



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 01:09 am GMT

PDB ID : 7P02  
EMDB ID : EMD-13141  
Title : Human Neurokinin 1 receptor (NK1R) substance P Gs complex  
Authors : Thom, C.; Ehrenmann, J.; Vacca, S.; Waltenspuhl, Y.; Schoppe, J.; Medalia, O.; Pluckthun, A.  
Deposited on : 2021-06-29  
Resolution : 2.87 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, 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

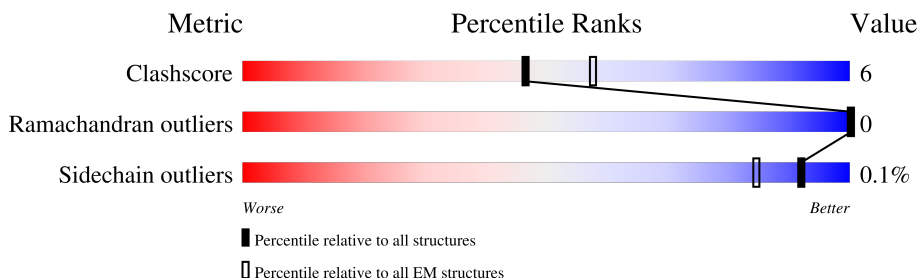
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.87 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	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 9062 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	51	Total	C	N	O	S	0	0
			396	249	70	74	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	226	Total	C	N	O	S	0	0
			1870	1183	334	345	8		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	linker	UNP P63096
A	21	LYS	-	linker	UNP P63096
A	22	GLN	-	linker	UNP P63096
A	23	LEU	-	linker	UNP P63096
A	24	GLN	-	linker	UNP P63096
A	25	LYS	-	linker	UNP P63096
A	26	ASP	-	linker	UNP P63096
A	27	LYS	-	linker	UNP P63096
A	28	GLN	-	linker	UNP P63096
A	29	VAL	-	linker	UNP P63096
A	30	TYR	-	linker	UNP P63096
A	31	ARG	-	linker	UNP P63096
A	32	ALA	-	linker	UNP P63096
A	33	THR	-	linker	UNP P63096
A	34	HIS	-	linker	UNP P63096
A	35	ARG	-	linker	UNP P63096
A	36	LEU	-	linker	UNP P63096
A	37	LEU	-	linker	UNP P63096
A	38	LEU	-	linker	UNP P63096
A	39	LEU	-	linker	UNP P63096
A	40	GLY	-	linker	UNP P63096
A	41	ALA	-	linker	UNP P63096
A	42	ASP	-	linker	UNP P63096
A	43	ASN	-	linker	UNP P63096
A	44	SER	-	linker	UNP P63096
A	45	GLY	-	linker	UNP P63096
A	46	LYS	-	linker	UNP P63096
A	47	SER	-	linker	UNP P63096
A	48	THR	-	linker	UNP P63096
A	49	ILE	-	linker	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
A	50	VAL	-	linker	UNP P63096
A	182	LYS	-	linker	UNP P63096
A	183	GLN	-	linker	UNP P63096
A	184	MET	-	linker	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	242	ASP	ALA	conflict	UNP P63092
A	245	ASP	SER	conflict	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	355	ALA	ILE	conflict	UNP P63092
A	358	ILE	VAL	conflict	UNP P63092

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	287	Total	C	N	O	S	0	0
			2347	1584	369	374	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	GLN	-	expression tag	UNP P25103
R	-1	GLY	-	expression tag	UNP P25103
R	0	PRO	-	expression tag	UNP P25103

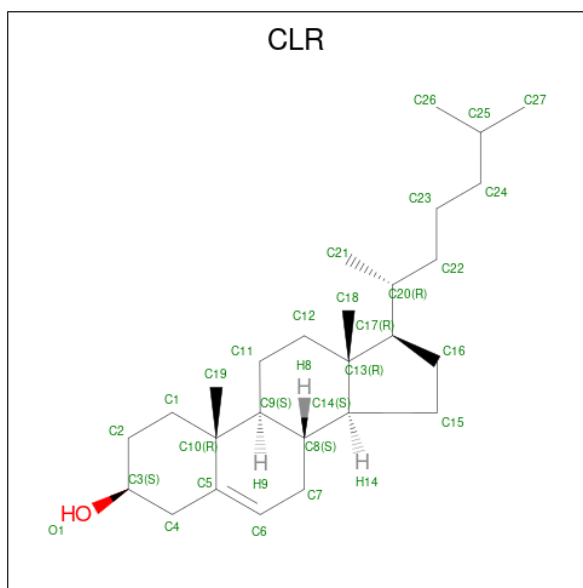
- Molecule 6 is a protein called Protachykinin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	10	Total	C	N	O	0	1
			77	52	13	11		

There is a discrepancy between the modelled and reference sequences:

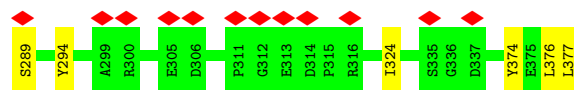
Chain	Residue	Modelled	Actual	Comment	Reference
P	12	NH2	-	amidation	UNP P20366

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

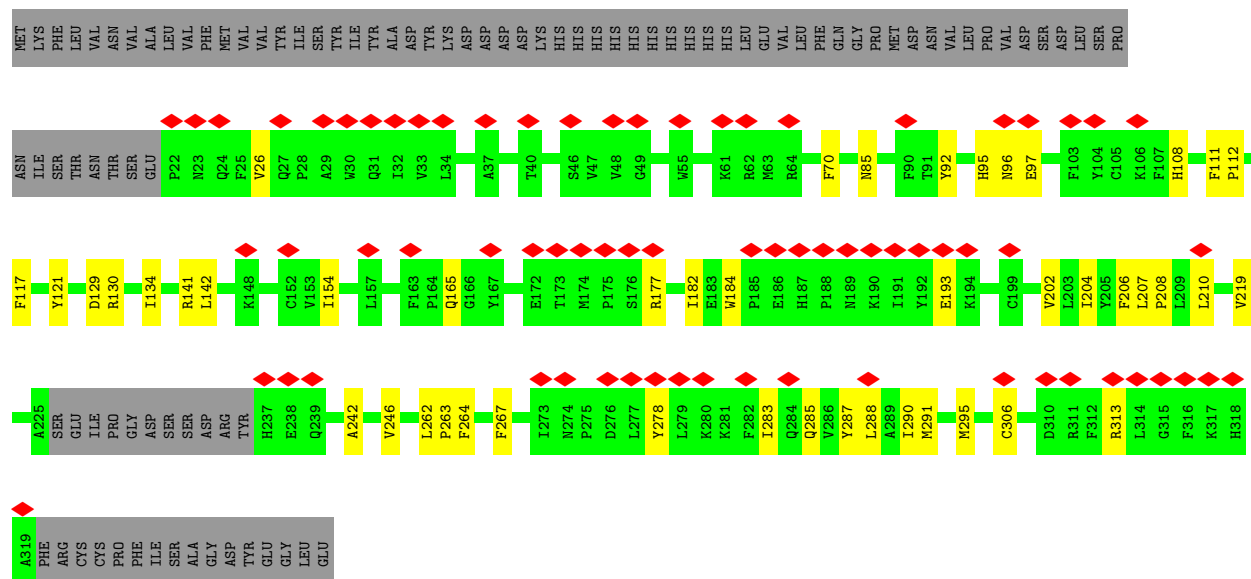


Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	

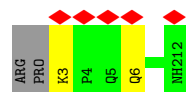
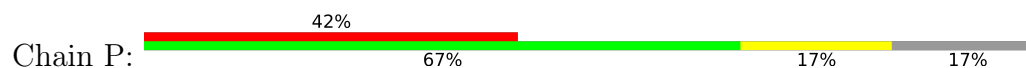




• Molecule 5: Substance-P receptor



• Molecule 6: Protachykinin-1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	395052	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 ( $e^-/\text{\AA}^2$ )	63.51	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	3.119	Depositor
Minimum map value	-1.897	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.251	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

### 5.1 Standard geometry

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	0.63	0/1829	0.64	0/2480
2	B	0.62	0/2606	0.68	0/3532
3	G	0.61	0/402	0.62	0/542
4	A	0.60	0/1907	0.60	0/2568
5	R	0.62	0/2426	0.63	0/3320
6	P	0.56	0/78	0.57	0/102
All	All	0.62	0/9248	0.64	0/12544

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	H	1785	0	1716	19	0
2	B	2559	0	2465	40	0
3	G	396	0	407	1	0
4	A	1870	0	1848	17	0
5	R	2347	0	2383	37	0
6	P	77	0	76	1	0
7	R	28	0	46	0	0
All	All	9062	0	8941	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 107 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)
2:B:61:MET:HE1	2:B:328:ALA:HB3	1.30	1.09
2:B:61:MET:CE	2:B:328:ALA:HB3	1.96	0.94
5:R:70:PHE:CD2	5:R:129:ASP:OD2	2.21	0.94
5:R:70:PHE:HD2	5:R:129:ASP:OD2	1.51	0.93
2:B:274:THR:CG2	2:B:314:ARG:HE	1.93	0.82

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%)	219 (96%)	9 (4%)	0	100	100
2	B	331/354 (94%)	317 (96%)	14 (4%)	0	100	100
3	G	49/71 (69%)	48 (98%)	1 (2%)	0	100	100
4	A	222/246 (90%)	210 (95%)	12 (5%)	0	100	100
5	R	283/382 (74%)	267 (94%)	16 (6%)	0	100	100
6	P	8/12 (67%)	8 (100%)	0	0	100	100
All	All	1121/1363 (82%)	1069 (95%)	52 (5%)	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%)	275 (100%)	1 (0%)	89	96
3	G	42/58 (72%)	42 (100%)	0	100	100
4	A	203/215 (94%)	203 (100%)	0	100	100
5	R	253/341 (74%)	253 (100%)	0	100	100
6	P	8/10 (80%)	8 (100%)	0	100	100
All	All	979/1164 (84%)	978 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	0.46	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	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.

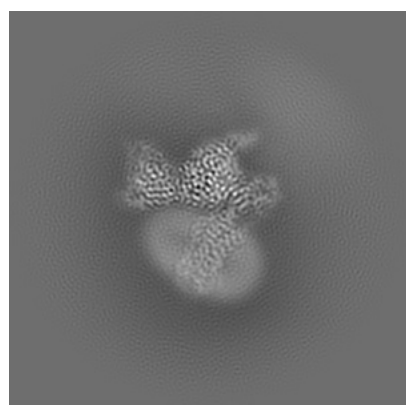
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13141. These allow visual inspection of the internal detail of the map and identification of artifacts.

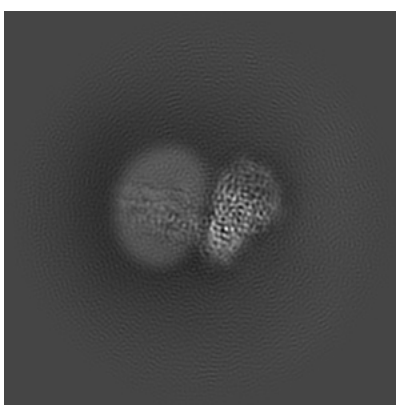
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

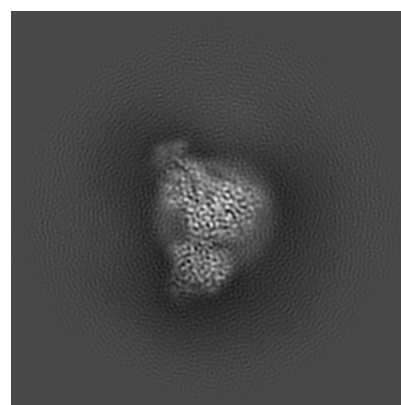
#### 6.1.1 Primary map



X



Y

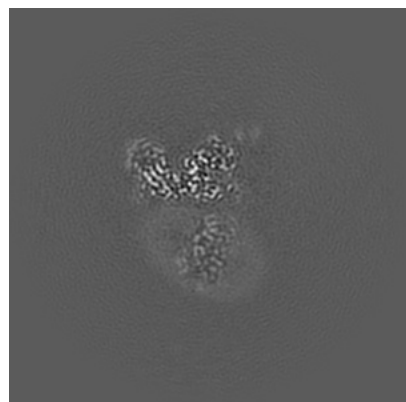


Z

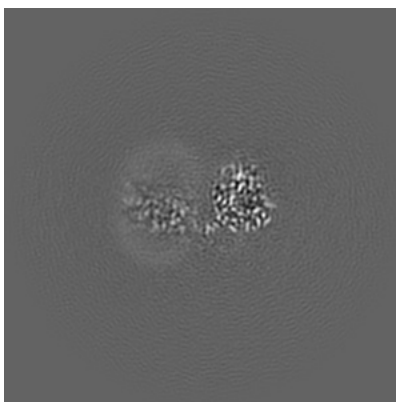
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

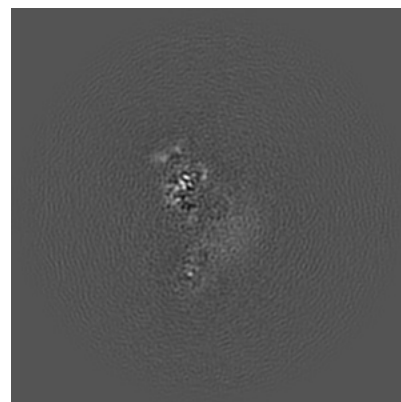
#### 6.2.1 Primary map



X Index: 208



Y Index: 208

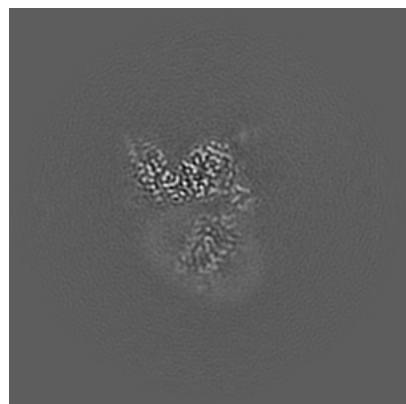


Z Index: 208

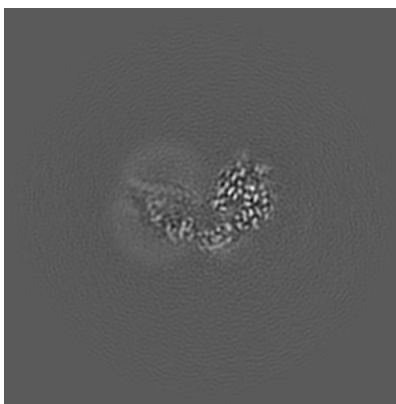
The images above show central slices of the map in three orthogonal directions.

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

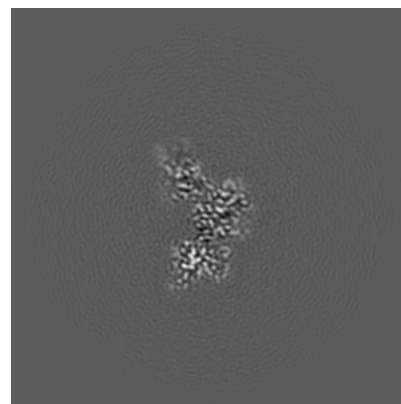
### 6.3.1 Primary map



X Index: 201



Y Index: 217

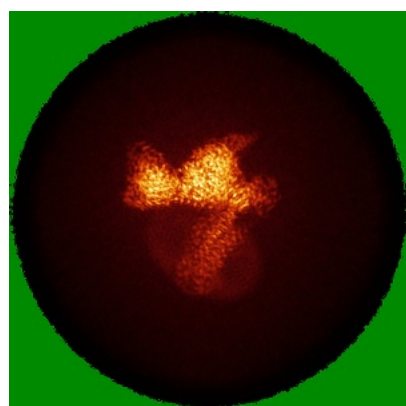


Z Index: 230

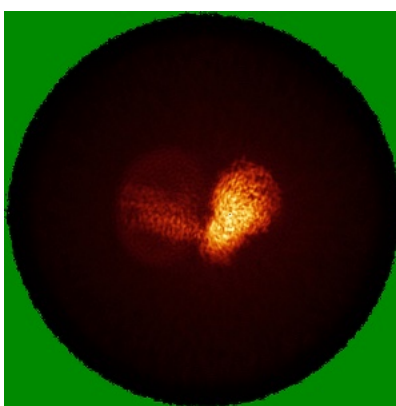
The images above show the largest variance slices of the map in three orthogonal directions.

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

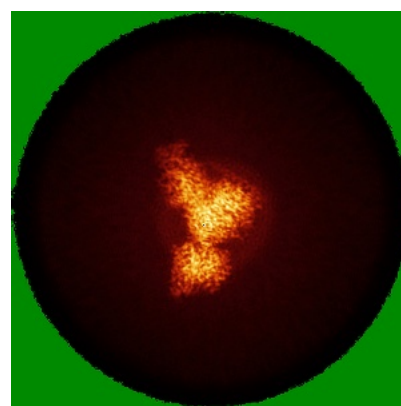
### 6.4.1 Primary map



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

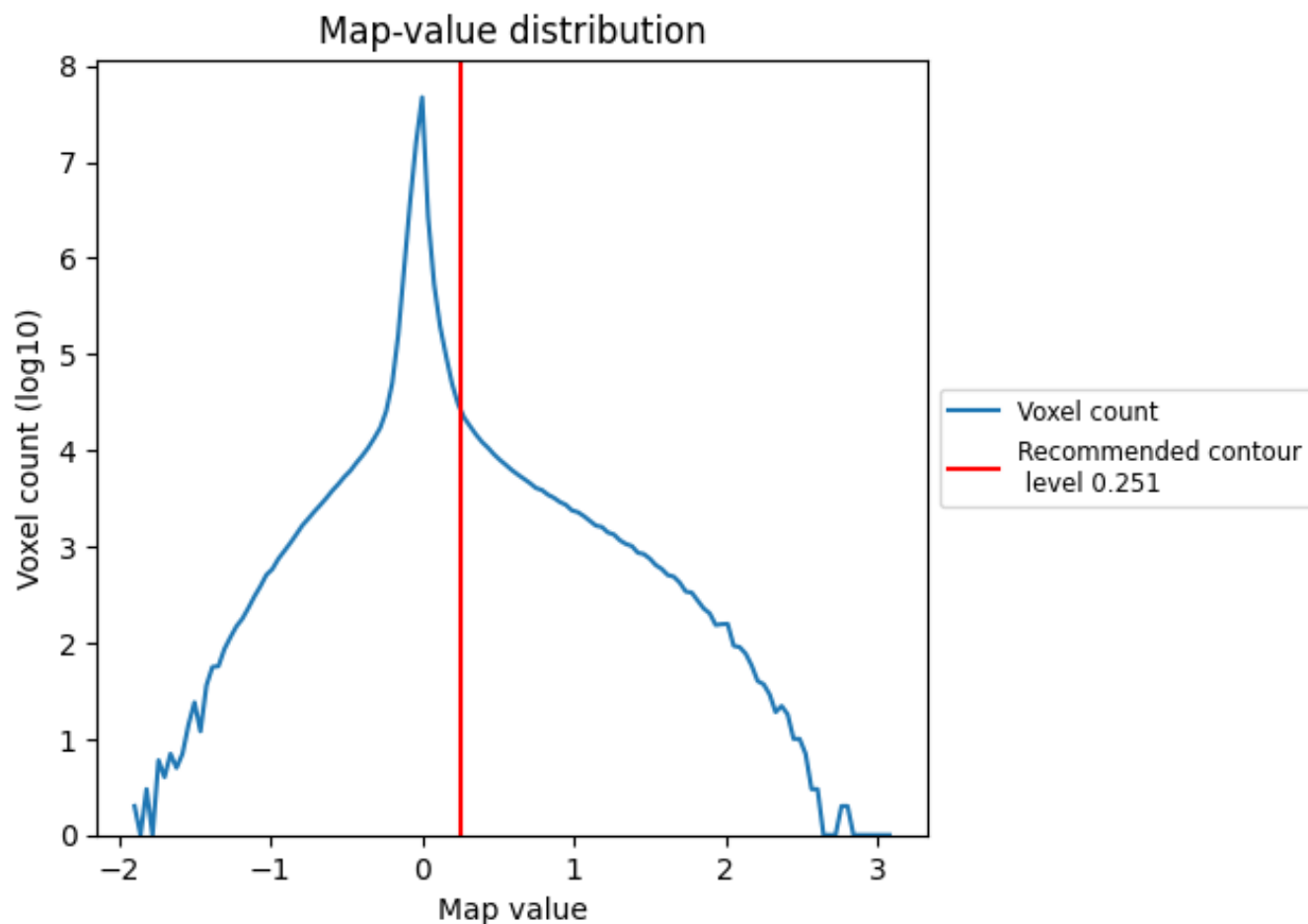
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

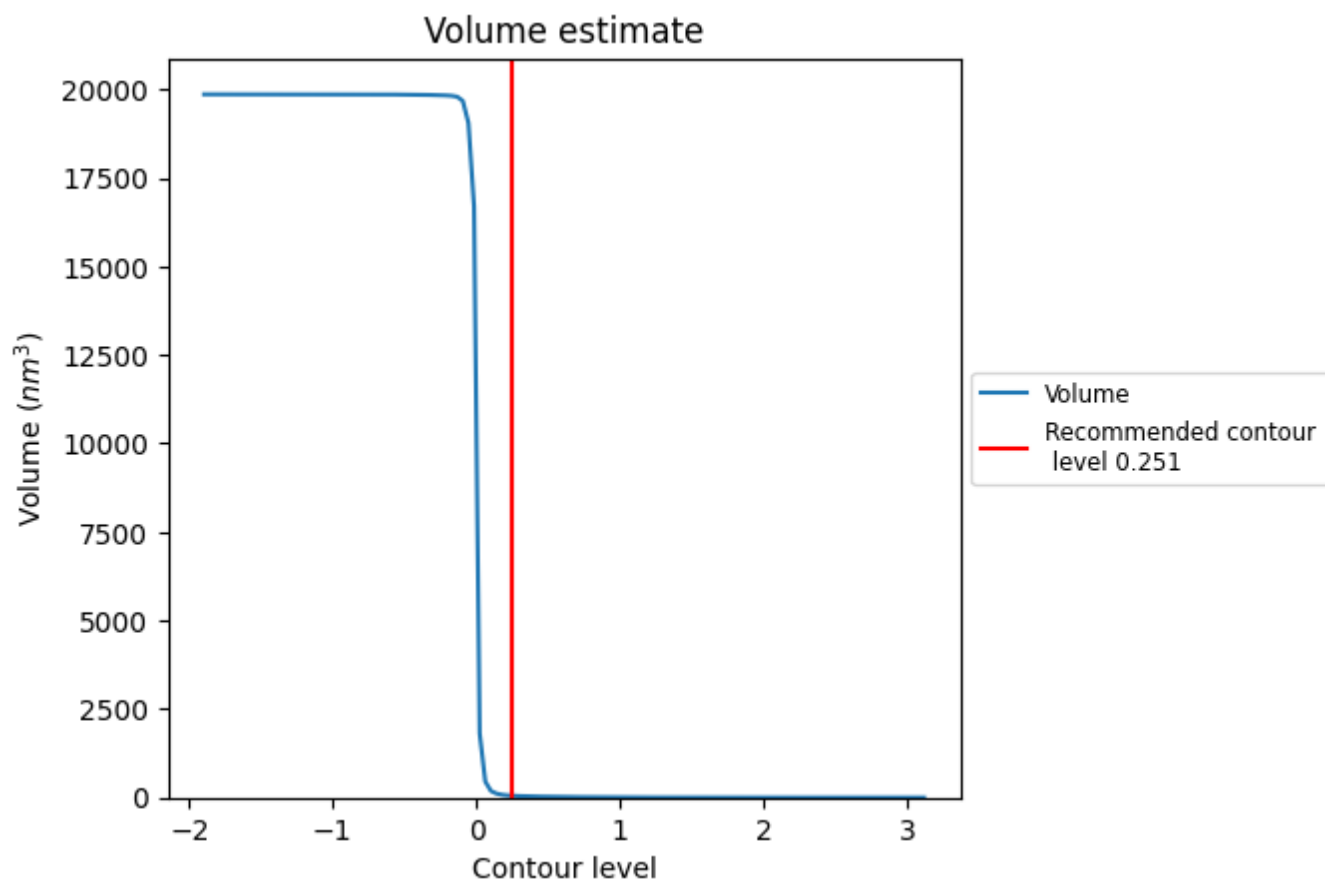
This section contains the results of statistical analysis of the map.

### 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.

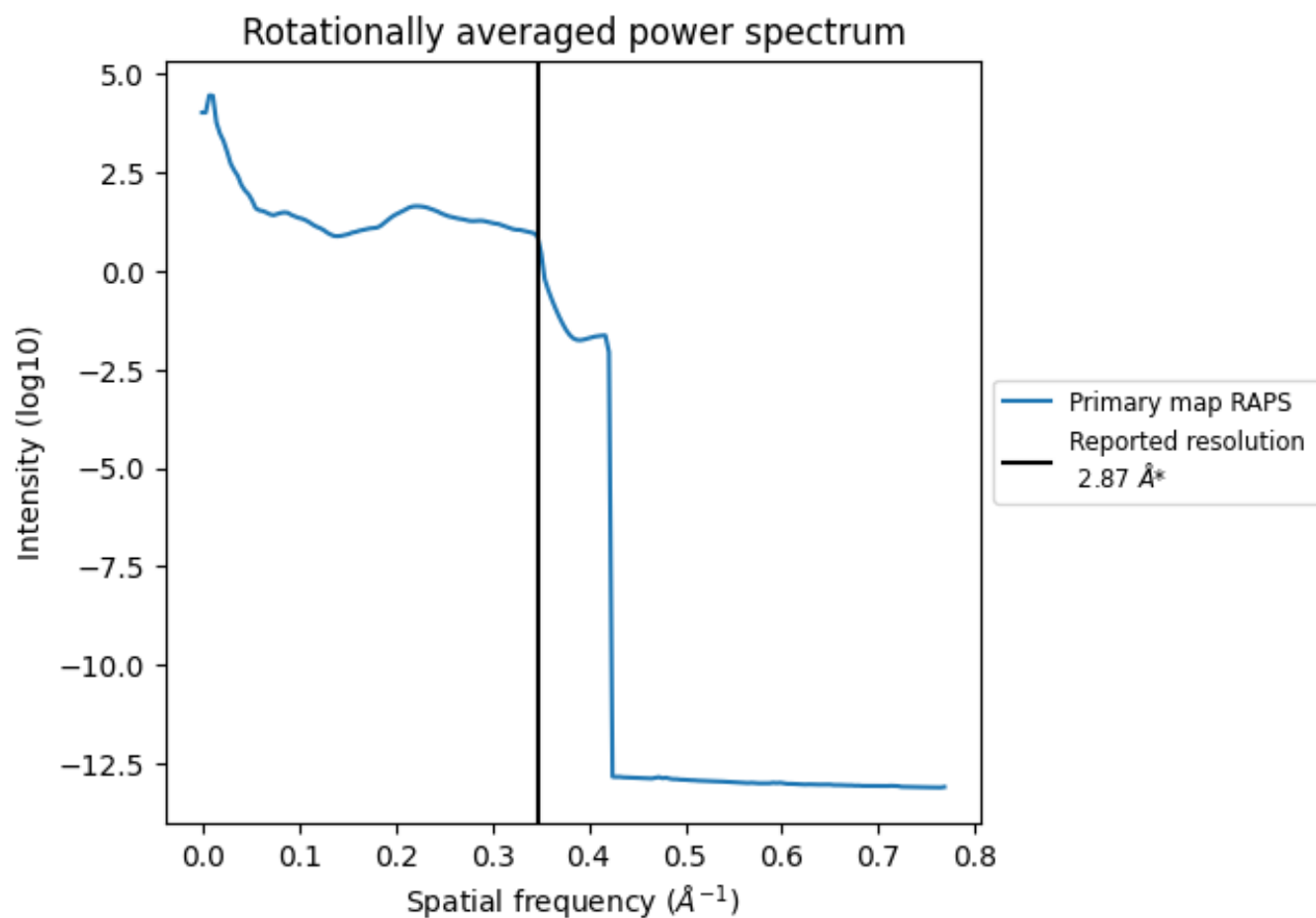
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm<sup>3</sup>; this corresponds to an approximate mass of 47 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 0.348 Å<sup>-1</sup>

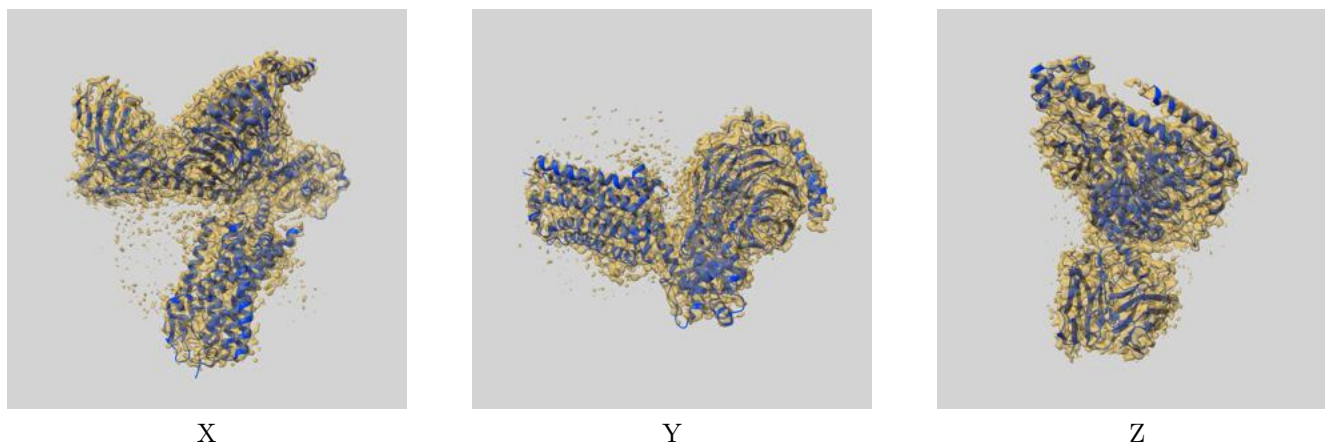
## 8 Fourier-Shell correlation ⓘ

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

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

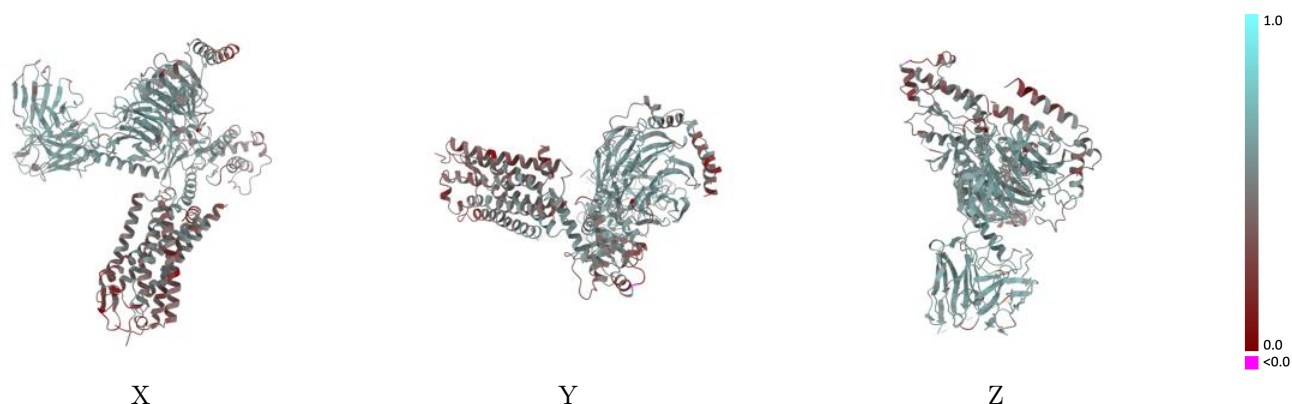
This section contains information regarding the fit between EMDB map EMD-13141 and PDB model 7P02. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



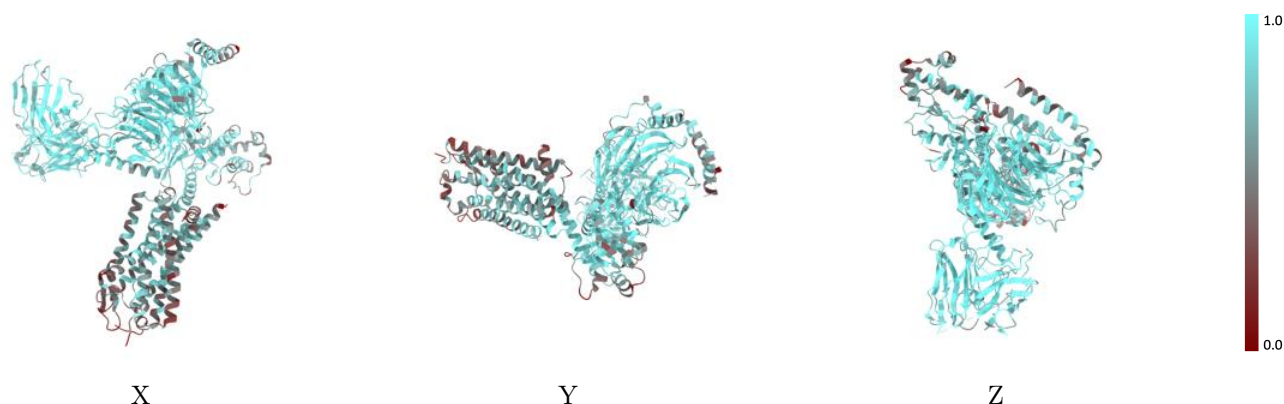
The images above show the 3D surface view of the map at the recommended contour level 0.251 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



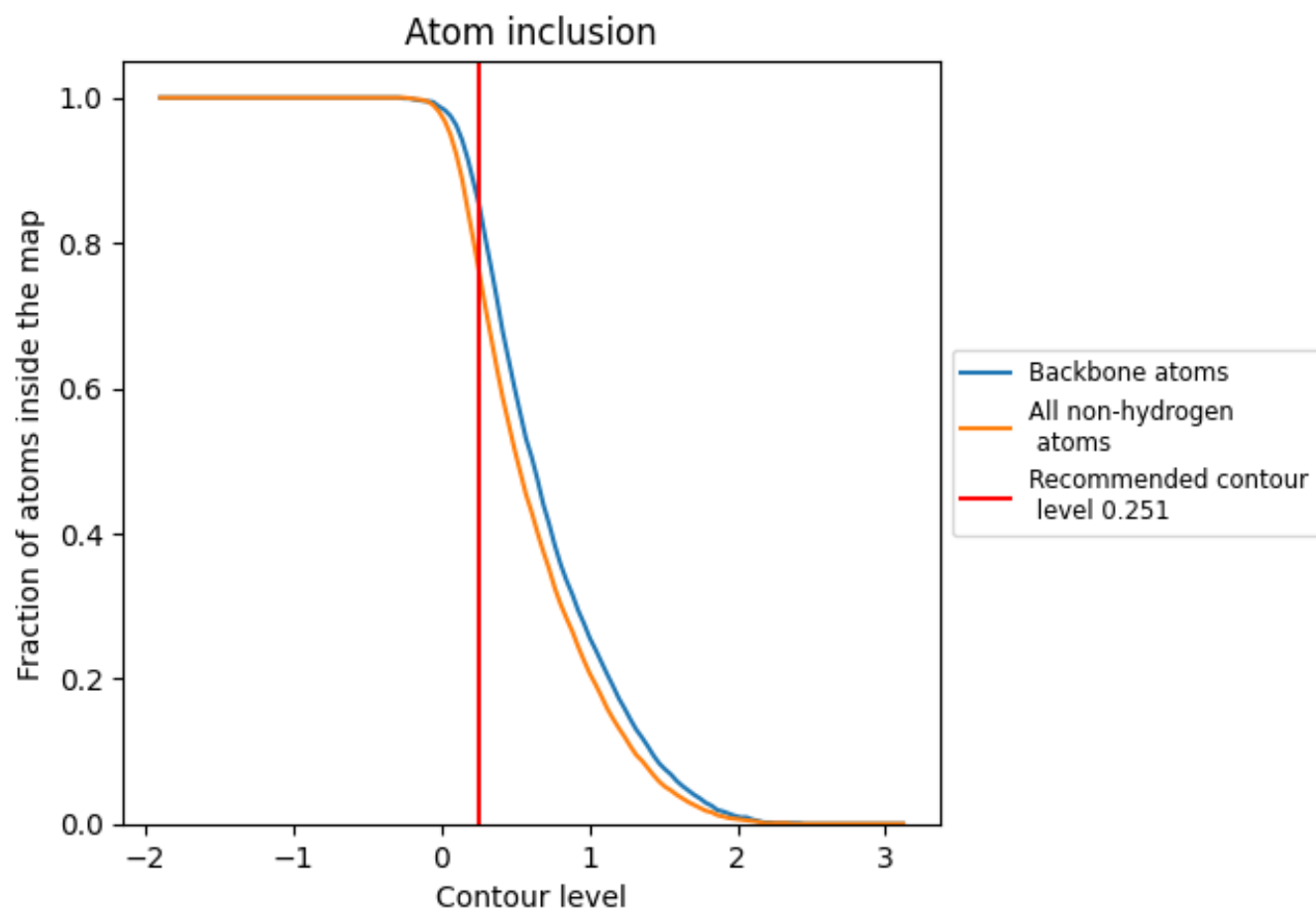
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.251).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.251) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7660</div>	<div><div></div>0.5020</div>
A	<div><div></div>0.7580</div>	<div><div></div>0.4840</div>
B	<div><div></div>0.8830</div>	<div><div></div>0.5590</div>
G	<div><div></div>0.7120</div>	<div><div></div>0.4680</div>
H	<div><div></div>0.8730</div>	<div><div></div>0.5670</div>
P	<div><div></div>0.5190</div>	<div><div></div>0.3890</div>
R	<div><div></div>0.5840</div>	<div><div></div>0.4130</div>

1.0

0.0

<0.0