



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:23 pm GMT

PDB ID : 7P00
EMDB ID : EMD-13140
Title : Human Neurokinin 1 receptor (NK1R) substance P Gq chimera (mGsqi) complex
Authors : Thom, C.; Ehrenmann, J.; Vacca, S.; Waltenspuhl, Y.; Schoppe, J.; Medalia, O.; Pluckthun, A.
Deposited on : 2021-06-29
Resolution : 2.71 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
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

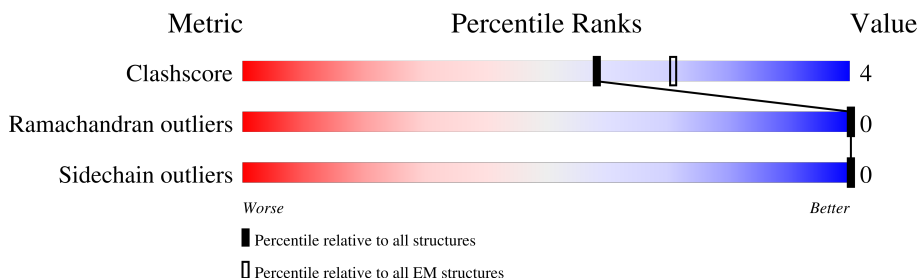
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

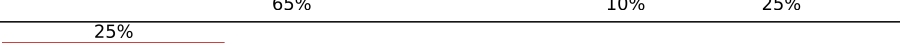
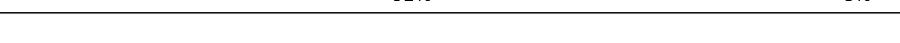
The reported resolution of this entry is 2.71 Å.

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	H	298	
2	B	354	
3	G	71	
4	A	246	
5	R	382	
6	P	12	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9110 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 Antibody fragment scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	232	Total	C	N	O	S	0	0
			1785	1132	295	348	10		

- 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	333	Total	C	N	O	S	0	0
			2559	1578	461	499	21		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	HIS	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- 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	G	52	Total	C	N	O	S	0	0
			405	254	71	77	3		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	228	Total	C	N	O	S	0	0
			1879	1190	332	349	8		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	ASP	engineered mutation	UNP P63096
A	21	LYS	ARG	engineered mutation	UNP P63096
A	22	GLN	ASN	engineered mutation	UNP P63096
A	24	GLN	ARG	engineered mutation	UNP P63096
A	25	LYS	GLU	engineered mutation	UNP P63096
A	27	LYS	GLY	engineered mutation	UNP P63096
A	28	GLN	GLU	engineered mutation	UNP P63096
A	29	VAL	LYS	engineered mutation	UNP P63096
A	30	TYR	ALA	engineered mutation	UNP P63096
A	31	ARG	ALA	engineered mutation	UNP P63096
A	32	ALA	ARG	engineered mutation	UNP P63096
A	33	THR	GLU	engineered mutation	UNP P63096
A	34	HIS	VAL	engineered mutation	UNP P63096
A	35	ARG	LYS	engineered mutation	UNP P63096
A	42	ASP	GLY	engineered mutation	UNP P63096
A	43	ASN	GLU	engineered mutation	UNP P63096
A	185	ARG	-	linker	UNP P63096
A	186	ILE	-	linker	UNP P63096
A	187	LEU	-	linker	UNP P63096
A	188	HIS	-	linker	UNP P63096
A	189	GLY	-	linker	UNP P63096
A	190	GLY	-	linker	UNP P63096
A	191	SER	-	linker	UNP P63096
A	192	GLY	-	linker	UNP P63096
A	193	GLY	-	linker	UNP P63096
A	194	SER	-	linker	UNP P63096
A	195	GLY	-	linker	UNP P63096
A	196	GLY	-	linker	UNP P63096
A	197	THR	-	linker	UNP P63096
A	198	SER	-	linker	UNP P63096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	linker	UNP P63096
A	242	ASP	ALA	engineered mutation	UNP A0A590UJY2
A	245	ASP	SER	engineered mutation	UNP A0A590UJY2
A	?	-	ASN	deletion	UNP A0A590UJY2
A	?	-	MET	deletion	UNP A0A590UJY2
A	?	-	VAL	deletion	UNP A0A590UJY2
A	?	-	ILE	deletion	UNP A0A590UJY2
A	?	-	ARG	deletion	UNP A0A590UJY2
A	?	-	GLU	deletion	UNP A0A590UJY2
A	?	-	ASP	deletion	UNP A0A590UJY2
A	?	-	ASN	deletion	UNP A0A590UJY2
A	?	-	GLN	deletion	UNP A0A590UJY2
A	?	-	THR	deletion	UNP A0A590UJY2
A	355	ALA	ILE	engineered mutation	UNP A0A590UJY2
A	358	ILE	VAL	engineered mutation	UNP A0A590UJY2
A	363	LYS	ARG	engineered mutation	UNP A0A590UJY2
A	367	LEU	GLN	engineered mutation	UNP A0A590UJY2
A	368	GLN	ARG	engineered mutation	UNP A0A590UJY2
A	370	ASN	HIS	engineered mutation	UNP A0A590UJY2
A	373	GLU	GLN	engineered mutation	UNP A0A590UJY2
A	375	ASN	GLU	engineered mutation	UNP A0A590UJY2
A	377	VAL	LEU	engineered mutation	UNP A0A590UJY2

- Molecule 5 is a protein called Substance-P receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	288	Total	C	N	O	S	0	0
			2359	1593	370	376	20		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-46	MET	-	initiating methionine	UNP P25103
R	-45	LYS	-	expression tag	UNP P25103
R	-44	PHE	-	expression tag	UNP P25103
R	-43	LEU	-	expression tag	UNP P25103
R	-42	VAL	-	expression tag	UNP P25103
R	-41	ASN	-	expression tag	UNP P25103
R	-40	VAL	-	expression tag	UNP P25103
R	-39	ALA	-	expression tag	UNP P25103
R	-38	LEU	-	expression tag	UNP P25103
R	-37	VAL	-	expression tag	UNP P25103

Continued on next page...

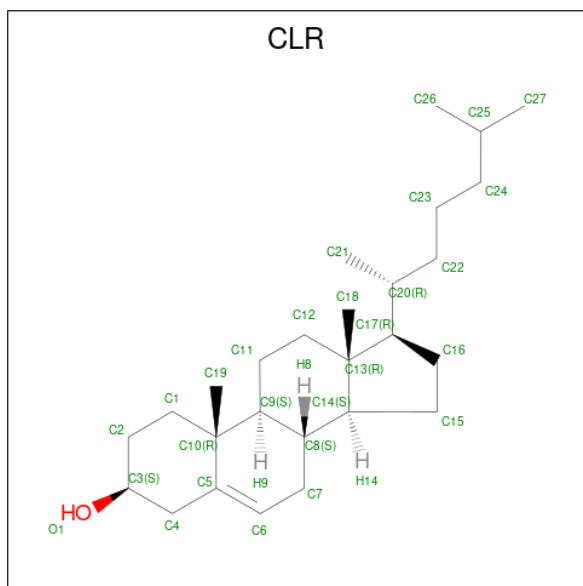
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-36	PHE	-	expression tag	UNP P25103
R	-35	MET	-	expression tag	UNP P25103
R	-34	VAL	-	expression tag	UNP P25103
R	-33	VAL	-	expression tag	UNP P25103
R	-32	TYR	-	expression tag	UNP P25103
R	-31	ILE	-	expression tag	UNP P25103
R	-30	SER	-	expression tag	UNP P25103
R	-29	TYR	-	expression tag	UNP P25103
R	-28	ILE	-	expression tag	UNP P25103
R	-27	TYR	-	expression tag	UNP P25103
R	-26	ALA	-	expression tag	UNP P25103
R	-25	ASP	-	expression tag	UNP P25103
R	-24	TYR	-	expression tag	UNP P25103
R	-23	LYS	-	expression tag	UNP P25103
R	-22	ASP	-	expression tag	UNP P25103
R	-21	ASP	-	expression tag	UNP P25103
R	-20	ASP	-	expression tag	UNP P25103
R	-19	ASP	-	expression tag	UNP P25103
R	-18	LYS	-	expression tag	UNP P25103
R	-17	HIS	-	expression tag	UNP P25103
R	-16	HIS	-	expression tag	UNP P25103
R	-15	HIS	-	expression tag	UNP P25103
R	-14	HIS	-	expression tag	UNP P25103
R	-13	HIS	-	expression tag	UNP P25103
R	-12	HIS	-	expression tag	UNP P25103
R	-11	HIS	-	expression tag	UNP P25103
R	-10	HIS	-	expression tag	UNP P25103
R	-9	HIS	-	expression tag	UNP P25103
R	-8	HIS	-	expression tag	UNP P25103
R	-7	LEU	-	expression tag	UNP P25103
R	-6	GLU	-	expression tag	UNP P25103
R	-5	VAL	-	expression tag	UNP P25103
R	-4	LEU	-	expression tag	UNP P25103
R	-3	PHE	-	expression tag	UNP P25103
R	-2	GLN	-	expression tag	UNP P25103
R	-1	GLY	-	expression tag	UNP P25103
R	0	PRO	-	expression tag	UNP P25103

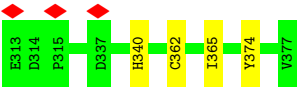
- Molecule 6 is a protein called Substance P.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	12	Total	C	N	O	S	
			95	63	18	13	1	0
								1

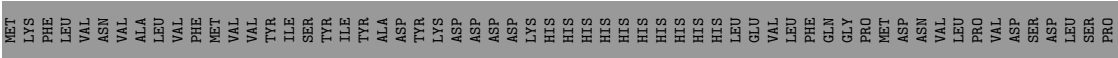
- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



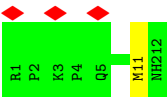
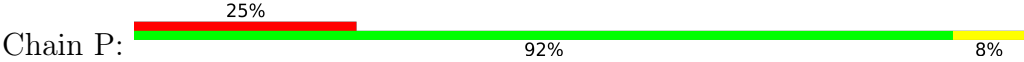
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	R	1	28	27	1	0



• Molecule 5: Substance-P receptor



• Molecule 6: Substance P



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	558058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62.51	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.331	Depositor
Minimum map value	-2.182	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.277	Depositor
Map size (Å)	270.816, 270.816, 270.816	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.651, 0.651, 0.651	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, CLR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.60	0/1829	0.77	0/2480
2	B	0.60	0/2606	0.80	0/3532
3	G	0.59	0/411	0.66	0/554
4	A	0.57	0/1915	0.70	0/2579
5	R	0.61	0/2439	0.66	0/3338
6	P	0.53	0/97	0.58	0/128
All	All	0.59	0/9297	0.73	0/12611

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	H	1785	0	1716	9	0
2	B	2559	0	2465	36	0
3	G	405	0	413	6	0
4	A	1879	0	1862	15	0
5	R	2359	0	2392	23	0
6	P	95	0	99	1	0
7	R	28	0	46	0	0
All	All	9110	0	8993	81	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 4.

The worst 5 of 81 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:H:172:VAL:HG21	1:H:262:LEU:HD21	1.60	0.83
4:A:224:ARG:O	4:A:228:ILE:HG12	1.79	0.82
4:A:227:TRP:CZ3	4:A:228:ILE:HD13	2.17	0.78
4:A:228:ILE:CG2	4:A:265:LEU:HD11	2.13	0.78
4:A:228:ILE:HG21	4:A:265:LEU:HD11	1.65	0.75

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	H	228/298 (76%)	222 (97%)	6 (3%)	0	100	100
2	B	331/354 (94%)	321 (97%)	10 (3%)	0	100	100
3	G	50/71 (70%)	48 (96%)	2 (4%)	0	100	100
4	A	224/246 (91%)	214 (96%)	10 (4%)	0	100	100
5	R	284/382 (74%)	274 (96%)	10 (4%)	0	100	100
6	P	10/12 (83%)	10 (100%)	0	0	100	100
All	All	1127/1363 (83%)	1089 (97%)	38 (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	H	197/245 (80%)	197 (100%)	0	100	100
2	B	276/295 (94%)	276 (100%)	0	100	100
3	G	43/58 (74%)	43 (100%)	0	100	100
4	A	205/215 (95%)	205 (100%)	0	100	100
5	R	254/341 (74%)	254 (100%)	0	100	100
6	P	10/10 (100%)	10 (100%)	0	100	100
All	All	985/1164 (85%)	985 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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](#)

1 ligand is 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	CLR	R	401	-	31,31,31	0.29	0	48,48,48	0.41	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	CLR	R	401	-	-	0/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

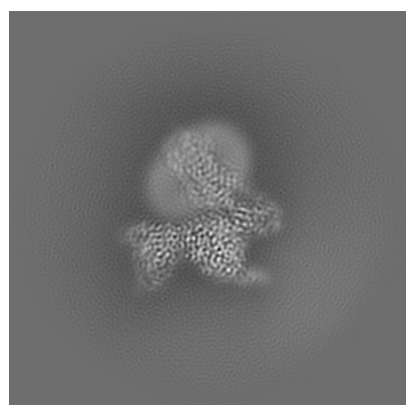
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13140. These allow visual inspection of the internal detail of the map and identification of artifacts.

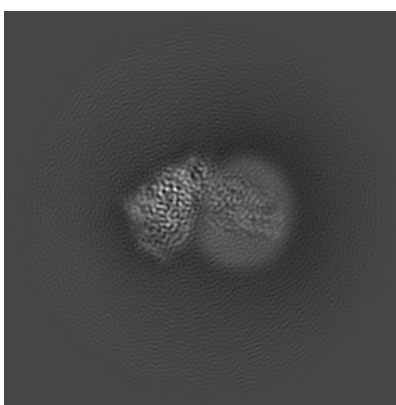
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

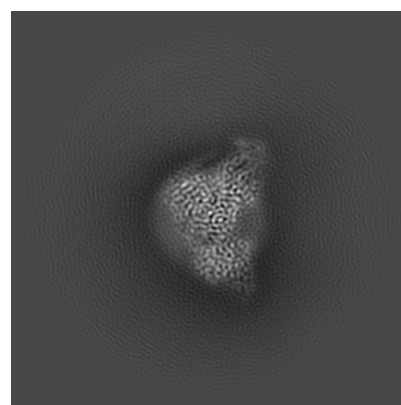
6.1.1 Primary map



X



Y

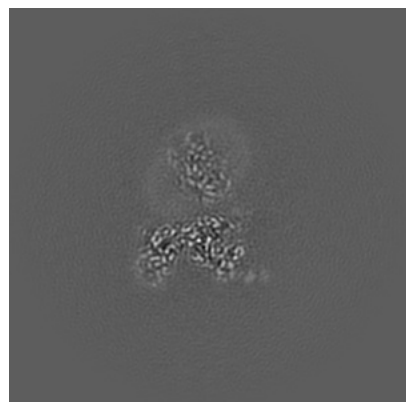


Z

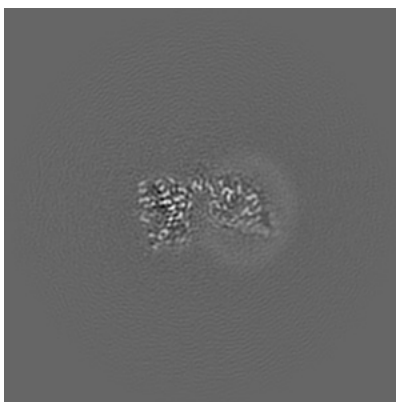
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

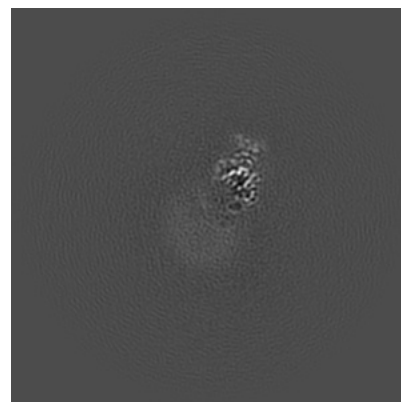
6.2.1 Primary map



X Index: 208



Y Index: 208

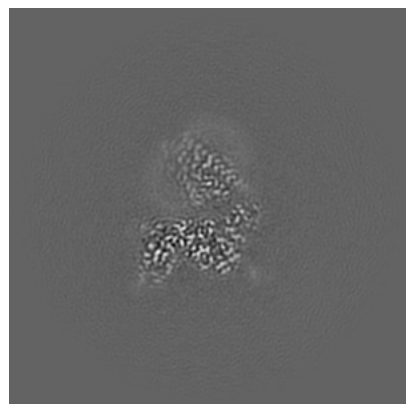


Z Index: 208

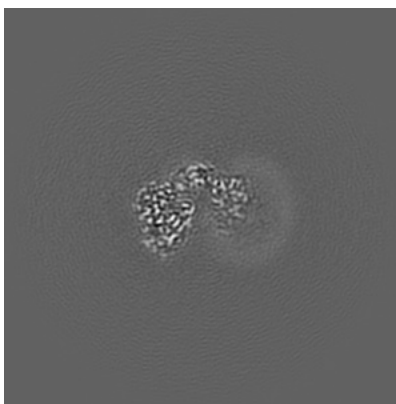
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

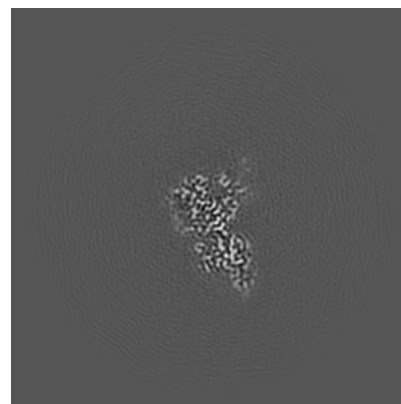
6.3.1 Primary map



X Index: 219



Y Index: 220

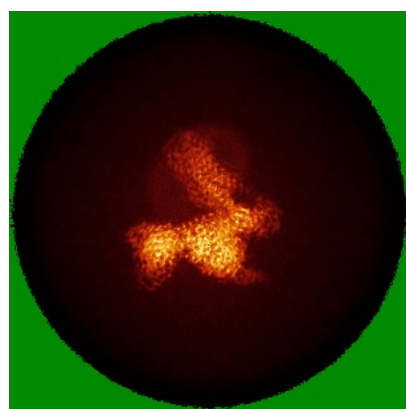


Z Index: 177

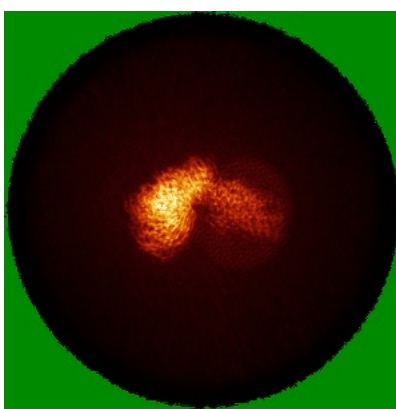
The images above show the largest variance slices of the map in three orthogonal directions.

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

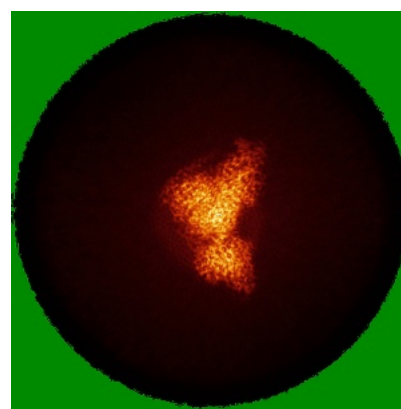
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.277. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

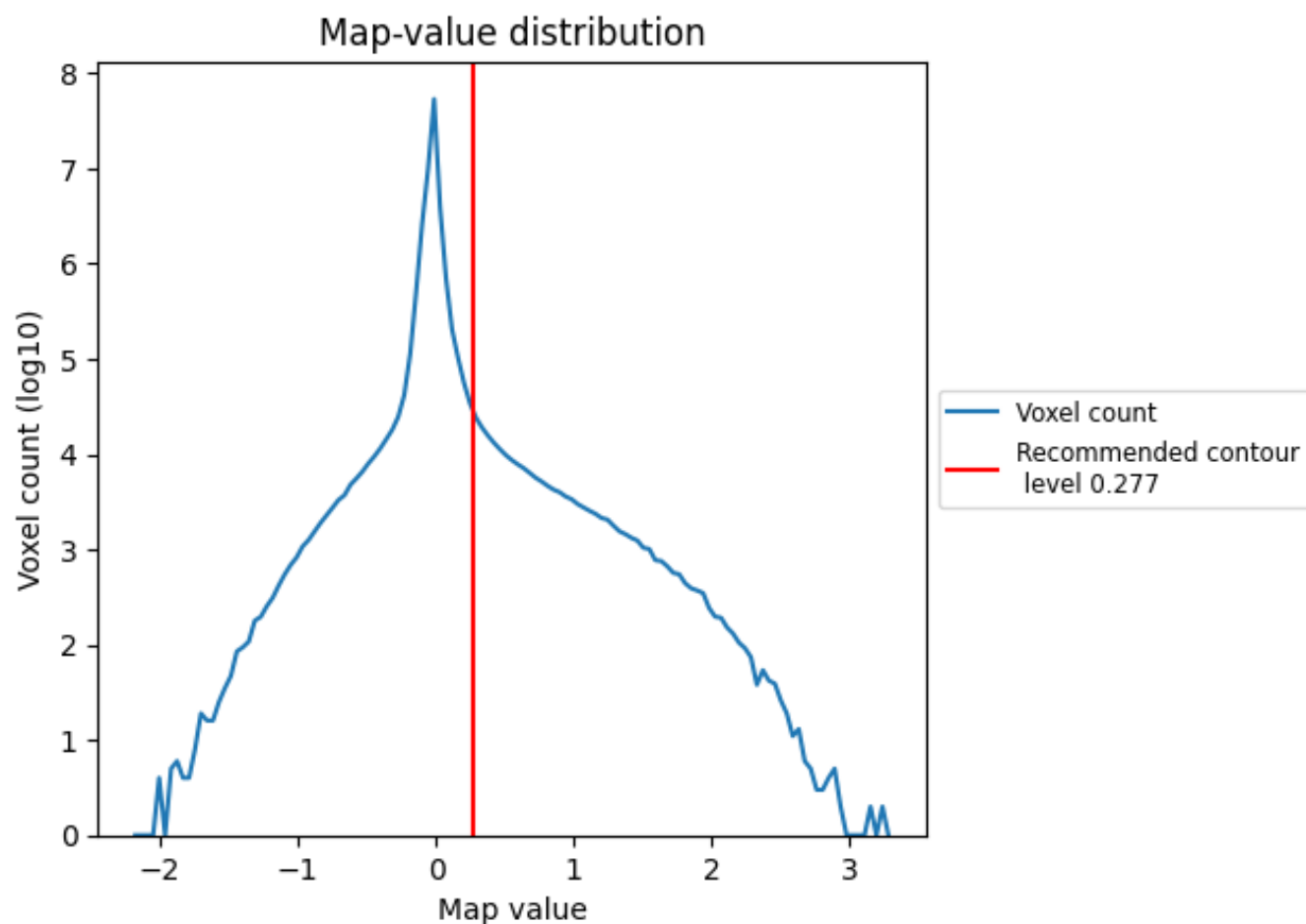
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

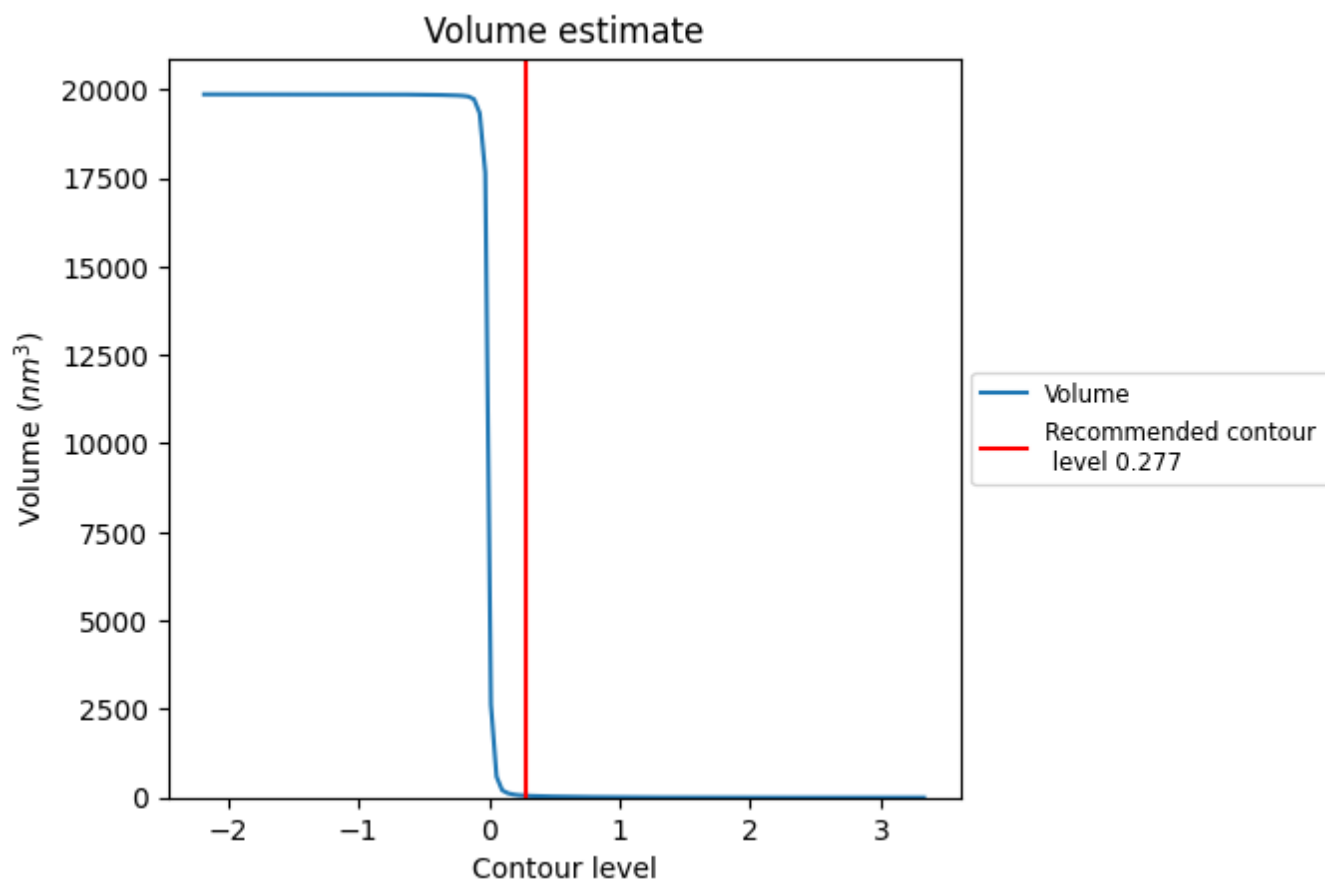
This section contains the results of statistical analysis of the map.

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.

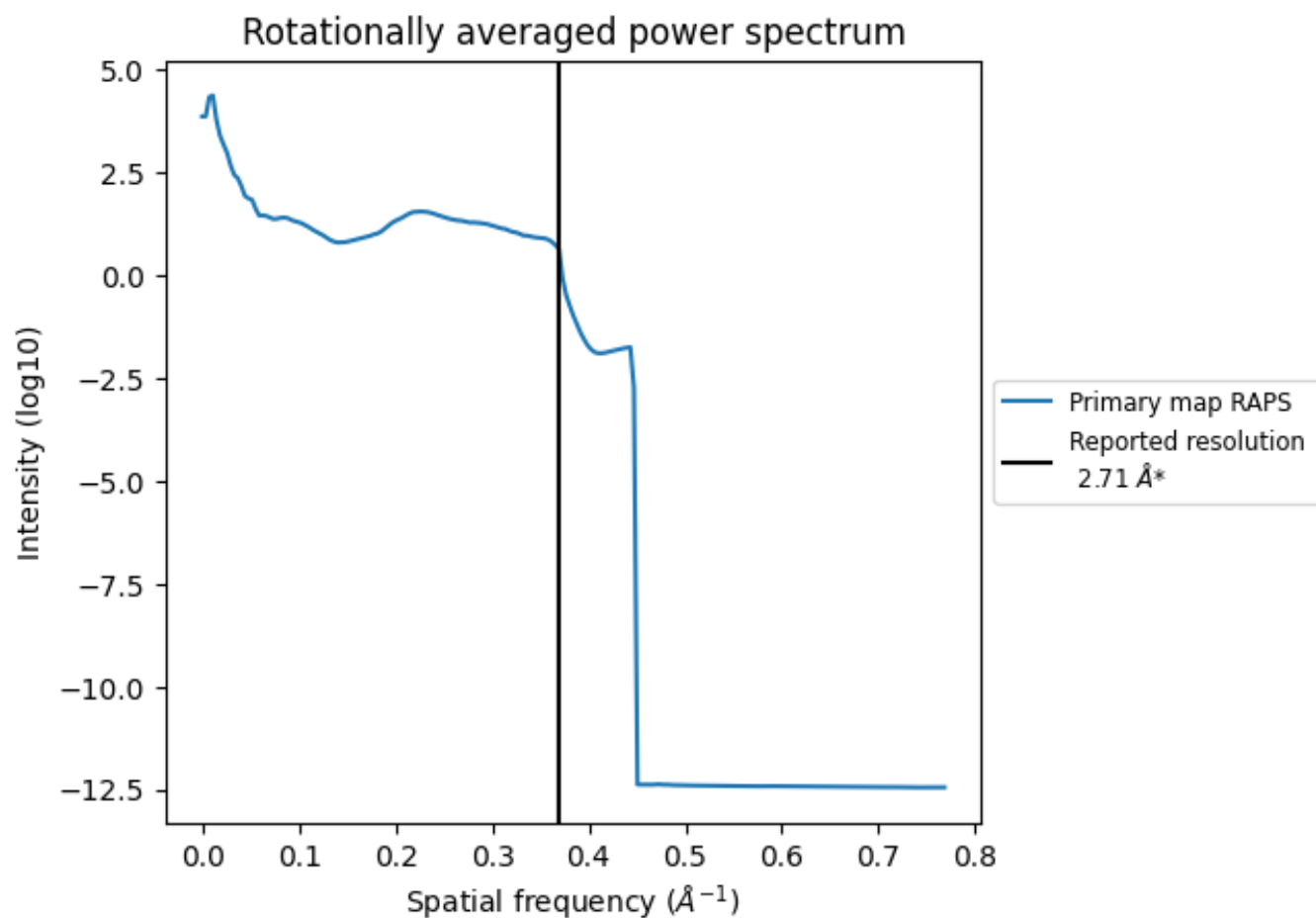
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 49 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 0.369 Å⁻¹

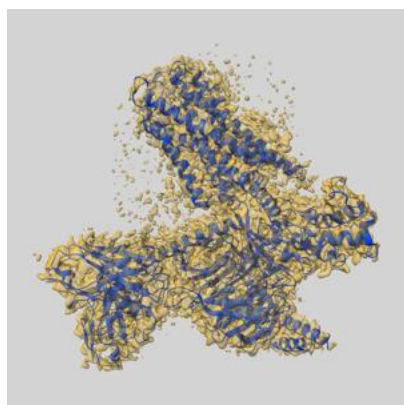
8 Fourier-Shell correlation

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

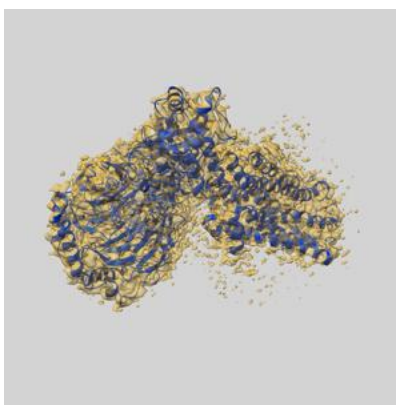
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13140 and PDB model 7P00. Per-residue inclusion information can be found in section [3](#) on page [8](#).

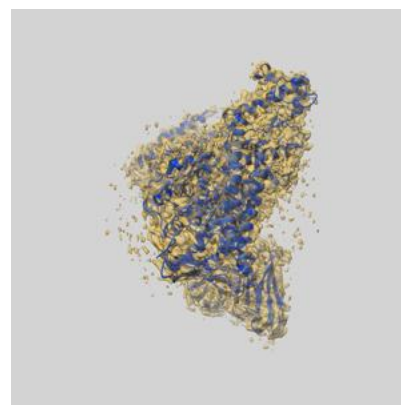
9.1 Map-model overlay [i](#)



X



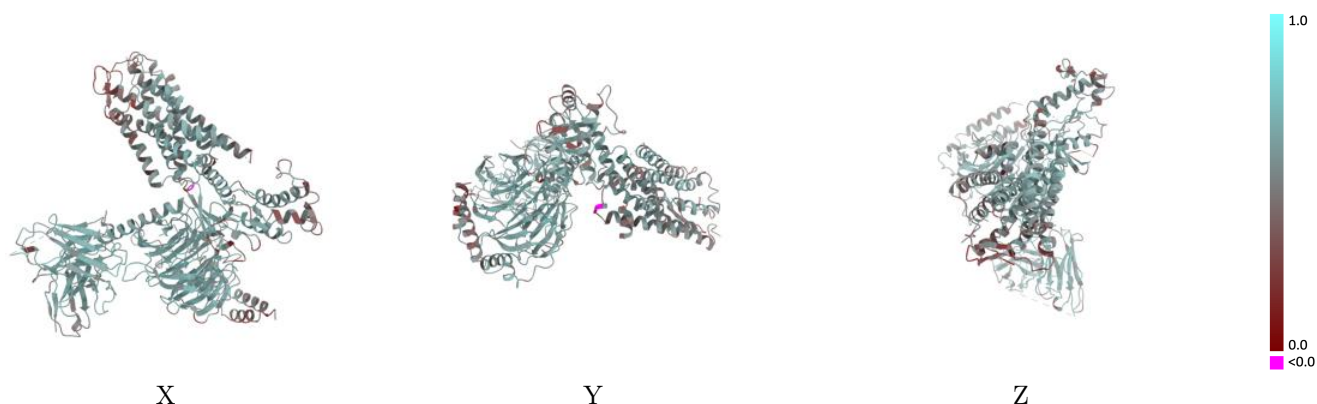
Y



Z

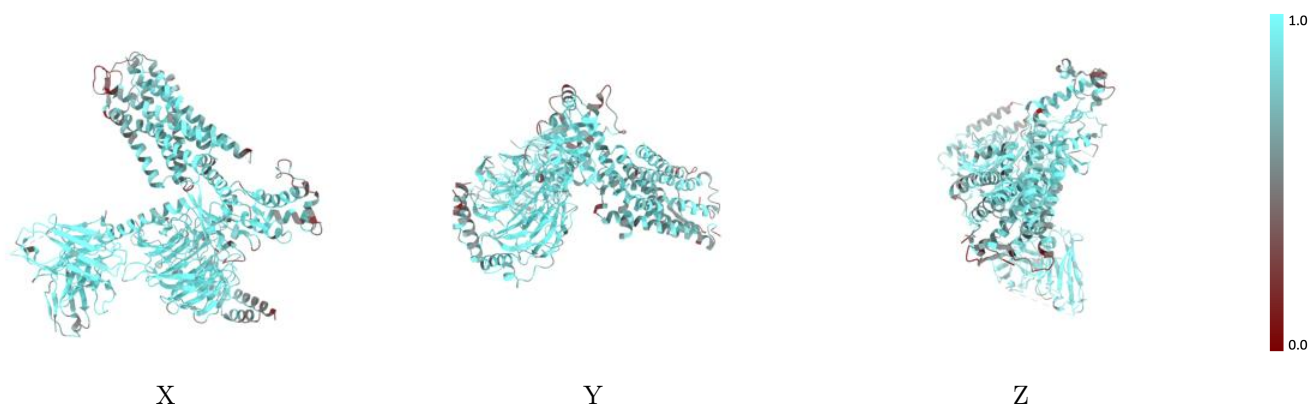
The images above show the 3D surface view of the map at the recommended contour level 0.277 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



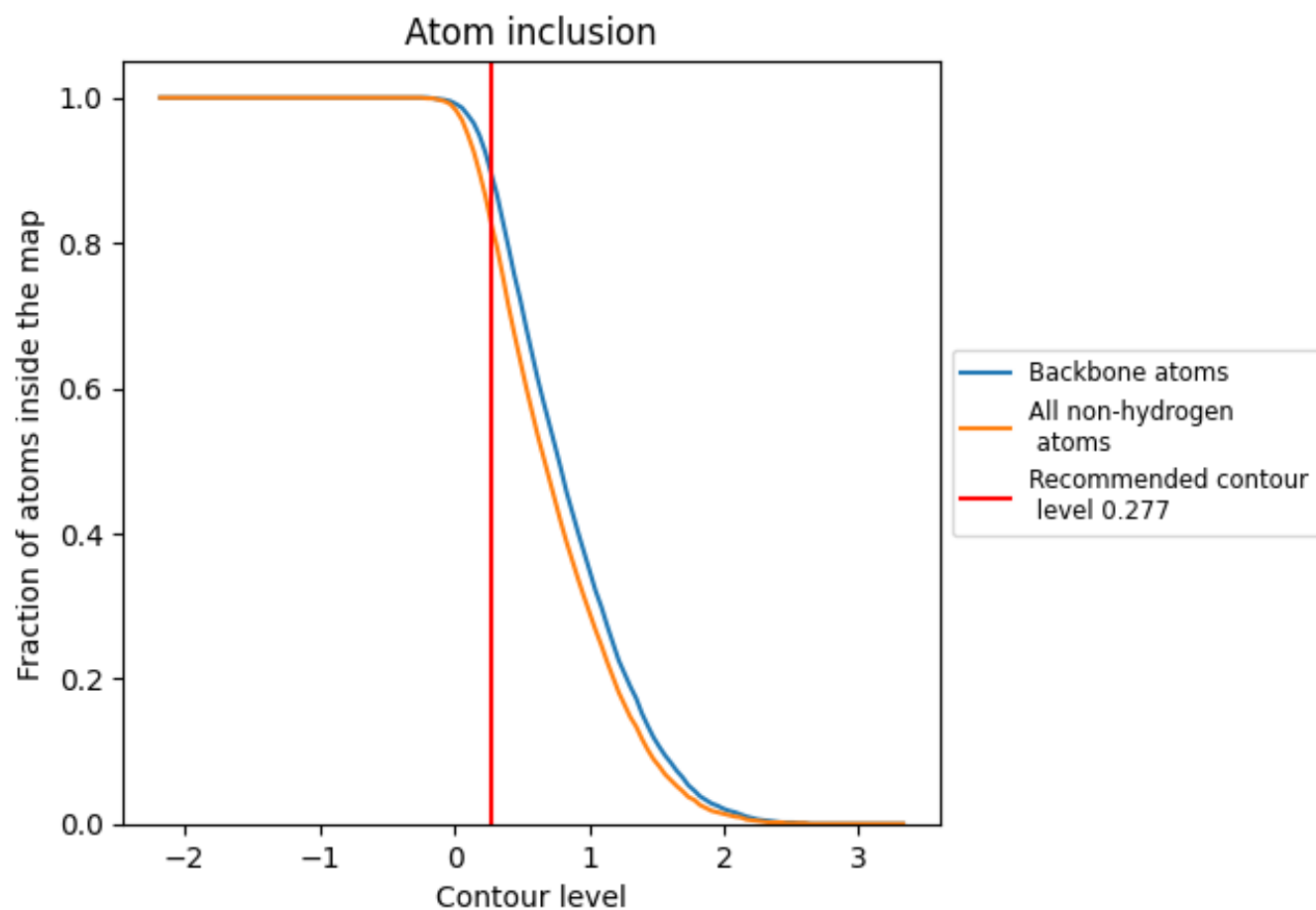
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.277).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.277) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8240	<div></div> 0.5460
A	<div></div> 0.8060	<div></div> 0.5340
B	<div></div> 0.9020	<div></div> 0.5910
G	<div></div> 0.7360	<div></div> 0.4880
H	<div></div> 0.8890	<div></div> 0.5890
P	<div></div> 0.6130	<div></div> 0.4190
R	<div></div> 0.7310	<div></div> 0.4890

