wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 06:36 AM JST

PDB ID	:	7WJ5
EMDB ID	:	EMD-32543
Title	:	Cryo-EM structure of human somatostatin receptor 2 complex with its agonist somatostatin delineates the ligand binding specificity
Authors	:	Heo, Y.S.; Yoon, E.J.; Jeon, Y.E.; Yun, J.-H.; Ishimoto, N.; Woo, H.; Park, S.Y.; Song, J.; Lee, W.T.
Deposited on	:	2022-01-05
Resolution	:	3.72 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

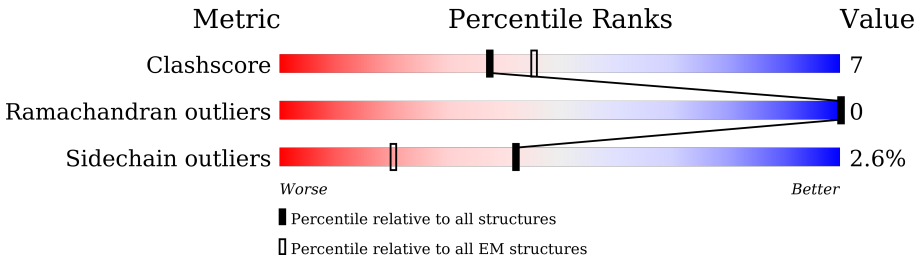
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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 <=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	29% 47% 14% 40%
2	B	358	8% 73% 19% 6%
3	C	71	24% 70% 25%
4	E	266	74% 12% 13%
5	R	518	14% 42% 12% 46%
6	S	14	7% 71% 14% 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8660 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
			Total	C	N	O	S		
1	A	214	1653	1057	284	300	12	0	0

- 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
			Total	C	N	O	S		
2	B	336	2547	1577	458	493	19	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	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
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- 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	C	53	Total	C	N	O	S	0	0
			381	243	67	68	3		

- Molecule 4 is a protein called Gai1 antibody (scfv16).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	232	Total	C	N	O	S	0	0
			1748	1116	295	328	9		

- Molecule 5 is a protein called Soluble cytochrome b562,Somatostatin receptor type 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	282	Total	C	N	O	S	0	0
			2226	1487	356	363	20		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-148	MET	-	initiating methionine	UNP P0ABE7
R	-147	LYS	-	expression tag	UNP P0ABE7
R	-146	THR	-	expression tag	UNP P0ABE7
R	-145	ILE	-	expression tag	UNP P0ABE7
R	-144	ILE	-	expression tag	UNP P0ABE7
R	-143	ALA	-	expression tag	UNP P0ABE7
R	-142	LEU	-	expression tag	UNP P0ABE7
R	-141	SER	-	expression tag	UNP P0ABE7
R	-140	TYR	-	expression tag	UNP P0ABE7
R	-139	ILE	-	expression tag	UNP P0ABE7
R	-138	PHE	-	expression tag	UNP P0ABE7
R	-137	CYS	-	expression tag	UNP P0ABE7
R	-136	LEU	-	expression tag	UNP P0ABE7
R	-135	VAL	-	expression tag	UNP P0ABE7
R	-134	PHE	-	expression tag	UNP P0ABE7
R	-133	ALA	-	expression tag	UNP P0ABE7
R	-132	ASP	-	expression tag	UNP P0ABE7
R	-131	TYR	-	expression tag	UNP P0ABE7
R	-130	LYS	-	expression tag	UNP P0ABE7
R	-129	ASP	-	expression tag	UNP P0ABE7
R	-128	ASP	-	expression tag	UNP P0ABE7
R	-127	ASP	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-126	ASP	-	expression tag	UNP P0ABE7
R	-125	LYS	-	expression tag	UNP P0ABE7
R	-124	HIS	-	expression tag	UNP P0ABE7
R	-123	HIS	-	expression tag	UNP P0ABE7
R	-122	HIS	-	expression tag	UNP P0ABE7
R	-121	HIS	-	expression tag	UNP P0ABE7
R	-120	HIS	-	expression tag	UNP P0ABE7
R	-119	HIS	-	expression tag	UNP P0ABE7
R	-118	HIS	-	expression tag	UNP P0ABE7
R	-117	HIS	-	expression tag	UNP P0ABE7
R	-116	LEU	-	expression tag	UNP P0ABE7
R	-115	GLU	-	expression tag	UNP P0ABE7
R	-114	VAL	-	expression tag	UNP P0ABE7
R	-113	LEU	-	expression tag	UNP P0ABE7
R	-112	PHE	-	expression tag	UNP P0ABE7
R	-111	GLN	-	expression tag	UNP P0ABE7
R	-110	GLY	-	expression tag	UNP P0ABE7
R	-109	PRO	-	expression tag	UNP P0ABE7
R	-108	GLY	-	expression tag	UNP P0ABE7
R	-107	ALA	-	expression tag	UNP P0ABE7
R	-106	PRO	-	expression tag	UNP P0ABE7
R	-99	TRP	MET	conflict	UNP P0ABE7
R	-4	ILE	HIS	conflict	UNP P0ABE7
R	0	LEU	-	linker	UNP P0ABE7

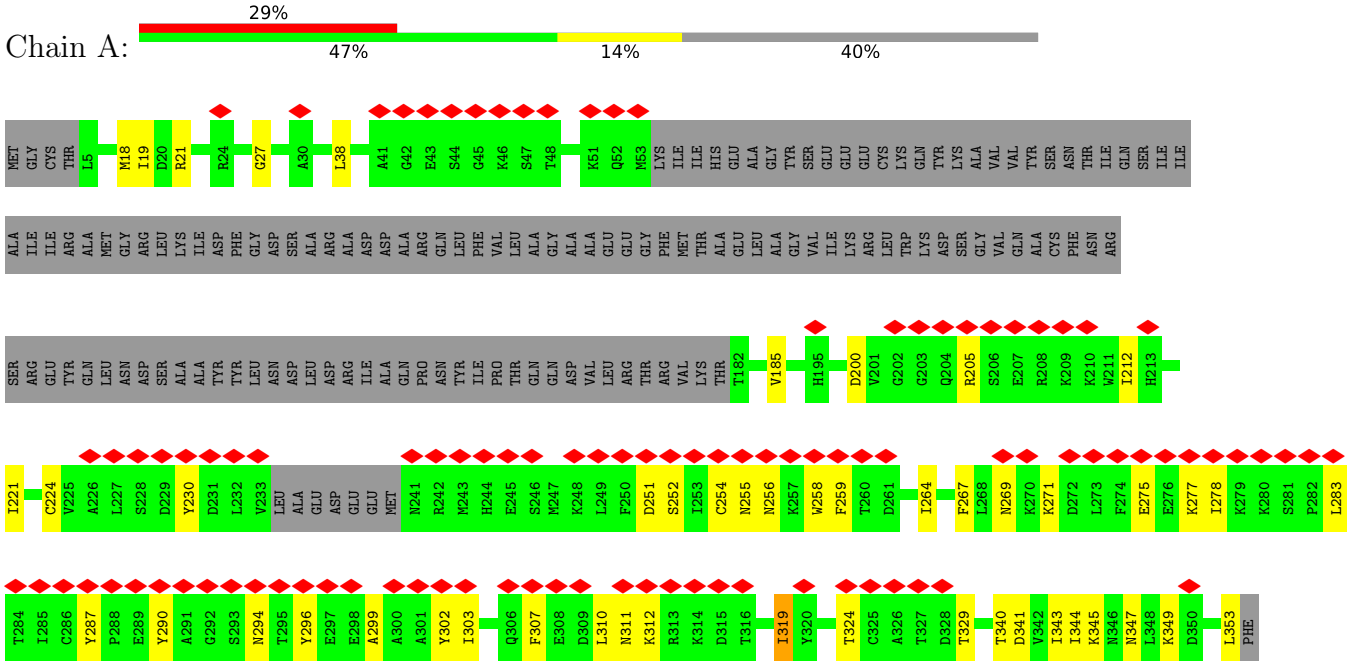
- Molecule 6 is a protein called Somatostatin-14 (SST-14).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	12	Total	C	N	O	S	0	0
			105	71	16	16	2		

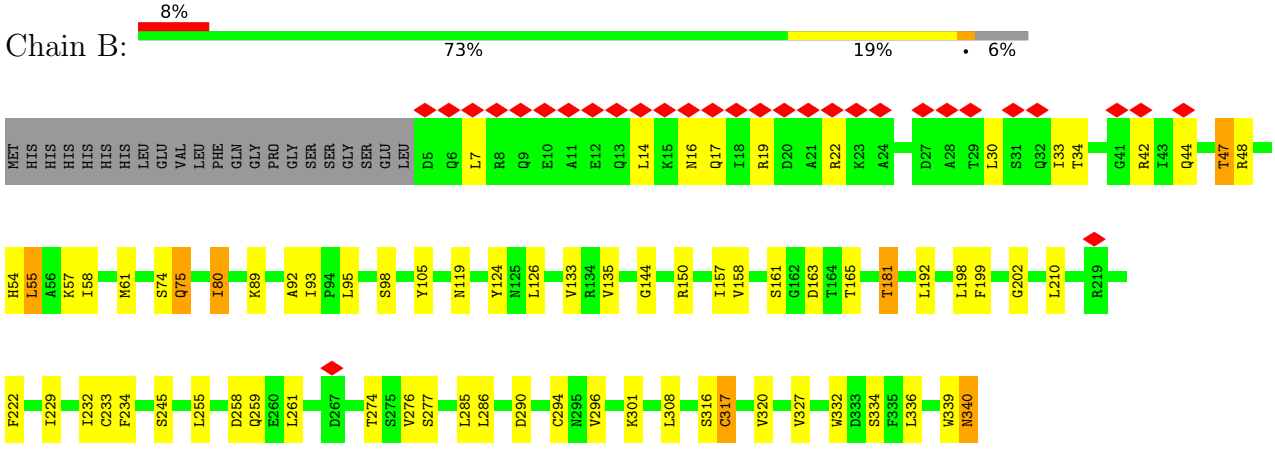
3 Residue-property plots (i)

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.

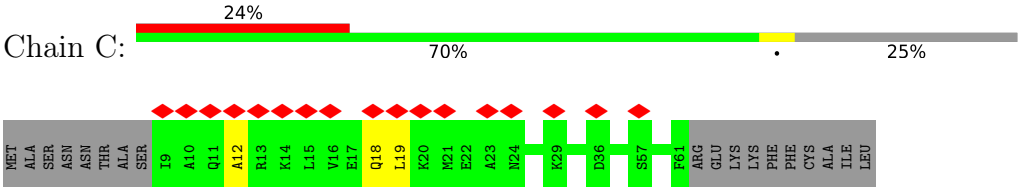
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



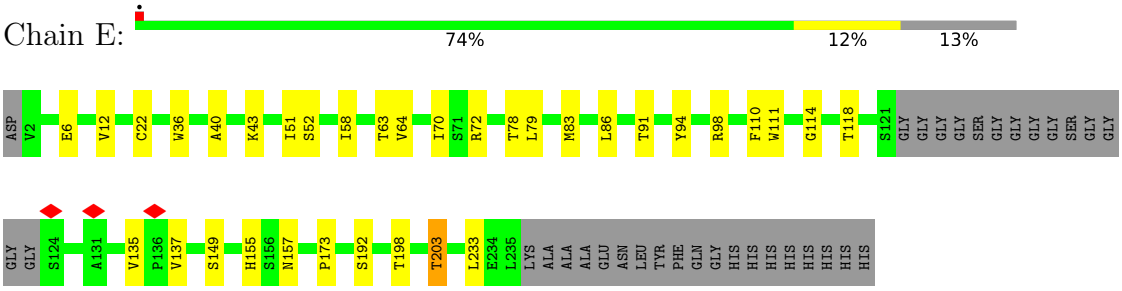
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



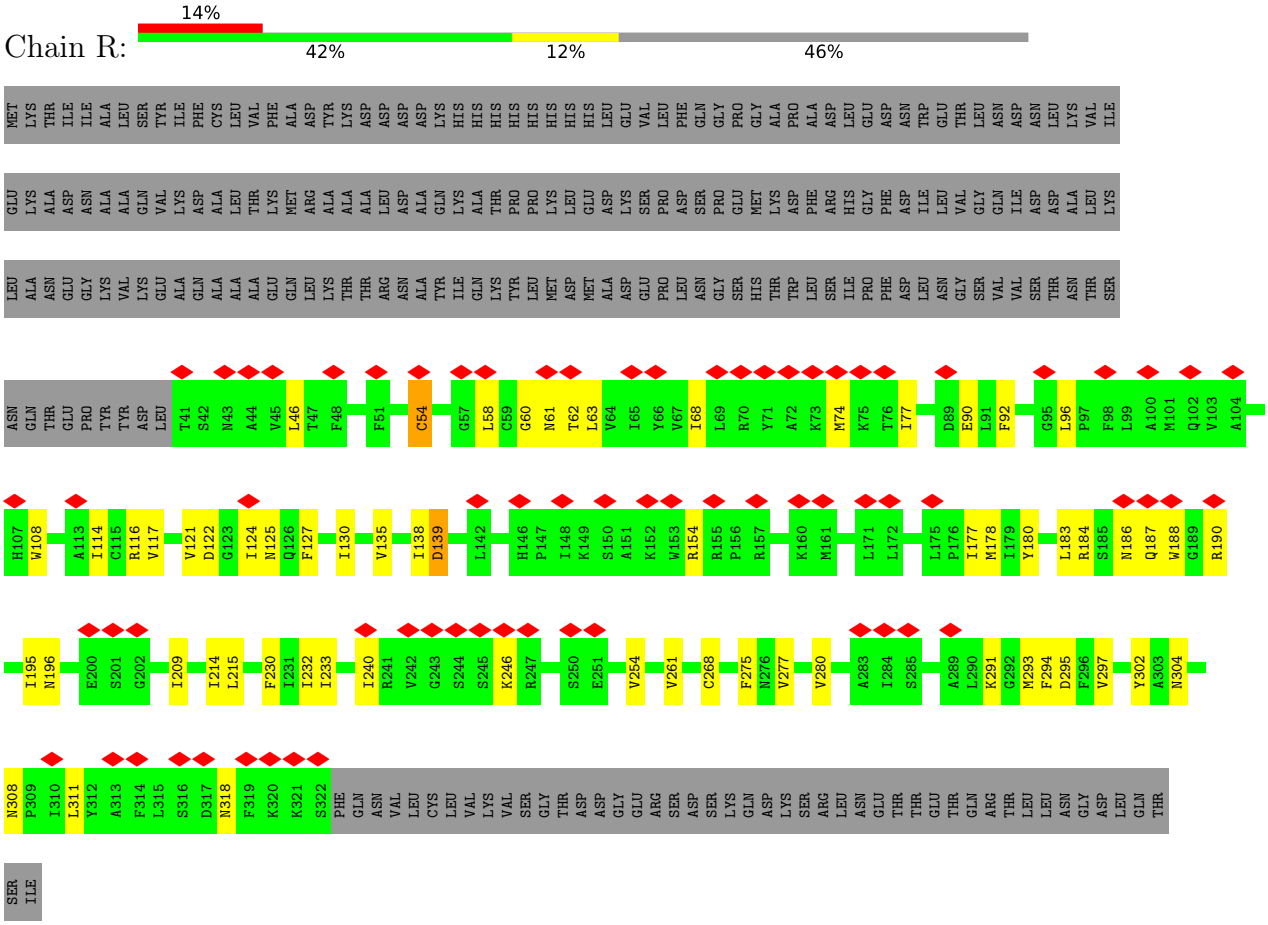
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



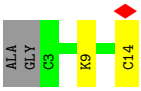
• Molecule 4: Gai1 antibody (scfv16)



• Molecule 5: Soluble cytochrome b562,Somatostatin receptor type 2



• Molecule 6: Somatostatin-14 (SST-14)


ALA
GLY
C3
K9
C14

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320885	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 ($e^-/Å^2$)	55.04	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	75000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	31.865	Depositor
Minimum map value	-19.582	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.033	Depositor
Recommended contour level	5	Depositor
Map size (Å)	212.224, 212.224, 212.224	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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	0.26	0/1681	0.46	0/2262
2	B	0.29	0/2594	0.55	0/3520
3	C	0.25	0/387	0.43	0/527
4	E	0.32	0/1792	0.50	0/2434
5	R	0.28	0/2283	0.47	0/3104
6	S	0.30	0/109	0.47	0/145
All	All	0.28	0/8846	0.50	0/11992

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

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	1653	0	1610	28	0
2	B	2547	0	2437	42	0
3	C	381	0	378	2	0
4	E	1748	0	1669	19	0
5	R	2226	0	2350	39	0
6	S	105	0	95	2	0
All	All	8660	0	8539	125	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.

The worst 5 of 125 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA3	2:B:55:LEU:HD11	1.55	0.86
1:A:221:ILE:HB	1:A:264:ILE:HG22	1.69	0.74
5:R:186:ASN:HD21	5:R:190:ARG:HB2	1.52	0.72
1:A:287:TYR:HB3	1:A:290:TYR:HB3	1.72	0.72
1:A:224:CYS:SG	1:A:269:ASN:ND2	2.63	0.71

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/354 (59%)	199 (96%)	9 (4%)	0	100	100
2	B	334/358 (93%)	319 (96%)	15 (4%)	0	100	100
3	C	51/71 (72%)	49 (96%)	2 (4%)	0	100	100
4	E	228/266 (86%)	220 (96%)	8 (4%)	0	100	100
5	R	280/518 (54%)	269 (96%)	11 (4%)	0	100	100
6	S	10/14 (71%)	9 (90%)	1 (10%)	0	100	100
All	All	1111/1581 (70%)	1065 (96%)	46 (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	170/305 (56%)	166 (98%)	4 (2%)	44	64
2	B	268/298 (90%)	255 (95%)	13 (5%)	21	47
3	C	36/58 (62%)	35 (97%)	1 (3%)	38	60
4	E	184/215 (86%)	182 (99%)	2 (1%)	70	80
5	R	248/453 (55%)	244 (98%)	4 (2%)	58	74
6	S	12/12 (100%)	12 (100%)	0	100	100
All	All	918/1341 (68%)	894 (97%)	24 (3%)	42	62

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	317	CYS
3	C	18	GLN
2	B	340	ASN
4	E	78	THR
2	B	75	GLN

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

Mol	Chain	Res	Type
1	A	255	ASN
5	R	186	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

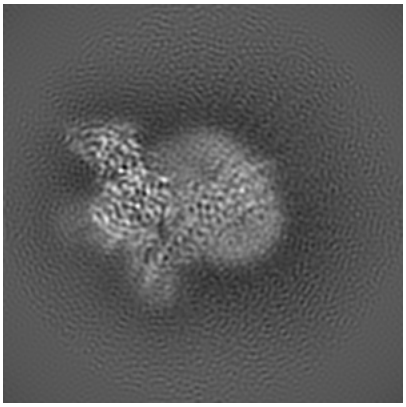
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32543. These allow visual inspection of the internal detail of the map and identification of artifacts.

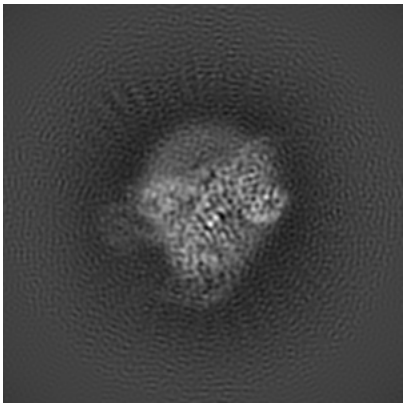
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

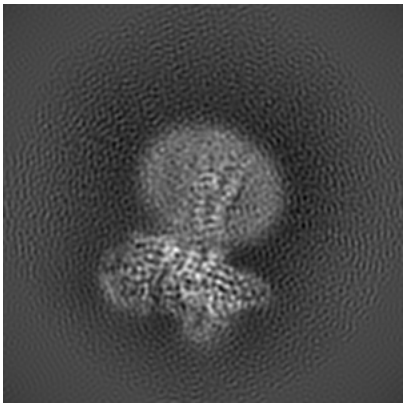
6.1.1 Primary map



X



Y

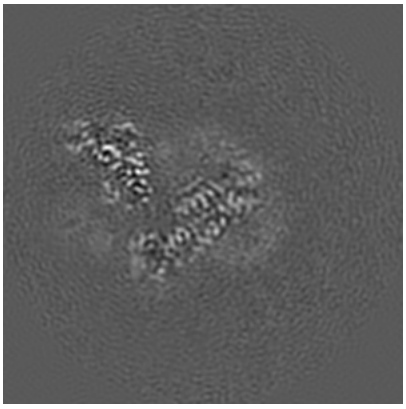


Z

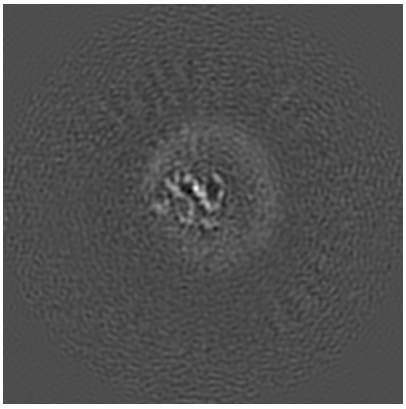
The images above show the map projected in three orthogonal directions.

6.2 Central slices

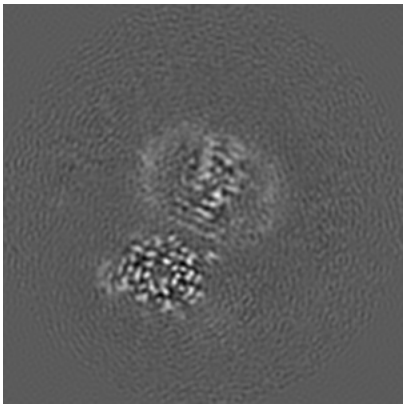
6.2.1 Primary map



X Index: 128



Y Index: 128

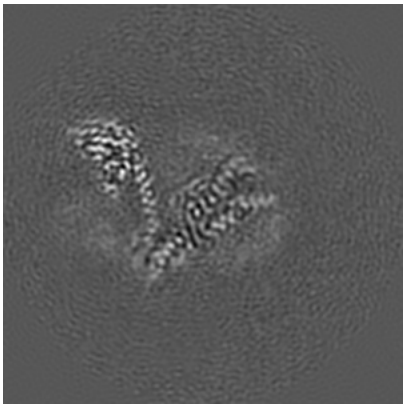


Z Index: 128

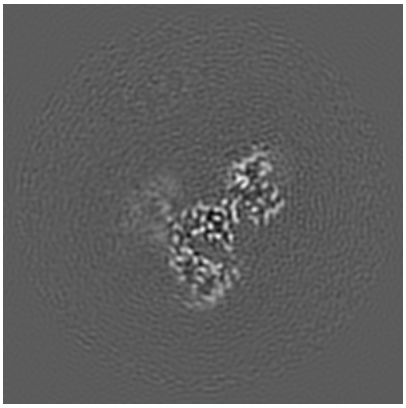
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

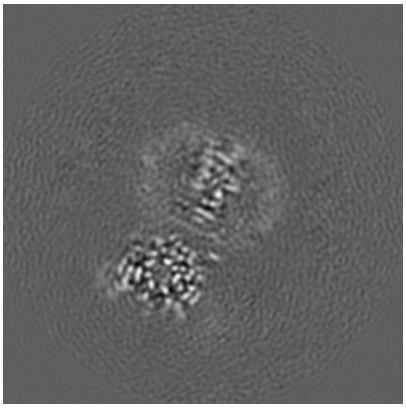
6.3.1 Primary map



X Index: 132



Y Index: 81

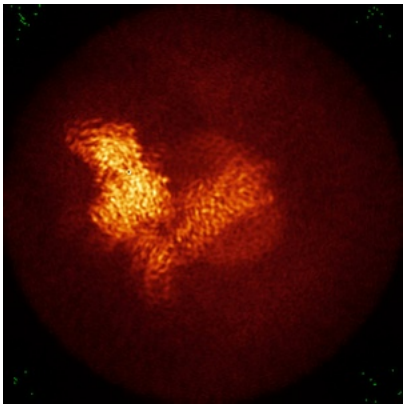


Z Index: 127

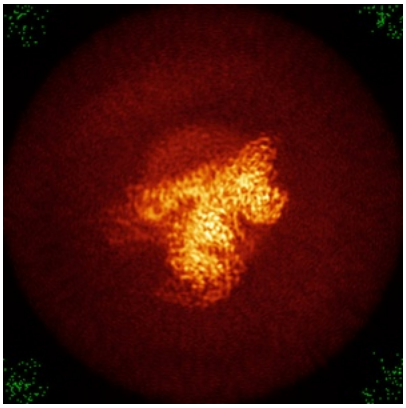
The images above show the largest variance slices of the map in three orthogonal directions.

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

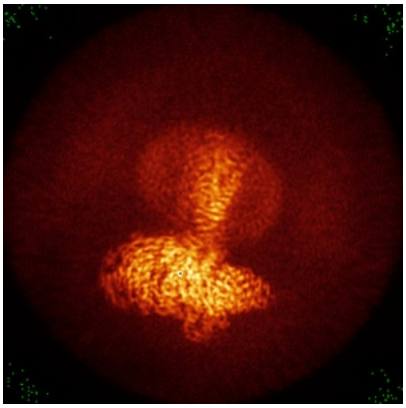
6.4.1 Primary map



X



Y



Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

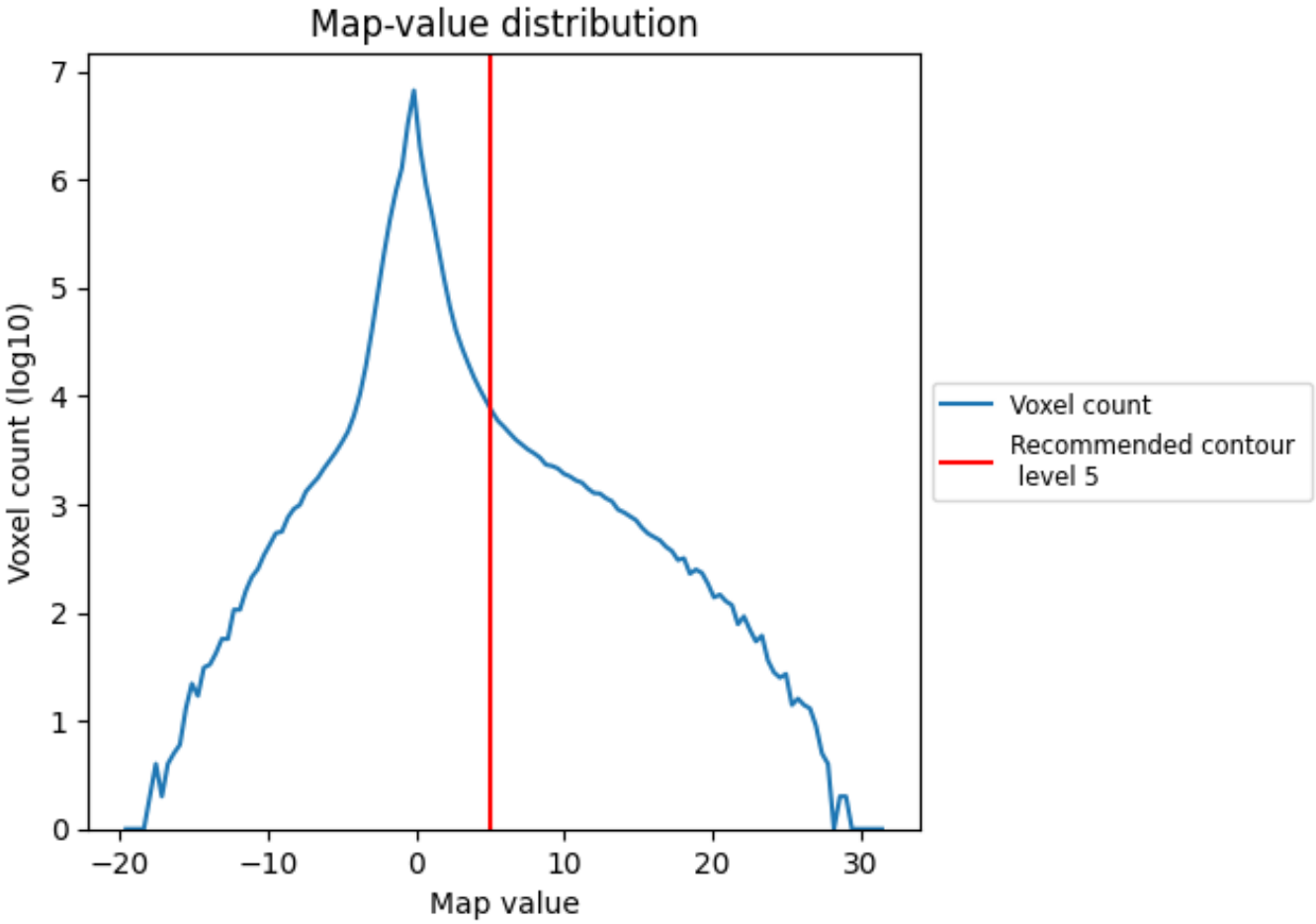
6.6 Mask visualisation (i)

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

7 Map analysis

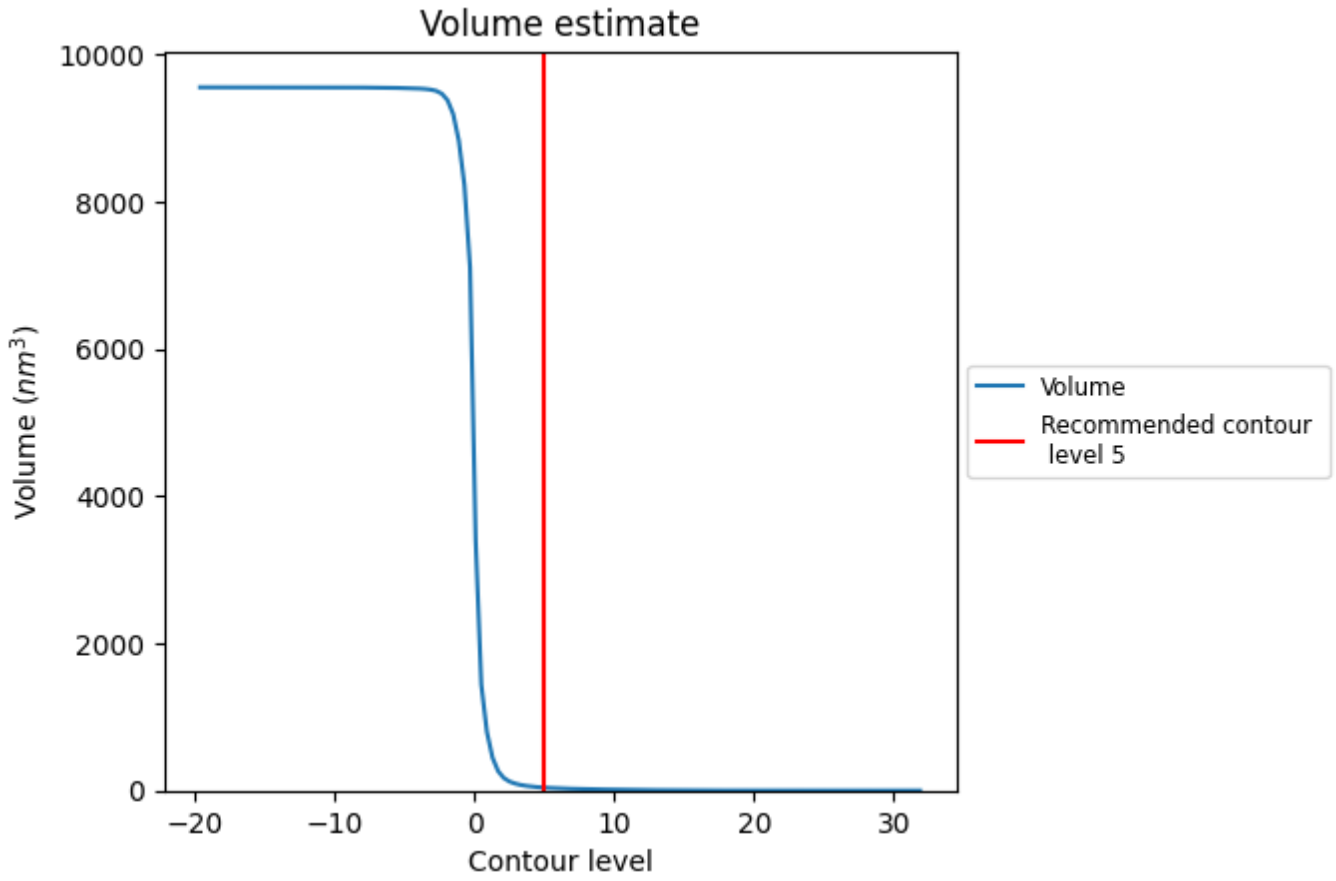
This section contains the results of statistical analysis of the map.

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.

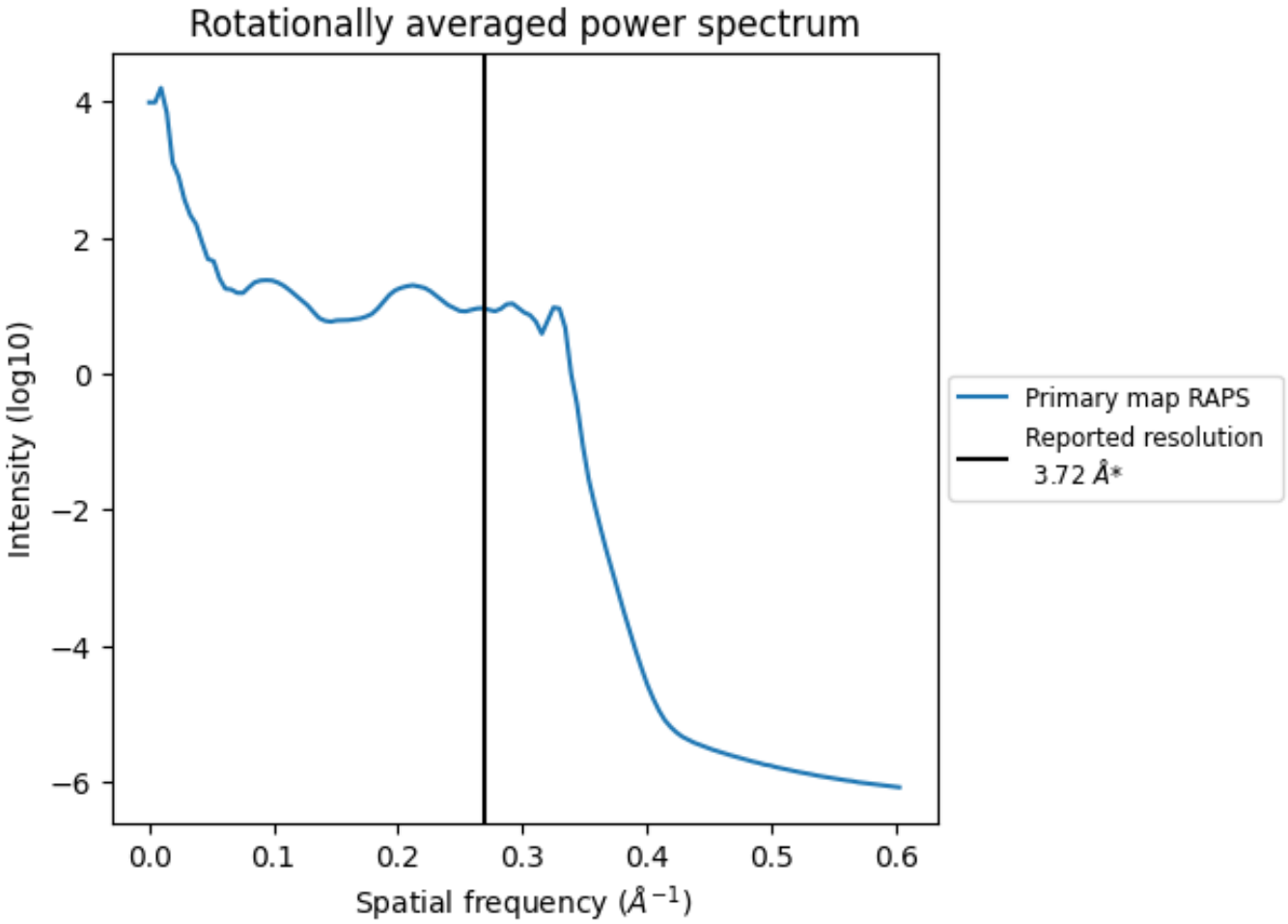
7.2 Volume estimate (i)



The volume at the recommended contour level is 40 nm^3; this corresponds to an approximate mass of 36 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 0.269 Å^{-1}

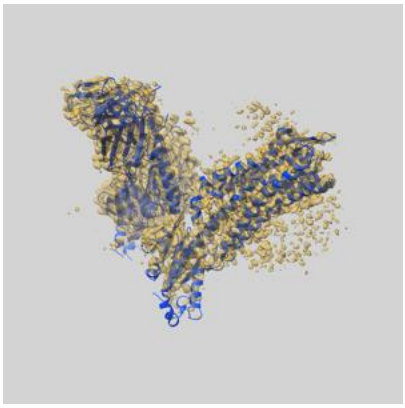
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

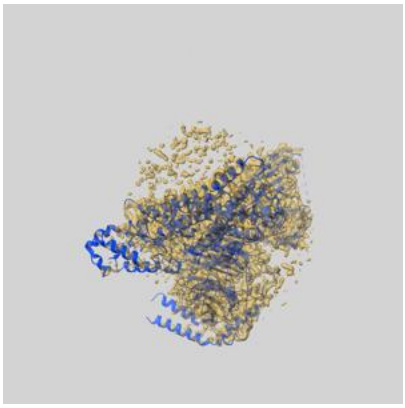
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32543 and PDB model 7WJ5. Per-residue inclusion information can be found in section 3 on page 6.

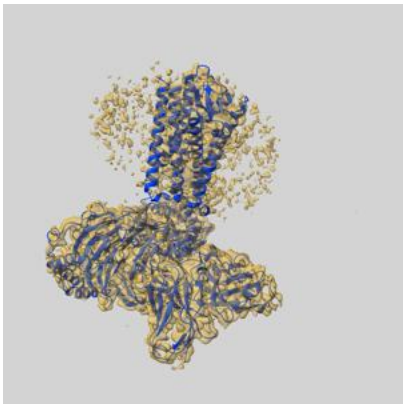
9.1 Map-model overlay



X



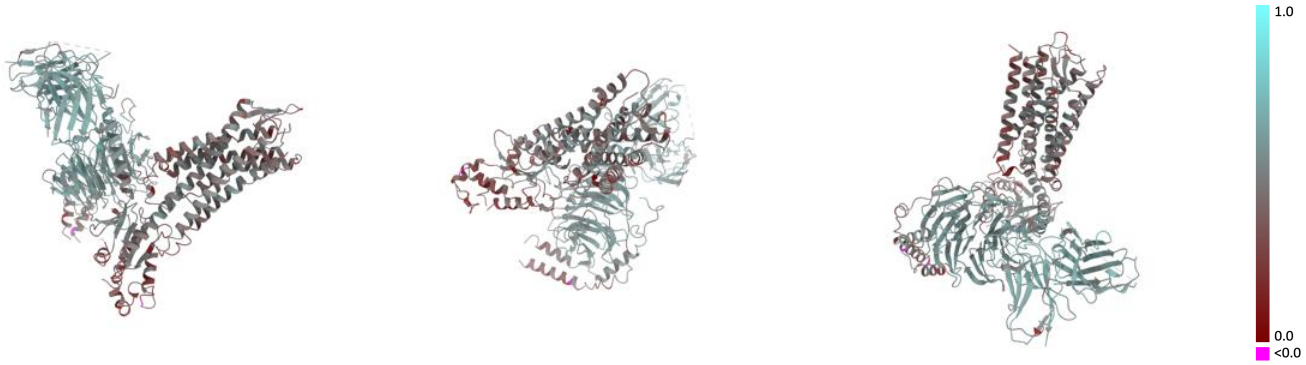
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

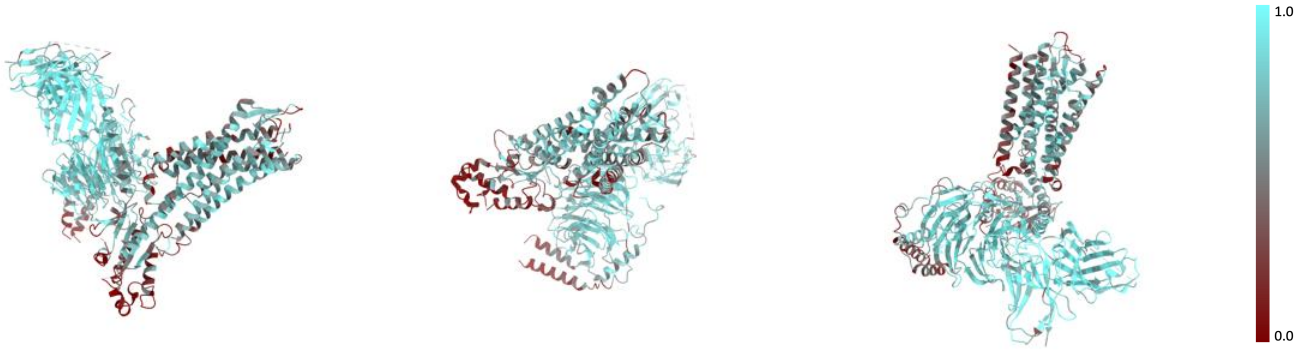
9.2 Q-score mapped to coordinate model (i)



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.

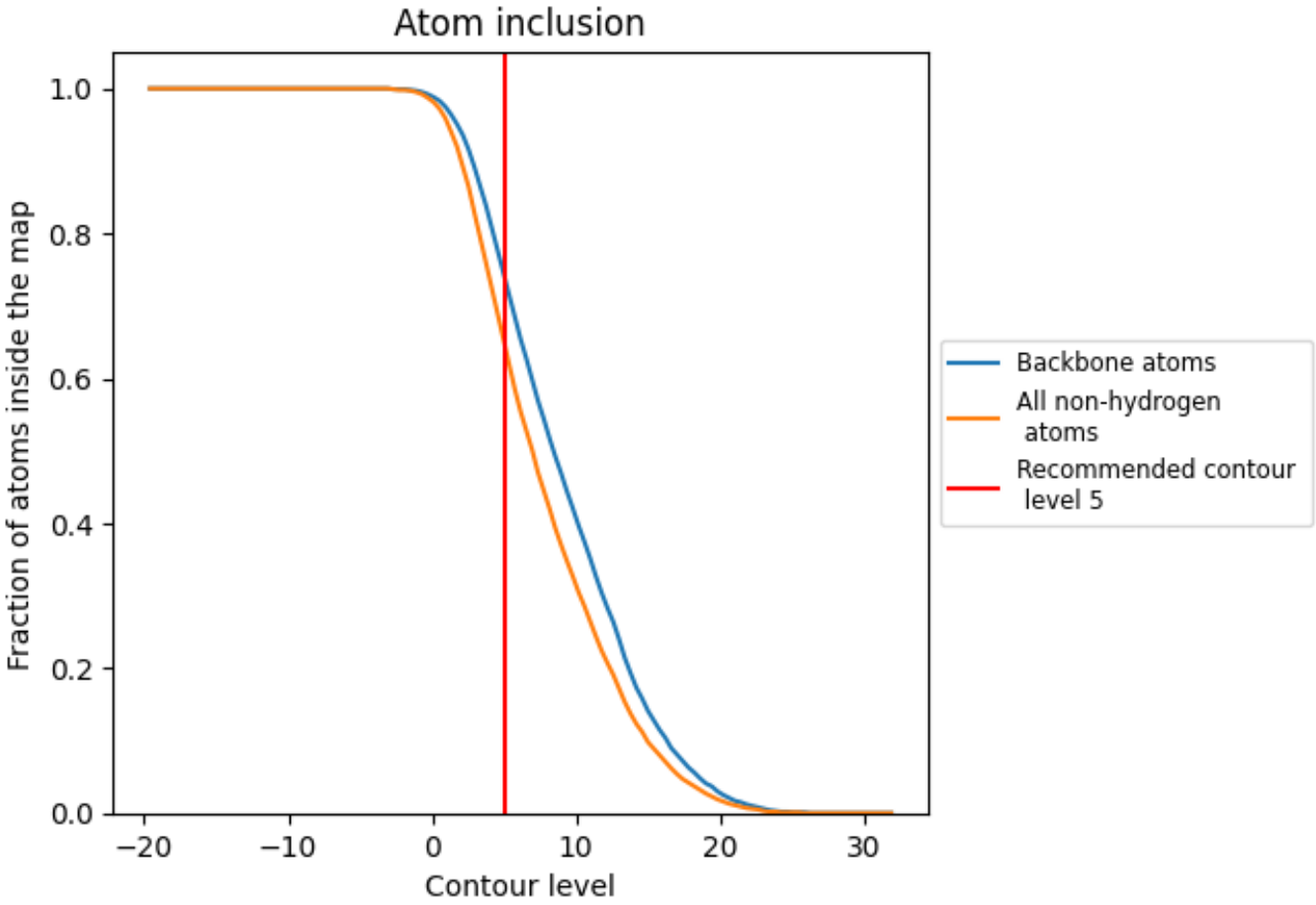
9.3 Atom inclusion mapped to coordinate model (i)



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 (5).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.4850
A	0.4020	0.3900
B	0.7660	0.5430
C	0.5400	0.4700
E	0.8450	0.5820
R	0.5600	0.4140
S	0.7120	0.4980