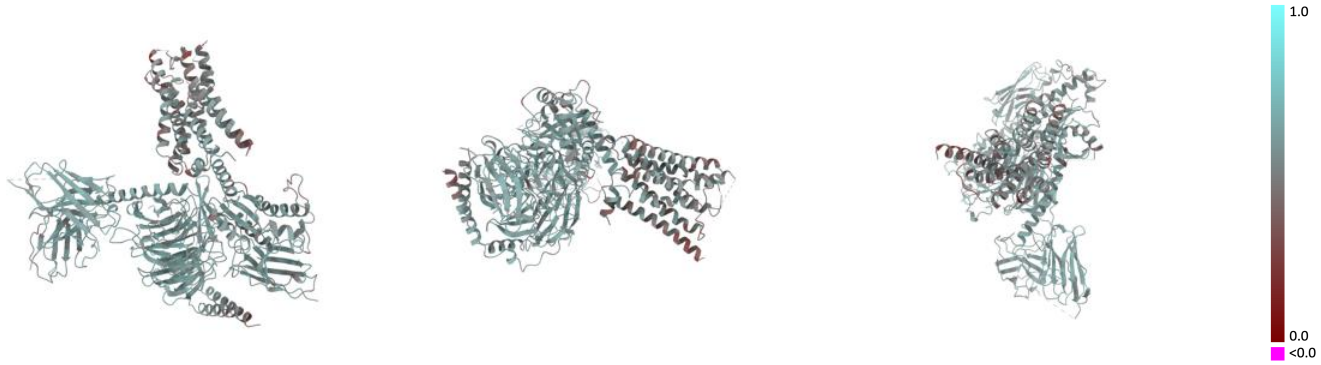
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

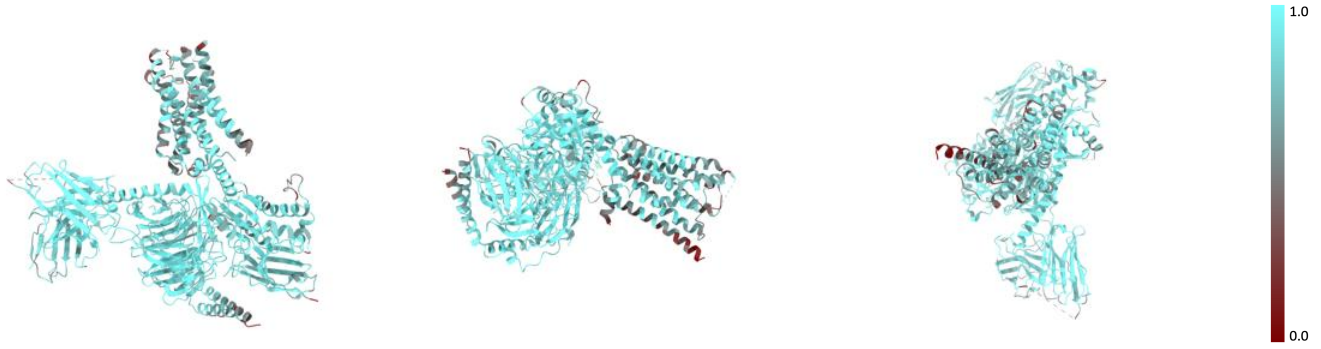
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

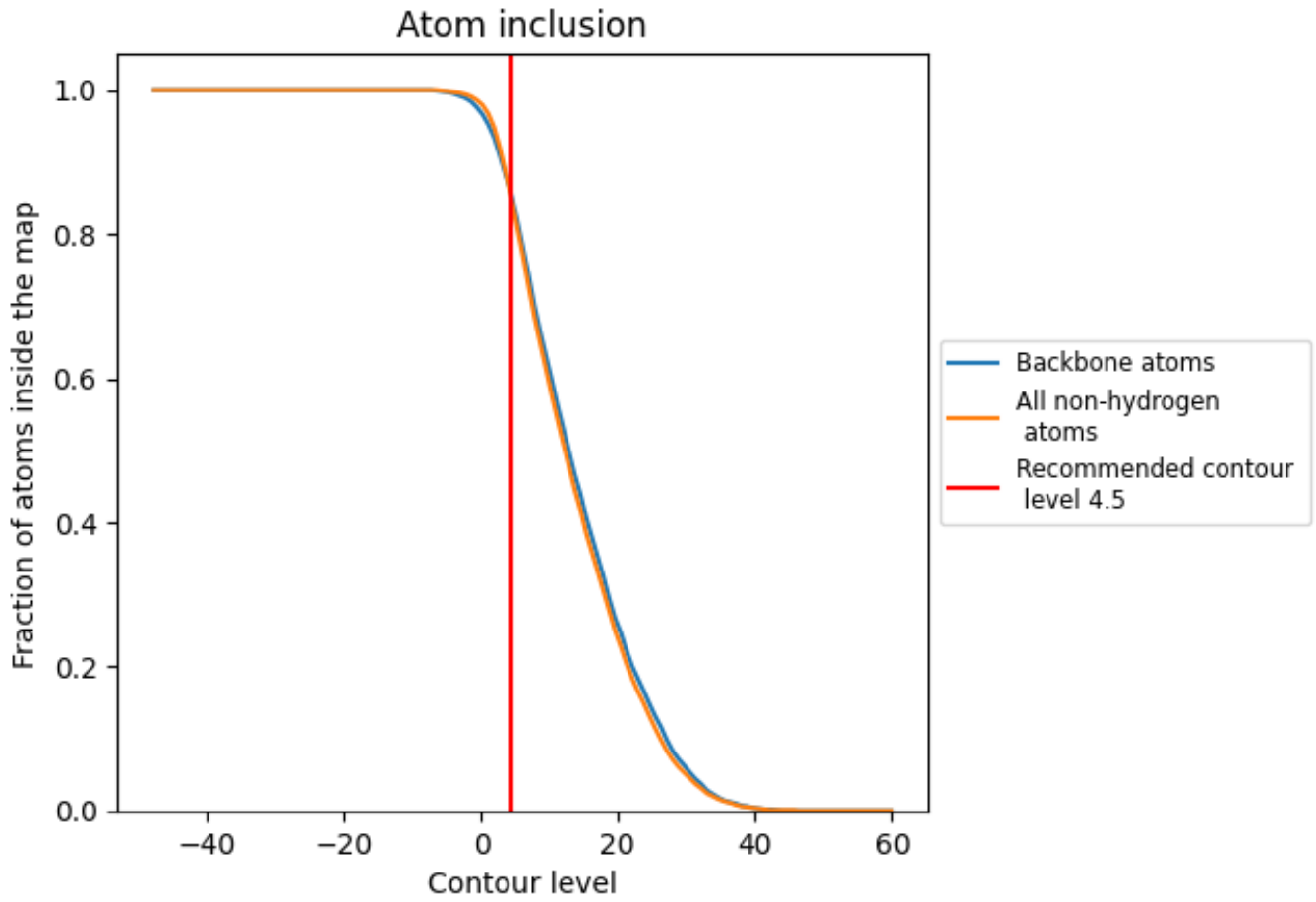
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8480	0.5520
A	0.8790	0.5590
B	0.9290	0.5860
C	0.8860	0.5750
G	0.8370	0.5520
N	0.8710	0.5690
R	0.6870	0.4800