



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 10:07 AM EDT

PDB ID : 9P0K / pdb_00009p0k
EMDB ID : EMD-71079
Title : Composite map of CXCL9-CXCR3-Gi-scFv16
Authors : Sun, D.; Masureel, M.; Johnson, M.
Deposited on : 2025-06-06
Resolution : 3.50 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:

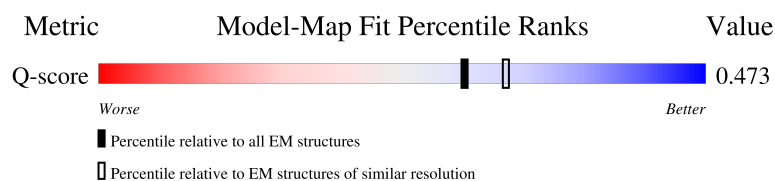
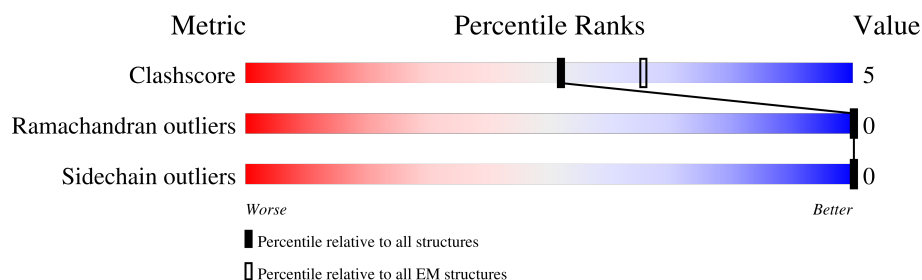
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	A	684	
2	B	103	
3	C	376	
4	D	357	

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Mol	Chain	Length	Quality of chain
5	E	71	<div><div></div><div>24%</div><div>61%</div><div>17%</div><div>23%</div></div>
6	F	269	<div><div></div><div>72%</div><div>14%</div><div>14%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18831 atoms, of which 9401 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 C-X-C chemokine receptor type 3, GFP-like fluorescent chro-moprotein FP506, related.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	298	4732	1525	2411	401	378	17	0	0

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	expression tag	UNP P49682
A	-33	LYS	-	expression tag	UNP P49682
A	-32	THR	-	expression tag	UNP P49682
A	-31	ILE	-	expression tag	UNP P49682
A	-30	ILE	-	expression tag	UNP P49682
A	-29	ALA	-	expression tag	UNP P49682
A	-28	LEU	-	expression tag	UNP P49682
A	-27	SER	-	expression tag	UNP P49682
A	-26	TYR	-	expression tag	UNP P49682
A	-25	ILE	-	expression tag	UNP P49682
A	-24	PHE	-	expression tag	UNP P49682
A	-23	CYS	-	expression tag	UNP P49682
A	-22	LEU	-	expression tag	UNP P49682
A	-21	VAL	-	expression tag	UNP P49682
A	-20	PHE	-	expression tag	UNP P49682
A	-19	ALA	-	expression tag	UNP P49682
A	-18	ASP	-	expression tag	UNP P49682
A	-17	TYR	-	expression tag	UNP P49682
A	-16	LYS	-	expression tag	UNP P49682
A	-15	ASP	-	expression tag	UNP P49682
A	-14	ASP	-	expression tag	UNP P49682
A	-13	ASP	-	expression tag	UNP P49682
A	-12	ASP	-	expression tag	UNP P49682
A	-11	LYS	-	expression tag	UNP P49682
A	-10	GLY	-	expression tag	UNP P49682
A	-9	SER	-	expression tag	UNP P49682
A	-8	GLU	-	expression tag	UNP P49682

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASN	-	expression tag	UNP P49682
A	-6	LEU	-	expression tag	UNP P49682
A	-5	TYR	-	expression tag	UNP P49682
A	-4	PHE	-	expression tag	UNP P49682
A	-3	GLN	-	expression tag	UNP P49682
A	-2	SER	-	expression tag	UNP P49682
A	-1	GLY	-	expression tag	UNP P49682
A	0	SER	-	expression tag	UNP P49682
A	260	ALA	VAL	conflict	UNP P49682
A	369	GLY	-	linker	UNP P49682
A	370	ASN	-	linker	UNP P49682
A	371	SER	-	linker	UNP P49682
A	372	LEU	-	linker	UNP P49682
A	373	GLU	-	linker	UNP P49682
A	374	VAL	-	linker	UNP P49682
A	375	LEU	-	linker	UNP P49682
A	376	PHE	-	linker	UNP P49682
A	377	GLN	-	linker	UNP P49682
A	378	GLY	-	linker	UNP P49682
A	379	PRO	-	linker	UNP P49682
A	426	LEU	PHE	conflict	UNP U6GSR1
A	444	LEU	PHE	conflict	UNP U6GSR1
A	449	GLN	MET	conflict	UNP U6GSR1
A	533	THR	MET	conflict	UNP U6GSR1
A	543	ALA	VAL	conflict	UNP U6GSR1
A	555	GLY	SER	conflict	UNP U6GSR1
A	586	LYS	ALA	conflict	UNP U6GSR1
A	619	GLY	-	expression tag	UNP U6GSR1
A	620	SER	-	expression tag	UNP U6GSR1
A	621	ALA	-	expression tag	UNP U6GSR1
A	622	TRP	-	expression tag	UNP U6GSR1
A	623	SER	-	expression tag	UNP U6GSR1
A	624	HIS	-	expression tag	UNP U6GSR1
A	625	PRO	-	expression tag	UNP U6GSR1
A	626	GLN	-	expression tag	UNP U6GSR1
A	627	PHE	-	expression tag	UNP U6GSR1
A	628	GLU	-	expression tag	UNP U6GSR1
A	629	LYS	-	expression tag	UNP U6GSR1
A	630	GLY	-	expression tag	UNP U6GSR1
A	631	GLY	-	expression tag	UNP U6GSR1
A	632	GLY	-	expression tag	UNP U6GSR1
A	633	SER	-	expression tag	UNP U6GSR1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	634	GLY	-	expression tag	UNP U6GSR1
A	635	GLY	-	expression tag	UNP U6GSR1
A	636	GLY	-	expression tag	UNP U6GSR1
A	637	SER	-	expression tag	UNP U6GSR1
A	638	GLY	-	expression tag	UNP U6GSR1
A	639	GLY	-	expression tag	UNP U6GSR1
A	640	SER	-	expression tag	UNP U6GSR1
A	641	ALA	-	expression tag	UNP U6GSR1
A	642	TRP	-	expression tag	UNP U6GSR1
A	643	SER	-	expression tag	UNP U6GSR1
A	644	HIS	-	expression tag	UNP U6GSR1
A	645	PRO	-	expression tag	UNP U6GSR1
A	646	GLN	-	expression tag	UNP U6GSR1
A	647	PHE	-	expression tag	UNP U6GSR1
A	648	GLU	-	expression tag	UNP U6GSR1
A	649	LYS	-	expression tag	UNP U6GSR1

- Molecule 2 is a protein called C-X-C motif chemokine 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total	C	H	N	O	S	0	0
			1134	346	580	98	106	4		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	217	Total	C	H	N	O	S	0	0
			3498	1113	1747	293	333	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP P63096
C	-20	LYS	-	expression tag	UNP P63096
C	-19	LYS	-	expression tag	UNP P63096
C	-18	HIS	-	expression tag	UNP P63096
C	-17	HIS	-	expression tag	UNP P63096
C	-16	HIS	-	expression tag	UNP P63096
C	-15	HIS	-	expression tag	UNP P63096
C	-14	HIS	-	expression tag	UNP P63096
C	-13	HIS	-	expression tag	UNP P63096
C	-12	HIS	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP P63096
C	-10	HIS	-	expression tag	UNP P63096
C	-9	HIS	-	expression tag	UNP P63096
C	-8	GLU	-	expression tag	UNP P63096
C	-7	ASN	-	expression tag	UNP P63096
C	-6	LEU	-	expression tag	UNP P63096
C	-5	TYR	-	expression tag	UNP P63096
C	-4	PHE	-	expression tag	UNP P63096
C	-3	GLN	-	expression tag	UNP P63096
C	-2	GLY	-	expression tag	UNP P63096
C	-1	GLY	-	expression tag	UNP P63096
C	0	SER	-	expression tag	UNP P63096

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	337	Total	C	H	N	O	S	0	0
			5092	1599	2500	466	506	21		

There are 18 discrepancies between the modelled and reference sequences:

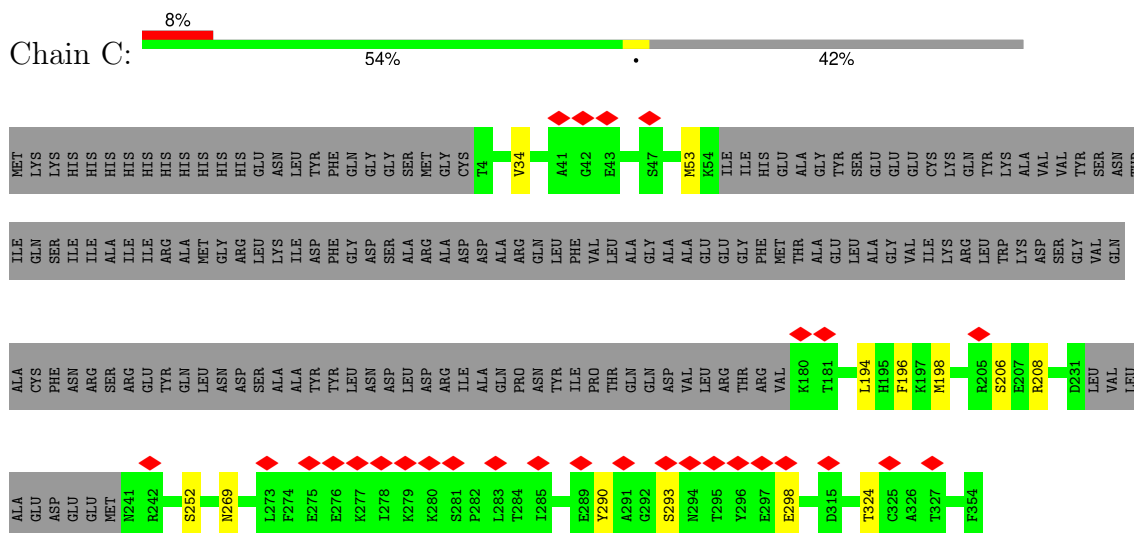
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	expression tag	UNP P62873
D	-15	HIS	-	expression tag	UNP P62873
D	-14	HIS	-	expression tag	UNP P62873
D	-13	HIS	-	expression tag	UNP P62873
D	-12	HIS	-	expression tag	UNP P62873
D	-11	HIS	-	expression tag	UNP P62873
D	-10	HIS	-	expression tag	UNP P62873
D	-9	HIS	-	expression tag	UNP P62873
D	-8	HIS	-	expression tag	UNP P62873
D	-7	GLY	-	expression tag	UNP P62873
D	-6	GLU	-	expression tag	UNP P62873
D	-5	ASN	-	expression tag	UNP P62873
D	-4	LEU	-	expression tag	UNP P62873
D	-3	TYR	-	expression tag	UNP P62873
D	-2	PHE	-	expression tag	UNP P62873
D	-1	GLN	-	expression tag	UNP P62873
D	0	GLY	-	expression tag	UNP P62873
D	1	SER	-	expression tag	UNP P62873

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

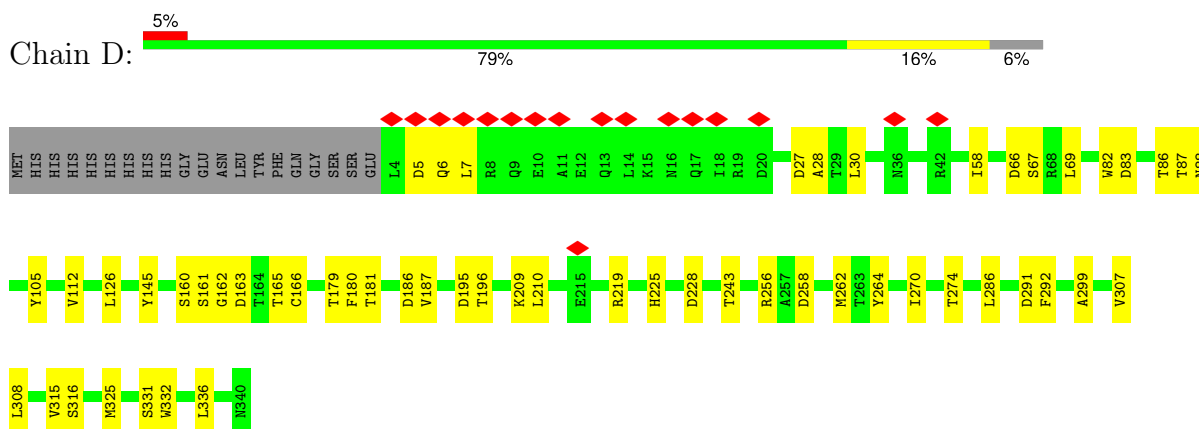
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	55	861	266	437	75	80	3	0	0

- Molecule 6 is a protein called scFV16.

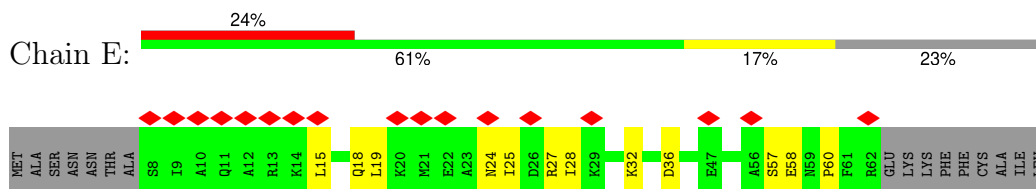
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	232	3514	1135	1726	296	347	10	0	0



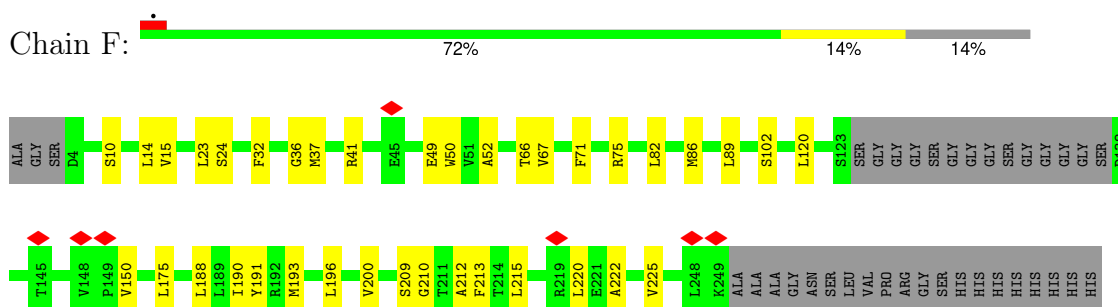
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



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



- Molecule 6: scFV16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51645	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.436	Depositor
Minimum map value	-1.491	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.276	Depositor
Map size (Å)	467.84, 467.84, 467.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.462, 1.462, 1.462	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/2377	0.37	0/3244
2	B	0.19	0/561	0.41	0/756
3	C	0.14	0/1780	0.26	0/2384
4	D	0.15	0/2639	0.30	0/3577
5	E	0.14	0/430	0.38	0/580
6	F	0.14	0/1832	0.29	0/2483
All	All	0.16	0/9619	0.32	0/13024

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	A	2321	2411	2410	22	0
2	B	554	580	580	9	0
3	C	1751	1747	1744	8	0
4	D	2592	2500	2499	38	0
5	E	424	437	436	9	0
6	F	1788	1726	1724	23	0
All	All	9430	9401	9393	102	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 5.

The worst 5 of 102 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:44:THR:OG1	2:B:50:GLN:OE1	2.00	0.80
4:D:274:THR:OG1	4:D:315:VAL:O	2.03	0.77
3:C:269:ASN:OD1	3:C:324:THR:OG1	2.03	0.77
4:D:209:LYS:NZ	5:E:18:GLN:OE1	2.19	0.75
3:C:293:SER:OG	3:C:298:GLU:OE2	2.04	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	A	296/684 (43%)	288 (97%)	8 (3%)	0	100	100
2	B	70/103 (68%)	63 (90%)	7 (10%)	0	100	100
3	C	211/376 (56%)	207 (98%)	4 (2%)	0	100	100
4	D	335/357 (94%)	326 (97%)	9 (3%)	0	100	100
5	E	53/71 (75%)	53 (100%)	0	0	100	100
6	F	228/269 (85%)	221 (97%)	7 (3%)	0	100	100
All	All	1193/1860 (64%)	1158 (97%)	35 (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	246/574 (43%)	246 (100%)	0	100	100
2	B	66/96 (69%)	66 (100%)	0	100	100
3	C	193/325 (59%)	193 (100%)	0	100	100
4	D	280/298 (94%)	280 (100%)	0	100	100
5	E	45/58 (78%)	45 (100%)	0	100	100
6	F	197/217 (91%)	197 (100%)	0	100	100
All	All	1027/1568 (66%)	1027 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
3	C	195	HIS
6	F	143	GLN
6	F	180	GLN

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.

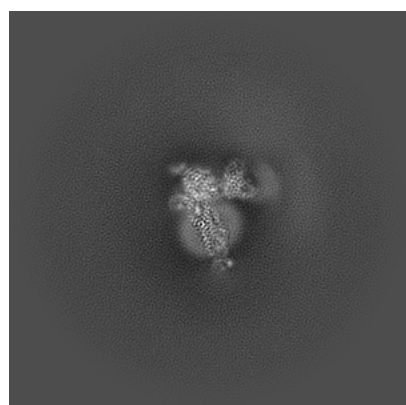
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71079. These allow visual inspection of the internal detail of the map and identification of artifacts.

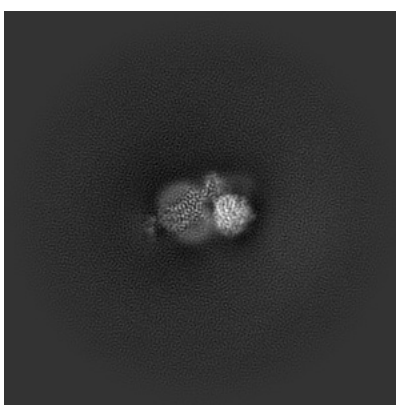
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

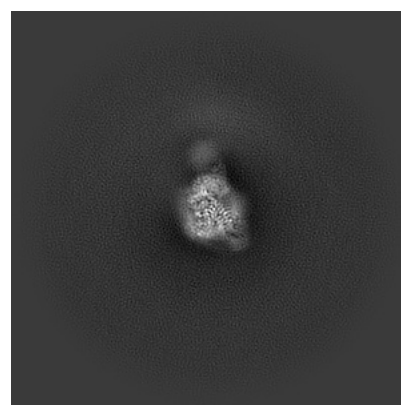
6.1.1 Primary map



X



Y

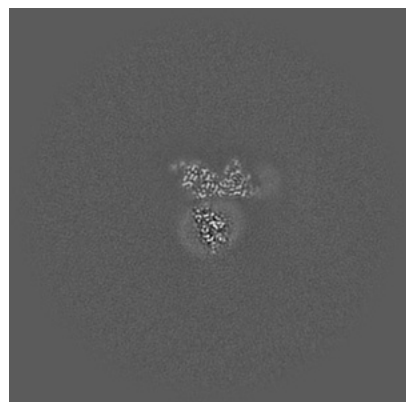


Z

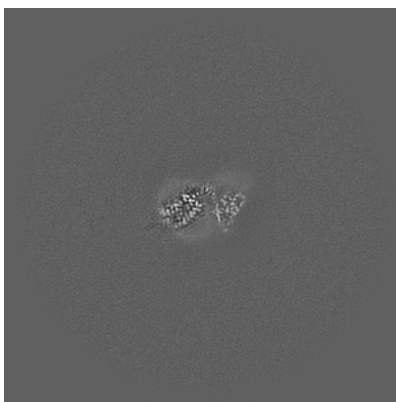
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

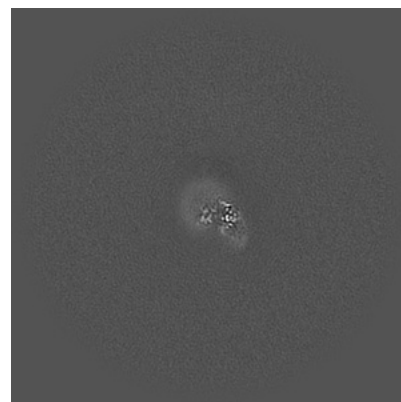
6.2.1 Primary map



X Index: 160



Y Index: 160

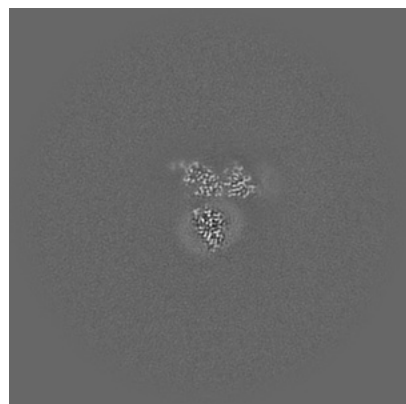


Z Index: 160

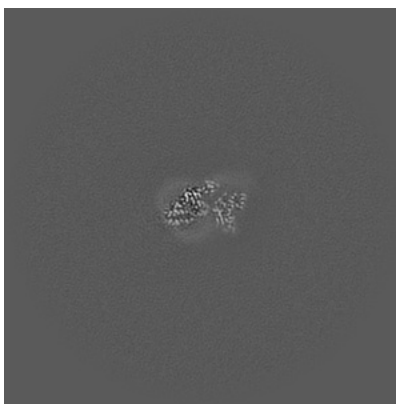
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

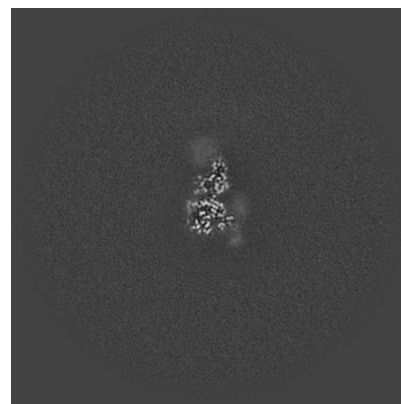
6.3.1 Primary map



X Index: 162



Y Index: 157

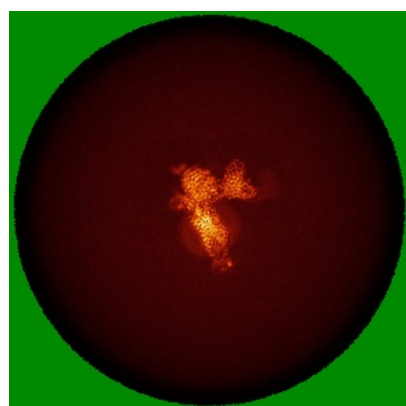


Z Index: 176

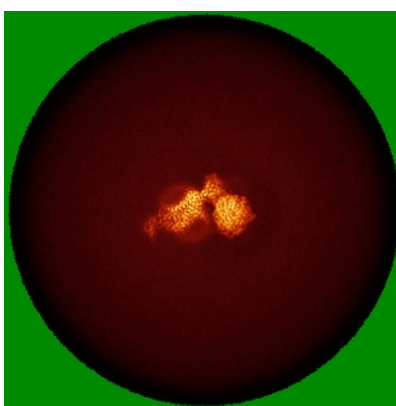
The images above show the largest variance slices of the map in three orthogonal directions.

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

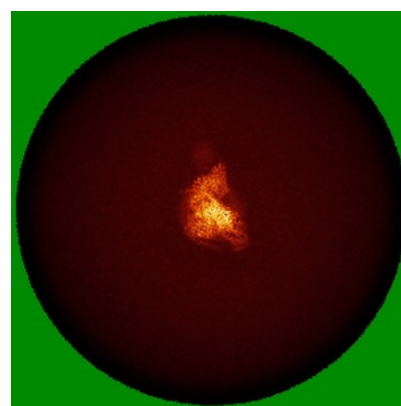
6.4.1 Primary map



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

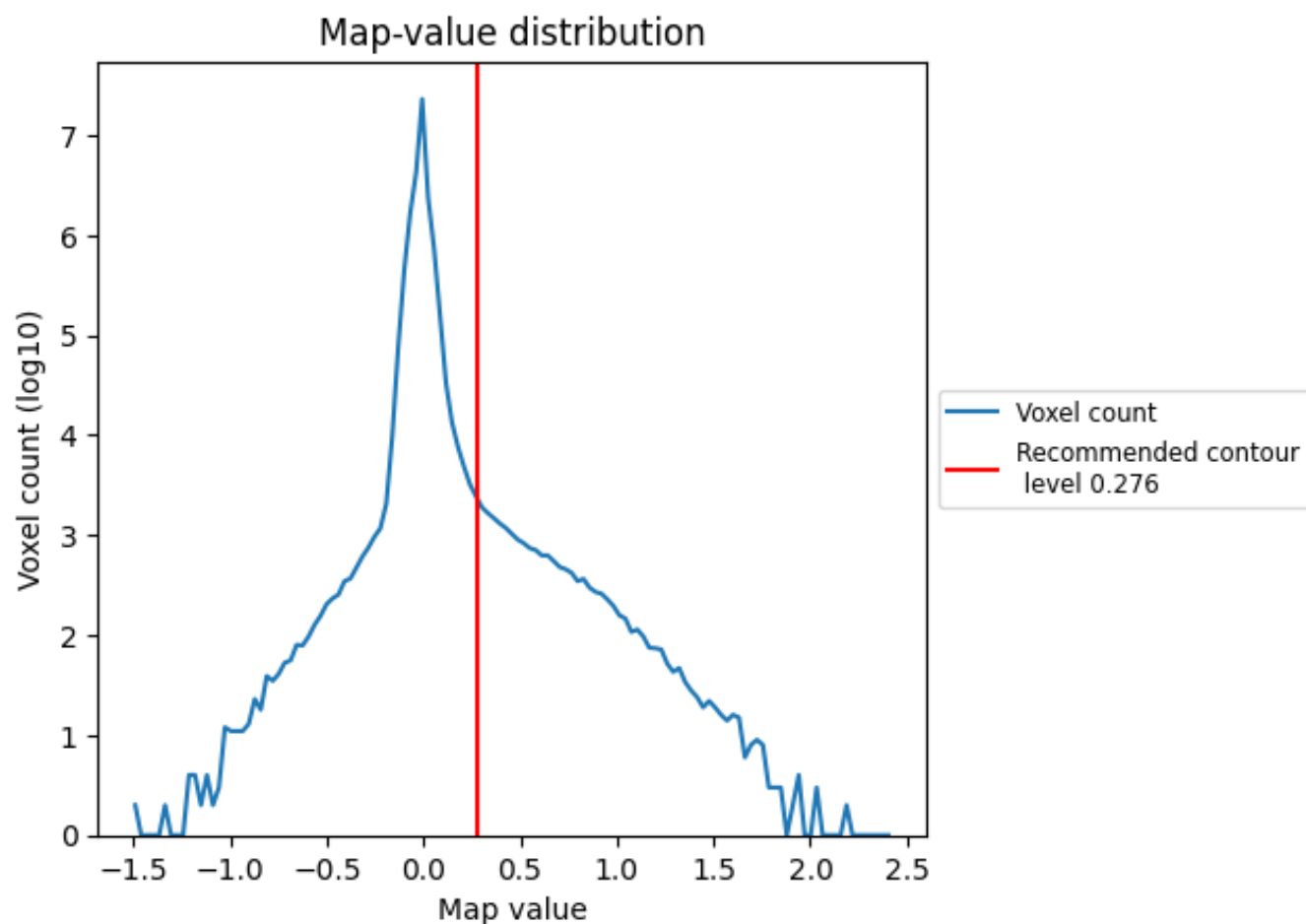
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

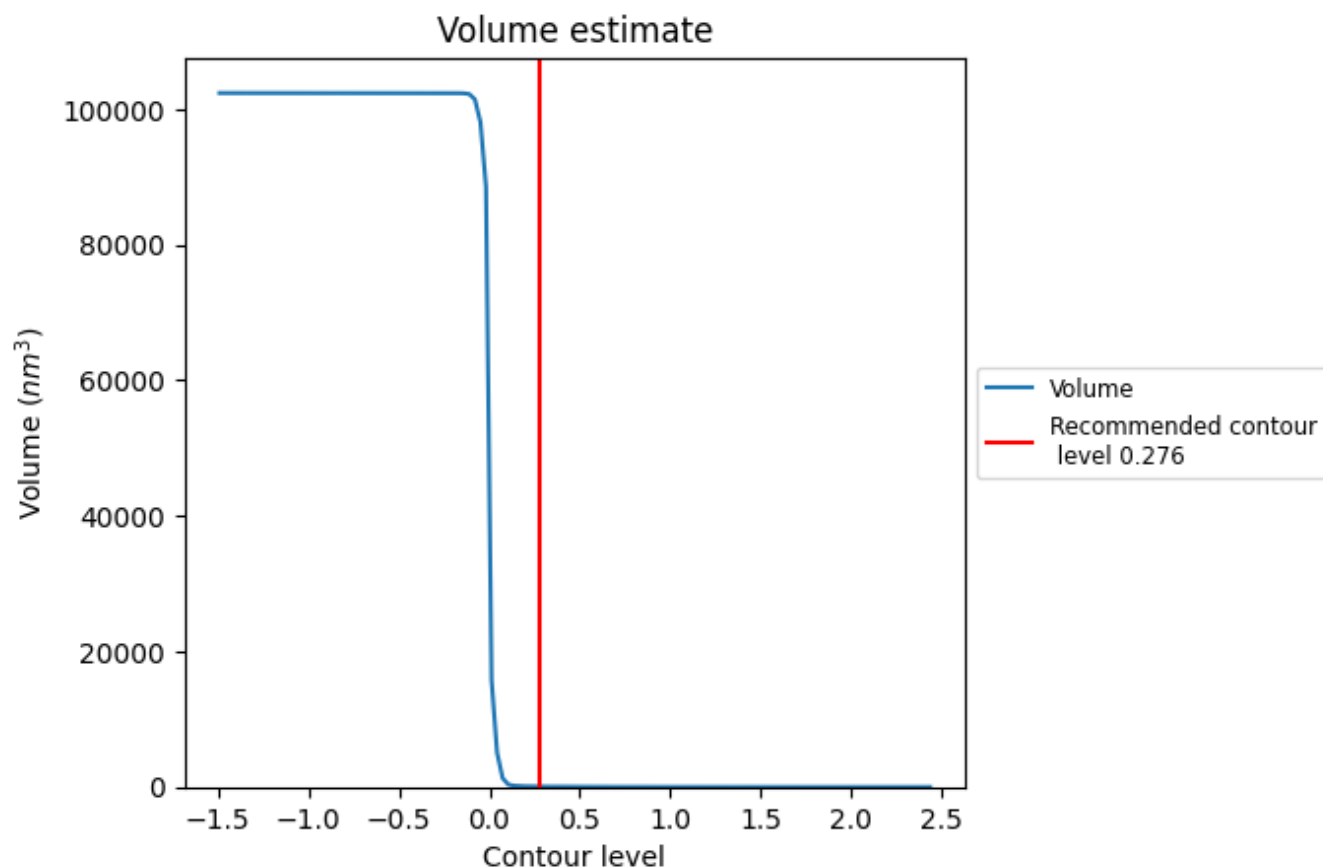
This section contains the results of statistical analysis of the map.

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.

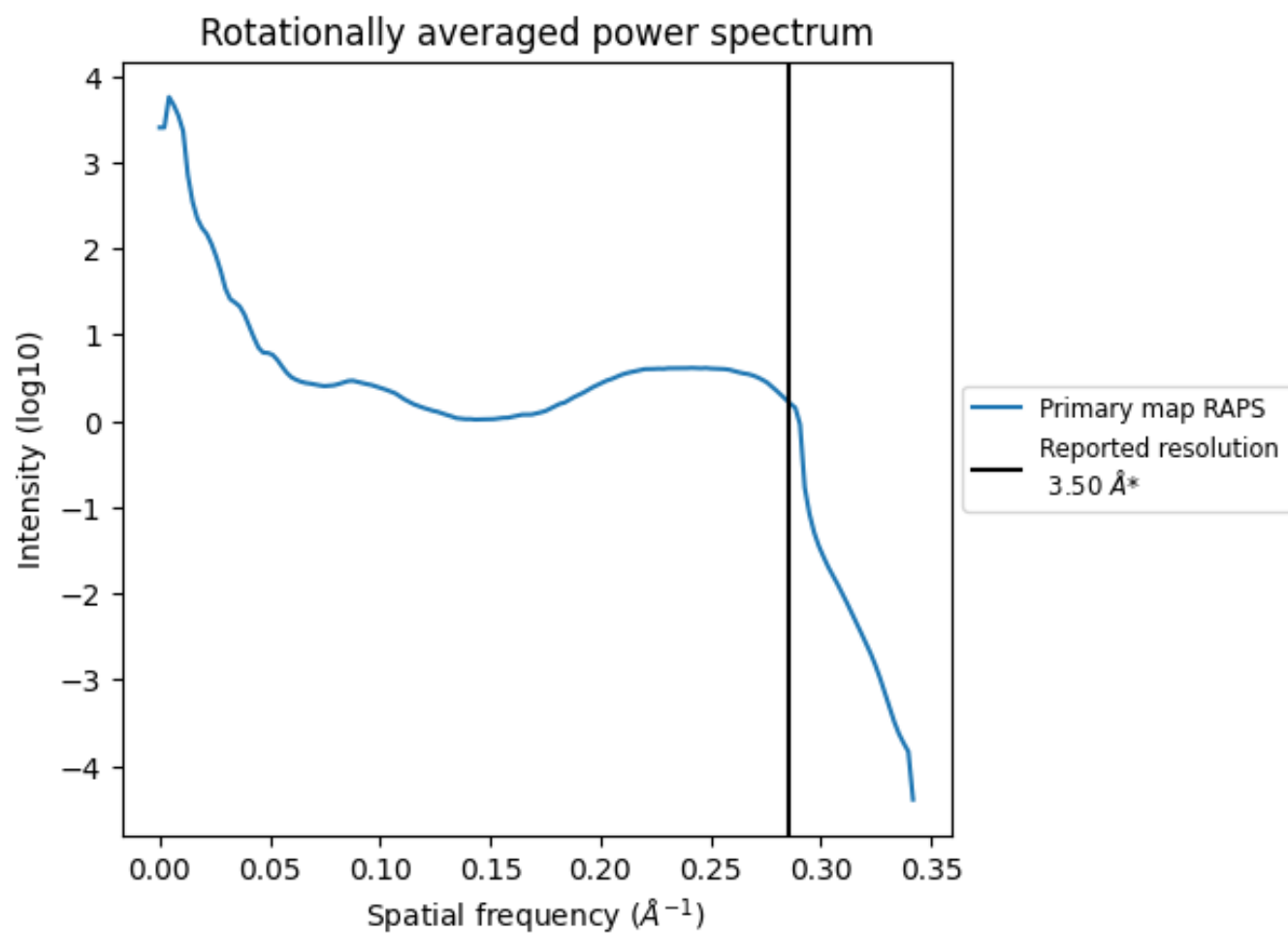
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm^3 ; this corresponds to an approximate mass of 57 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 0.286 Å⁻¹

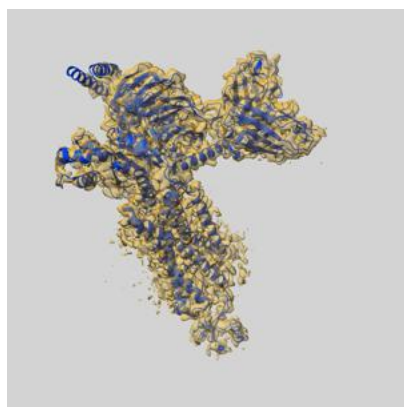
8 Fourier-Shell correlation

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

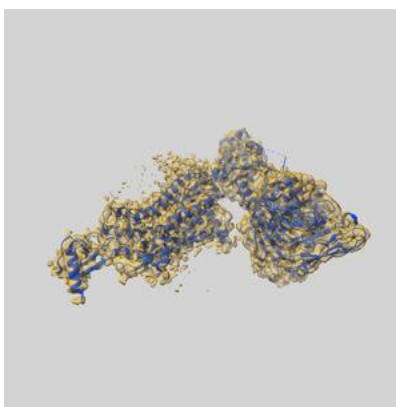
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71079 and PDB model 9P0K. Per-residue inclusion information can be found in section [3](#) on page [9](#).

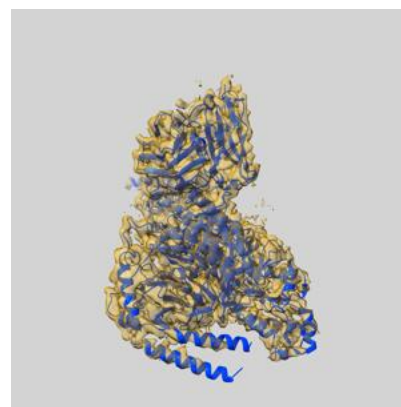
9.1 Map-model overlay [i](#)



X



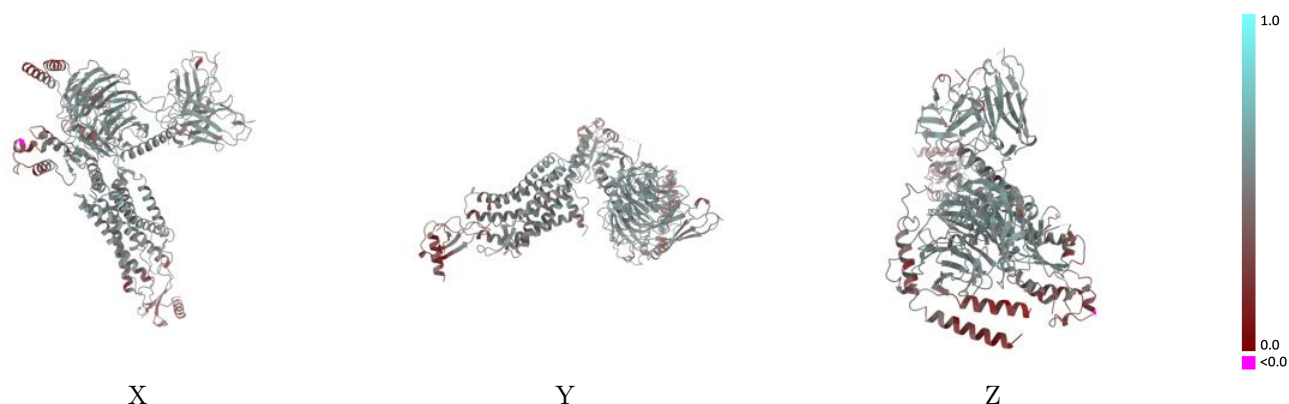
Y



Z

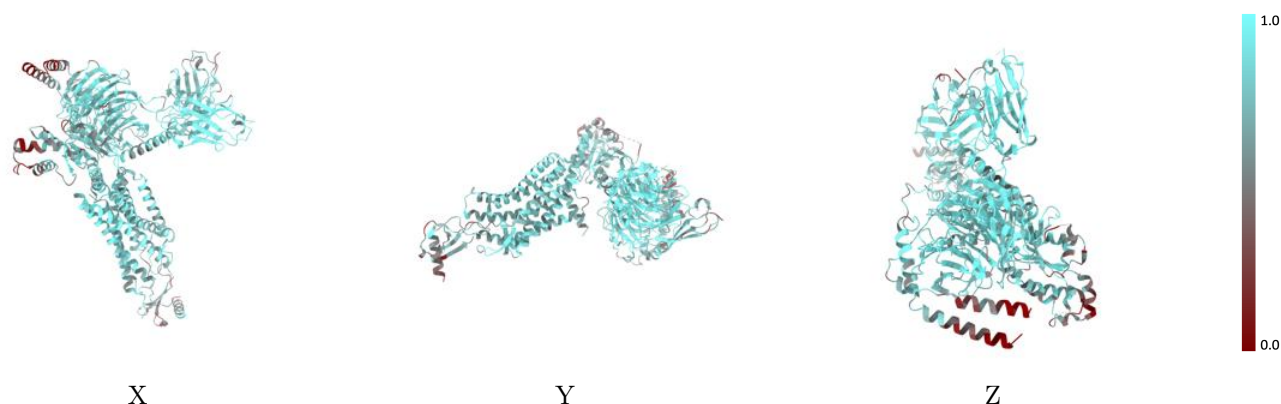
The images above show the 3D surface view of the map at the recommended contour level 0.276 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



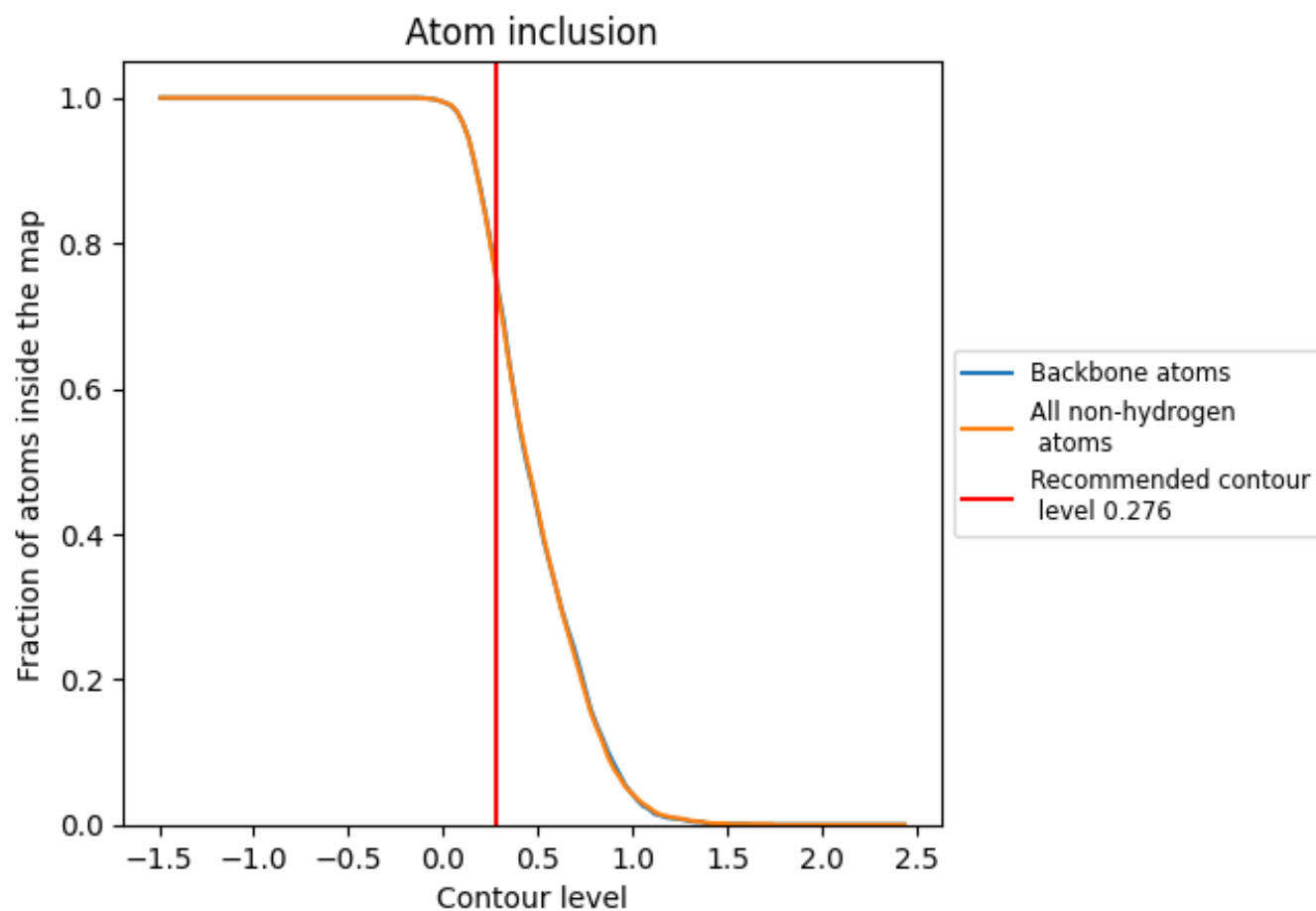
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.276).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.276) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7580</div>	<div><div></div>0.4730</div>
A	<div><div></div>0.7900</div>	<div><div></div>0.4860</div>
B	<div><div></div>0.5350</div>	<div><div></div>0.3410</div>
C	<div><div></div>0.7000</div>	<div><div></div>0.4520</div>
D	<div><div></div>0.8170</div>	<div><div></div>0.5010</div>
E	<div><div></div>0.5730</div>	<div><div></div>0.3440</div>
F	<div><div></div>0.8300</div>	<div><div></div>0.5050</div>

1.0

0.0

<0.0