



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 09:17 PM UTC

PDB ID : 9OAB / pdb_00009oab
EMDB ID : EMD-70278
Title : C3 reconstruction of the thermophilic bacteriophage P74-26 Neck
Authors : Sedivy, E.L.; Agnello, E.; Song, K.; Xu, C.; Kelch, B.A.
Deposited on : 2025-04-21
Resolution : 2.60 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

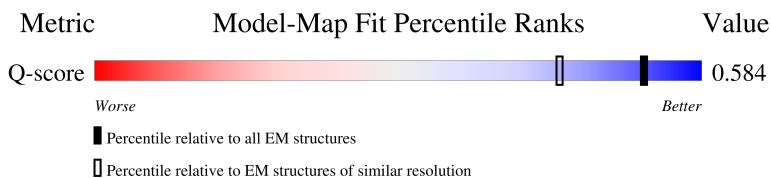
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



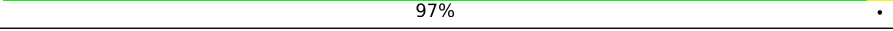
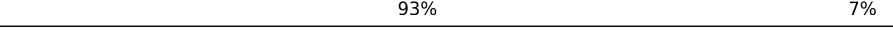
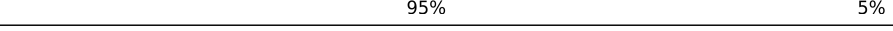
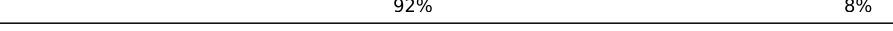
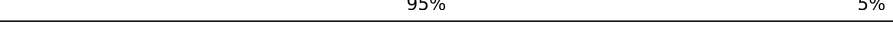
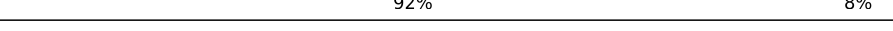
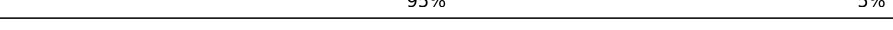
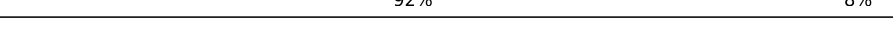
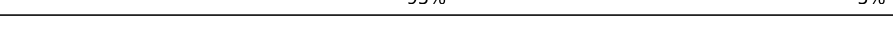
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	Da	448	 89% 5% 6%
1	Db	448	 89% 5% 6%
1	Dc	448	 88% 6% 6%
1	Dd	448	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	De	448	 90% 6% 6%
1	Df	448	 88% 6% 6%
1	Dg	448	 88% 6% 6%
1	Dh	448	 89% 6% 6%
1	Di	448	 88% 7% 6%
1	Dj	448	 88% 6% 6%
1	Dk	448	 89% 6% 6%
1	Dl	448	 88% 6% 6%
2	Ea	130	 92% 8%
2	Eb	130	 97% .
2	Ec	130	 93% 7%
2	Ed	130	 95% 5%
2	Ee	130	 92% 8%
2	Ef	130	 95% 5%
2	Eg	130	 92% 8%
2	Eh	130	 95% 5%
2	Ei	130	 92% 8%
2	Ej	130	 95% 5%
2	Ek	130	 92% 8%
2	El	130	 95% 5%
3	Fa	155	 88% 12%
3	Fb	155	 87% 13%
3	Fc	155	 87% 13%
3	Fd	155	 87% 13%
3	Fe	155	 88% 12%

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Mol	Chain	Length	Quality of chain
3	Ff	155	
4	Ga	146	
4	Gb	146	
4	Gc	146	
4	Gd	146	
4	Ge	146	
4	Gf	146	
4	Gg	146	
4	Gh	146	
4	Gi	146	
4	Gj	146	
4	Gk	146	
4	Gl	146	
4	Ha	146	
4	Hb	146	
4	Hc	146	
4	Hd	146	
4	He	146	
4	Hf	146	
4	Hg	146	
4	Hh	146	
4	Hi	146	
4	Hj	146	
4	Hk	146	
4	Hl	146	

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Mol	Chain	Length	Quality of chain
5	Ia	348	 91% 9%
5	Ib	348	 90% 10%
5	Ic	348	 90% 10%
5	Id	348	 91% 9%
5	Ie	348	 91% 9%
5	If	348	 91% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 100014 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Da	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Db	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dc	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dd	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	De	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Df	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dg	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dh	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Di	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dj	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dk	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		
1	Dl	423	Total	C	N	O	S	0	0
			3287	2117	551	609	10		

- Molecule 2 is a protein called Adaptor (P74p90).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ea	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Eb	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ec	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ed	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ee	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ef	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Eg	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Eh	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ei	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ej	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	Ek	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		
2	El	130	Total	C	N	O	S	0	0
			1027	655	180	189	3		

- Molecule 3 is a protein called Tail terminator.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Fa	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
3	Fb	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
3	Fc	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
3	Fd	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
3	Fe	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		
3	Ff	155	Total	C	N	O	S	0	0
			1244	799	210	232	3		

- Molecule 4 is a protein called Collar (P74p112).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ga	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Gb	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Gc	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Gd	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Ge	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Gf	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Gg	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Gh	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Gi	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Gj	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Gk	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Gl	87	Total	C	N	O	S	0	0
			695	452	115	126	2		
4	Ha	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hb	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hc	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hd	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	He	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hf	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hg	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hh	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hi	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hj	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		
4	Hk	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Hl	146	Total	C	N	O	S	0	0
			1141	739	188	211	3		

- Molecule 5 is a protein called Tail Tube Protein gp93.

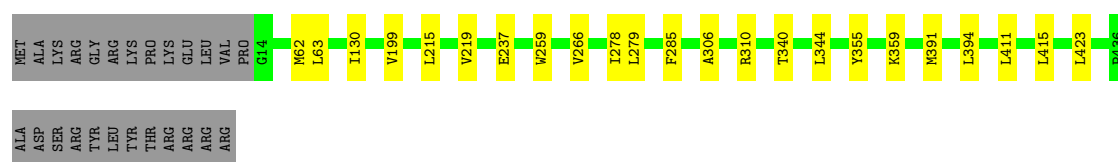
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ia	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
5	Ib	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
5	Ic	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
5	Id	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
5	Ie	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		
5	If	348	Total	C	N	O	S	0	0
			2679	1707	454	512	6		

3 Residue-property plots

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.

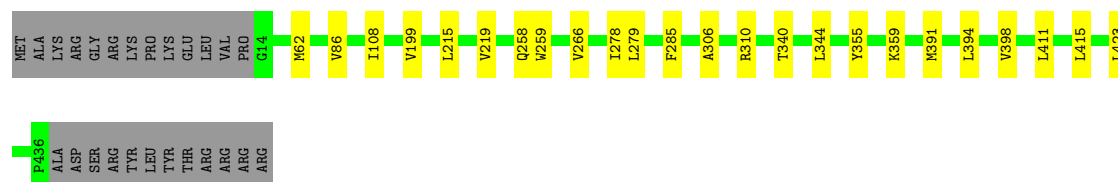
- Molecule 1: Portal protein

Chain Da: 



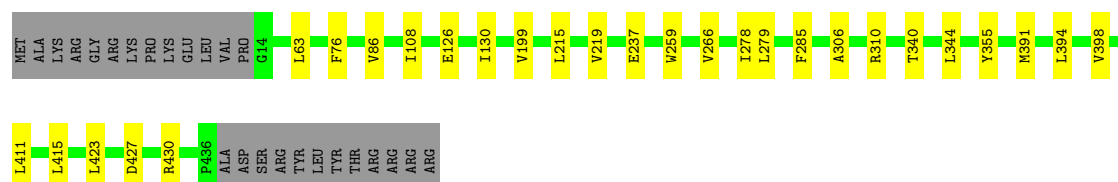
- Molecule 1: Portal protein

Chain Db: 



- Molecule 1: Portal protein

Chain Dc: 



- Molecule 1: Portal protein

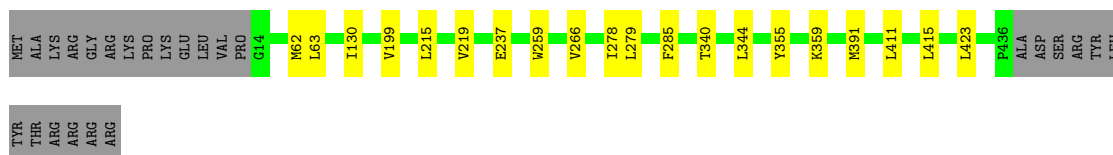
Chain Dd: 





- Molecule 1: Portal protein

Chain De: 90% 6%



- Molecule 1: Portal protein

Chain Df: 88% 6% 6%



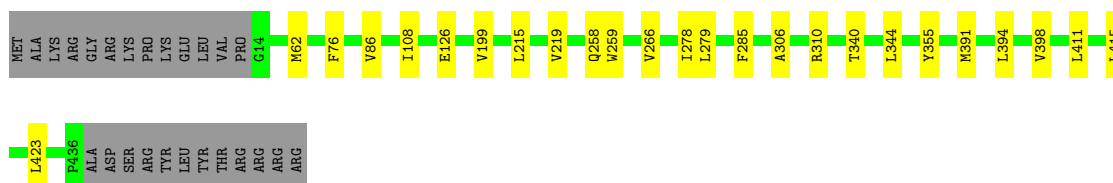
- Molecule 1: Portal protein

Chain Dg: 88% 6% 6%



- Molecule 1: Portal protein

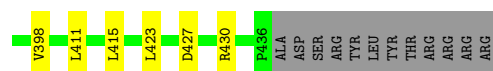
Chain Dh: 89% 6% 6%



- Molecule 1: Portal protein

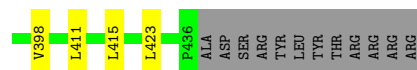
Chain Di: 88% 7% 6%





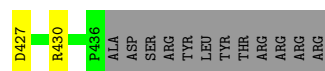
- Molecule 1: Portal protein

Chain Dj: 88% 6% 6%



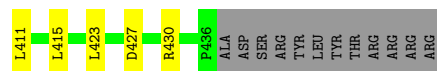
- Molecule 1: Portal protein

Chain Dk: 89% 6% 6%



- Molecule 1: Portal protein

Chain Dl: 88% 6% 6%



- Molecule 2: Adaptor (P74p90)

Chain Ea: 92% 8%



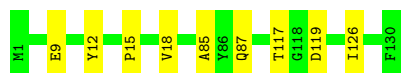
- Molecule 2: Adaptor (P74p90)

Chain Eb: 97%

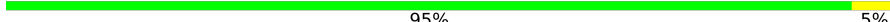


- Molecule 2: Adaptor (P74p90)

Chain Ec:  93% 7%



- Molecule 2: Adaptor (P74p90)

Chain Ed:  95% 5%



- Molecule 2: Adaptor (P74p90)

Chain Ee:  92% 8%



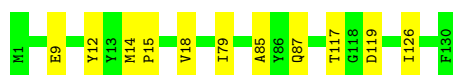
- Molecule 2: Adaptor (P74p90)

Chain Ef:  95% 5%

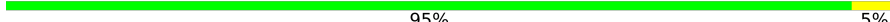


- Molecule 2: Adaptor (P74p90)

Chain Eg:  92% 8%



- Molecule 2: Adaptor (P74p90)

Chain Eh:  95% 5%

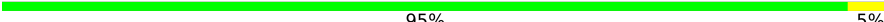


- Molecule 2: Adaptor (P74p90)

Chain Ei:  92% 8%



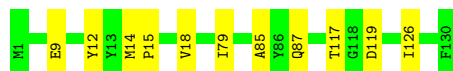
- Molecule 2: Adaptor (P74p90)

Chain Ej:  95% 5%

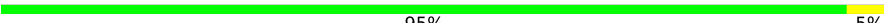


- Molecule 2: Adaptor (P74p90)

Chain Ek:  92% 8%



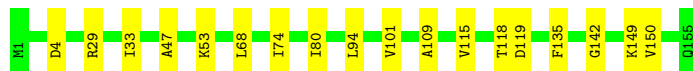
- Molecule 2: Adaptor (P74p90)

Chain El:  95% 5%



- Molecule 3: Tail terminator

Chain Fa:  88% 12%



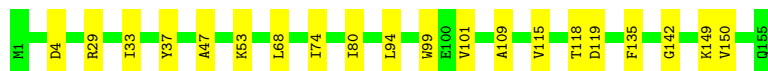
- Molecule 3: Tail terminator

Chain Fb:  87% 13%



- Molecule 3: Tail terminator

Chain Fc:  87% 13%



- Molecule 3: Tail terminator

Chain Fd:  87% 13%

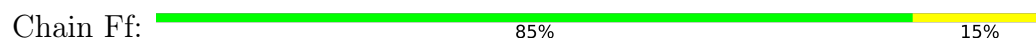


- Molecule 3: Tail terminator

Chain Fe:  88% 12%



- Molecule 3: Tail terminator



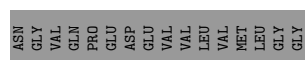
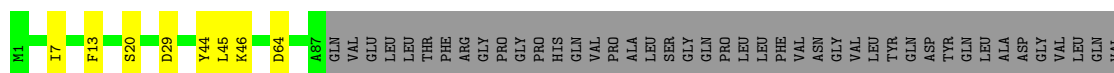
- Molecule 4: Collar (P74p112)



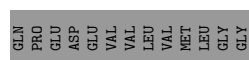
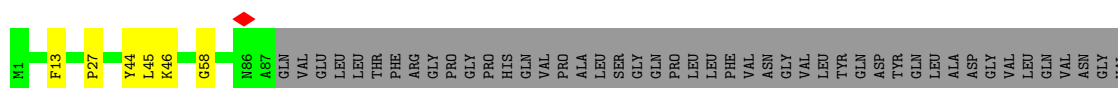
- Molecule 4: Collar (P74p112)



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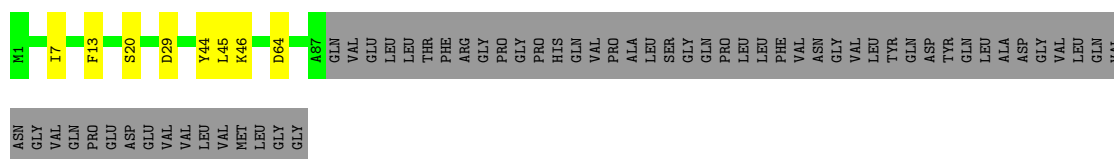




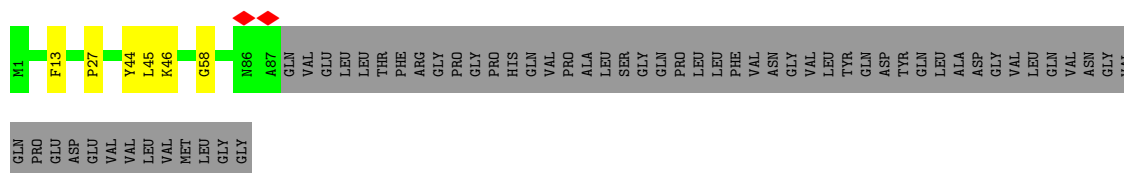
- Molecule 4: Collar (P74p112)



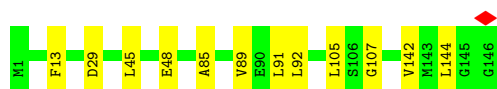
- Molecule 4: Collar (P74p112)



- Molecule 4: Collar (P74p112)



- Molecule 4: Collar (P74p112)

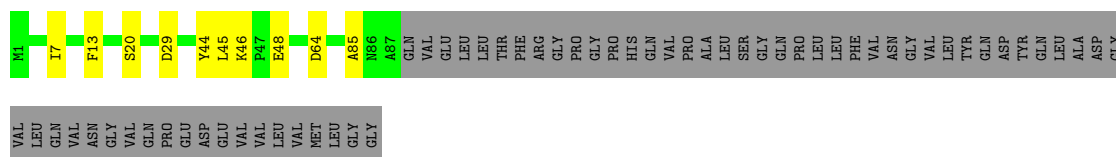


- Molecule 4: Collar (P74p112)

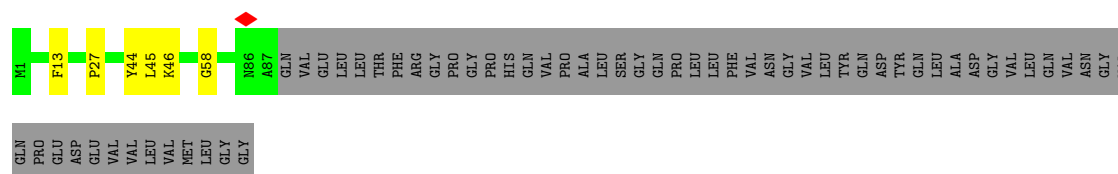


- Molecule 4: Collar (P74p112)





• Molecule 4: Collar (P74p112)



• Molecule 4: Collar (P74p112)



• Molecule 4: Collar (P74p112)



• Molecule 4: Collar (P74p112)



• Molecule 4: Collar (P74p112)



• Molecule 4: Collar (P74p112)

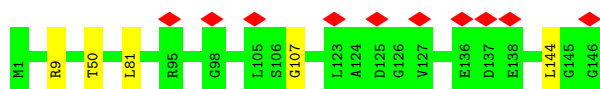




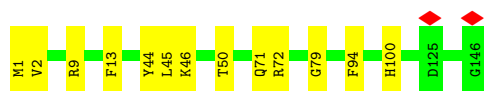
- Molecule 4: Collar (P74p112)



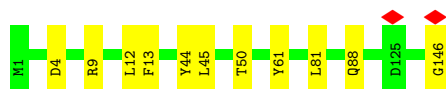
- Molecule 4: Collar (P74p112)



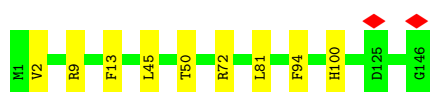
- Molecule 4: Collar (P74p112)



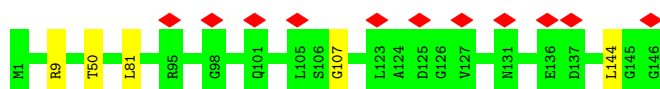
- Molecule 4: Collar (P74p112)



- Molecule 4: Collar (P74p112)

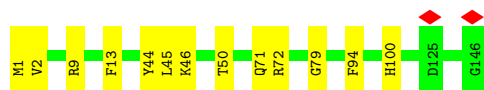


- Molecule 4: Collar (P74p112)



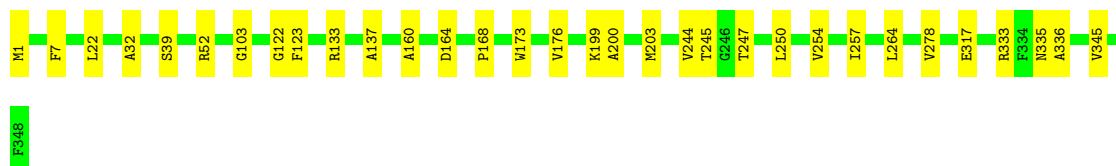
- Molecule 4: Collar (P74p112)

Chain Hl:  91% 9%



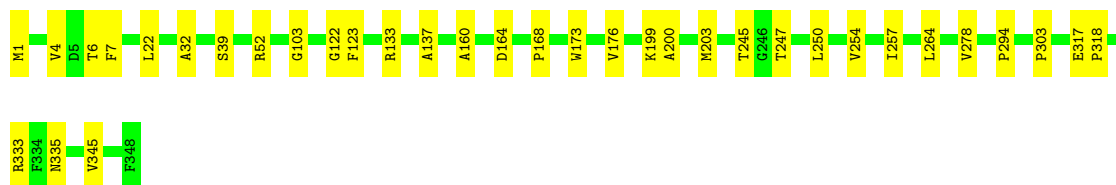
- Molecule 5: Tail Tube Protein gp93

Chain Ia:  91% 9%



- Molecule 5: Tail Tube Protein gp93

Chain Ib:  90% 10%



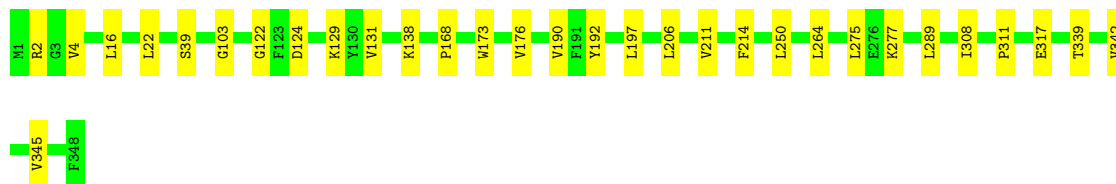
- Molecule 5: Tail Tube Protein gp93

Chain Ic:  90% 10%



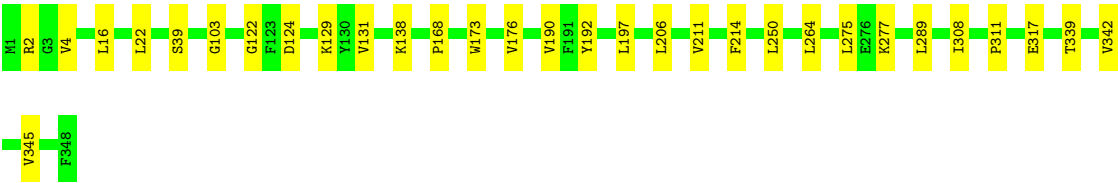
- Molecule 5: Tail Tube Protein gp93

Chain Id:  91% 9%

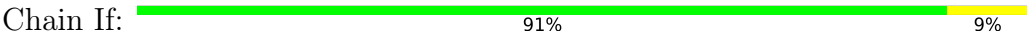


- Molecule 5: Tail Tube Protein gp93

Chain Ie:  91% 9%



• Molecule 5: Tail Tube Protein gp93



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	30748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.0571	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.024	Depositor
Minimum map value	-0.402	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	Da	0.14	0/3361	0.34	0/4567
1	Db	0.14	0/3361	0.34	0/4567
1	Dc	0.14	0/3361	0.34	0/4567
1	Dd	0.14	0/3361	0.34	0/4567
1	De	0.14	0/3361	0.34	0/4567
1	Df	0.14	0/3361	0.34	0/4567
1	Dg	0.14	0/3361	0.34	0/4567
1	Dh	0.14	0/3361	0.33	0/4567
1	Di	0.14	0/3361	0.33	0/4567
1	Dj	0.14	0/3361	0.33	0/4567
1	Dk	0.14	0/3361	0.33	0/4567
1	Dl	0.14	0/3361	0.34	0/4567
2	Ea	0.11	0/1050	0.28	0/1426
2	Eb	0.10	0/1050	0.24	0/1426
2	Ec	0.11	0/1050	0.28	0/1426
2	Ed	0.10	0/1050	0.24	0/1426
2	Ee	0.11	0/1050	0.28	0/1426
2	Ef	0.10	0/1050	0.24	0/1426
2	Eg	0.11	0/1050	0.28	0/1426
2	Uh	0.10	0/1050	0.25	0/1426
2	Ei	0.11	0/1050	0.28	0/1426
2	Ej	0.10	0/1050	0.24	0/1426
2	Ek	0.11	0/1050	0.27	0/1426
2	El	0.10	0/1050	0.25	0/1426
3	Fa	0.13	0/1279	0.32	0/1739
3	Fb	0.14	0/1279	0.32	0/1739
3	Fc	0.13	0/1279	0.32	0/1739
3	Fd	0.14	0/1279	0.31	0/1739
3	Fe	0.14	0/1279	0.32	0/1739
3	Ff	0.13	0/1279	0.30	0/1739
4	Ga	0.10	0/1168	0.30	0/1591
4	Gb	0.10	0/1168	0.28	0/1591
4	Gc	0.10	0/712	0.31	0/967
4	Gd	0.10	0/712	0.30	0/967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Ge	0.10	0/1168	0.30	0/1591
4	Gf	0.10	0/1168	0.29	0/1591
4	Gg	0.10	0/712	0.31	0/967
4	Gh	0.10	0/712	0.30	0/967
4	Gi	0.10	0/1168	0.30	0/1591
4	Gj	0.10	0/1168	0.29	0/1591
4	Gk	0.10	0/712	0.31	0/967
4	Gl	0.10	0/712	0.30	0/967
4	Ha	0.11	0/1168	0.32	0/1591
4	Hb	0.11	0/1168	0.33	0/1591
4	Hc	0.11	0/1168	0.31	0/1591
4	Hd	0.11	0/1168	0.34	0/1591
4	He	0.11	0/1168	0.32	0/1591
4	Hf	0.11	0/1168	0.33	0/1591
4	Hg	0.11	0/1168	0.31	0/1591
4	Hh	0.11	0/1168	0.34	0/1591
4	Hi	0.11	0/1168	0.32	0/1591
4	Hj	0.11	0/1168	0.33	0/1591
4	Hk	0.11	0/1168	0.32	0/1591
4	Hl	0.11	0/1168	0.34	0/1591
5	Ia	0.12	0/2737	0.32	0/3719
5	Ib	0.12	0/2737	0.32	0/3719
5	Ic	0.12	0/2737	0.32	0/3719
5	Id	0.10	0/2737	0.29	0/3719
5	Ie	0.10	0/2737	0.29	0/3719
5	If	0.10	0/2737	0.29	0/3719
All	All	0.12	0/102324	0.32	0/139104

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	Da	3287	0	3319	15	0
1	Db	3287	0	3319	17	0
1	Dc	3287	0	3319	16	0
1	Dd	3287	0	3319	21	0
1	De	3287	0	3319	13	0
1	Df	3287	0	3319	18	0
1	Dg	3287	0	3319	18	0
1	Dh	3287	0	3319	15	0
1	Di	3287	0	3319	18	0
1	Dj	3287	0	3319	20	0
1	Dk	3287	0	3319	15	0
1	Dl	3287	0	3319	18	0
2	Ea	1027	0	1017	7	0
2	Eb	1027	0	1017	3	0
2	Ec	1027	0	1017	7	0
2	Ed	1027	0	1017	5	0
2	Ee	1027	0	1017	7	0
2	Ef	1027	0	1017	4	0
2	Eg	1027	0	1017	8	0
2	Eh	1027	0	1017	4	0
2	Ei	1027	0	1017	7	0
2	Ej	1027	0	1017	4	0
2	Ek	1027	0	1017	8	0
2	El	1027	0	1017	5	0
3	Fa	1244	0	1200	12	0
3	Fb	1244	0	1200	15	0
3	Fc	1244	0	1200	13	0
3	Fd	1244	0	1200	15	0
3	Fe	1244	0	1200	13	0
3	Ff	1244	0	1200	16	0
4	Ga	1141	0	1140	6	0
4	Gb	1141	0	1140	5	0
4	Gc	695	0	696	5	0
4	Gd	695	0	696	3	0
4	Ge	1141	0	1140	6	0
4	Gf	1141	0	1140	5	0
4	Gg	695	0	696	5	0
4	Gh	695	0	696	3	0
4	Gi	1141	0	1140	7	0
4	Gj	1141	0	1140	5	0
4	Gk	695	0	696	6	0
4	Gl	695	0	696	3	0
4	Ha	1141	0	1140	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Hb	1141	0	1140	5	0
4	Hc	1141	0	1140	4	0
4	Hd	1141	0	1140	7	0
4	He	1141	0	1140	9	0
4	Hf	1141	0	1140	4	0
4	Hg	1141	0	1140	3	0
4	Hh	1141	0	1140	7	0
4	Hi	1141	0	1140	7	0
4	Hj	1141	0	1140	5	0
4	Hk	1141	0	1140	3	0
4	Hl	1141	0	1140	7	0
5	Ia	2679	0	2643	19	0
5	Ib	2679	0	2643	22	0
5	Ic	2679	0	2643	22	0
5	Id	2679	0	2643	19	0
5	Ie	2679	0	2643	19	0
5	If	2679	0	2643	19	0
All	All	100014	0	99786	521	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 3.

All (521) 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)
3:Fa:33:ILE:HG12	3:Fa:47:ALA:HB3	1.65	0.78
3:Fe:33:ILE:HG12	3:Fe:47:ALA:HB3	1.65	0.78
3:Fc:33:ILE:HG12	3:Fc:47:ALA:HB3	1.66	0.76
3:Fb:33:ILE:HG12	3:Fb:47:ALA:HB3	1.68	0.76
3:Ff:33:ILE:HG12	3:Ff:47:ALA:HB3	1.70	0.74
3:Fd:33:ILE:HG12	3:Fd:47:ALA:HB3	1.70	0.73
1:Dl:259:TRP:HZ2	2:El:119:ASP:HB2	1.56	0.70
1:Dj:259:TRP:HZ2	2:Ej:119:ASP:HB2	1.57	0.69
5:If:197:LEU:HB3	5:If:206:LEU:HB3	1.74	0.69
5:Id:197:LEU:HB3	5:Id:206:LEU:HB3	1.75	0.69
1:Df:259:TRP:HZ2	2:Ef:119:ASP:HB2	1.57	0.68
1:Db:259:TRP:HZ2	2:Eb:119:ASP:HB2	1.58	0.68
1:Dh:259:TRP:HZ2	2:Eh:119:ASP:HB2	1.58	0.68
5:Ie:197:LEU:HB3	5:Ie:206:LEU:HB3	1.76	0.68
1:Dd:259:TRP:HZ2	2:Ed:119:ASP:HB2	1.57	0.67
1:Da:259:TRP:HZ2	2:Ea:119:ASP:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dg:259:TRP:HZ2	2:Eg:119:ASP:HB2	1.60	0.67
1:Dc:259:TRP:HZ2	2:Ec:119:ASP:HB2	1.59	0.67
3:Fe:4:ASP:HB3	3:Fe:74:ILE:HD13	1.77	0.67
1:Di:259:TRP:HZ2	2:Ei:119:ASP:HB2	1.61	0.66
1:Dk:259:TRP:HZ2	2:Ek:119:ASP:HB2	1.61	0.66
3:Fd:4:ASP:HB3	3:Fd:74:ILE:HD13	1.78	0.65
3:Fa:4:ASP:HB3	3:Fa:74:ILE:HD13	1.78	0.65
4:Hh:9:ARG:HA	4:Hh:50:THR:HG22	1.79	0.65
3:Fc:4:ASP:HB3	3:Fc:74:ILE:HD13	1.79	0.64
3:Fb:4:ASP:HB3	3:Fb:74:ILE:HD13	1.79	0.64
3:Ff:4:ASP:HB3	3:Ff:74:ILE:HD13	1.77	0.64
4:Hi:9:ARG:HA	4:Hi:50:THR:HG22	1.80	0.64
1:De:259:TRP:HZ2	2:Ee:119:ASP:HB2	1.61	0.63
4:Hd:9:ARG:HA	4:Hd:50:THR:HG22	1.81	0.63
4:Hk:9:ARG:HA	4:Hk:50:THR:HG22	1.82	0.62
5:Ia:247:THR:HG22	5:Ia:333:ARG:HG2	1.80	0.62
4:Hc:9:ARG:HA	4:Hc:50:THR:HG22	1.81	0.62
5:Ic:247:THR:HG22	5:Ic:333:ARG:HG2	1.80	0.62
4:Hg:9:ARG:HA	4:Hg:50:THR:HG22	1.82	0.62
4:Hi:9:ARG:HA	4:Hi:50:THR:HG22	1.82	0.62
4:He:9:ARG:HA	4:He:50:THR:HG22	1.82	0.61
5:Ib:247:THR:HG22	5:Ib:333:ARG:HG2	1.81	0.61
5:Ib:39:SER:HB2	5:Ic:317:GLU:OE1	2.01	0.61
4:Ha:9:ARG:HA	4:Ha:50:THR:HG22	1.83	0.60
5:Ia:39:SER:HB2	5:Ib:317:GLU:OE1	2.00	0.60
5:Ia:317:GLU:OE1	5:Ic:39:SER:HB2	2.00	0.60
4:Hb:9:ARG:HA	4:Hb:50:THR:HG22	1.82	0.60
4:Hf:9:ARG:HA	4:Hf:50:THR:HG22	1.83	0.60
4:Hj:9:ARG:HA	4:Hj:50:THR:HG22	1.84	0.60
3:Fb:63:MET:HE3	5:Ia:32:ALA:HB2	1.85	0.59
3:Fd:63:MET:HE3	5:Ib:32:ALA:HB2	1.86	0.58
3:Ff:63:MET:HE3	5:Ic:32:ALA:HB2	1.85	0.57
2:Eg:87:GLN:HG3	3:Fd:135:PHE:HB3	1.87	0.55
3:Ff:80:ILE:HD11	3:Ff:101:VAL:HG11	1.89	0.55
4:Ge:48:GLU:HG2	4:Ge:85:ALA:HA	1.88	0.55
5:Ic:22:LEU:HD22	5:Ic:176:VAL:HG21	1.89	0.55
2:Ec:87:GLN:HG3	3:Fb:135:PHE:HB3	1.88	0.55
5:Ic:137:ALA:HA	5:Ic:160:ALA:HA	1.89	0.55
5:Ia:137:ALA:HA	5:Ia:160:ALA:HA	1.89	0.55
5:Ib:22:LEU:HD22	5:Ib:176:VAL:HG21	1.88	0.55
3:Fb:80:ILE:HD11	3:Fb:101:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ea:87:GLN:HG3	3:Fa:135:PHE:HB3	1.89	0.54
5:Ia:22:LEU:HD22	5:Ia:176:VAL:HG21	1.89	0.54
5:Ie:16:LEU:HD13	5:Ie:138:LYS:HE3	1.89	0.54
3:Fc:94:LEU:HD11	3:Fc:142:GLY:HA3	1.90	0.54
4:Gb:89:VAL:HG13	4:Gb:142:VAL:HG13	1.89	0.54
2:Ek:87:GLN:HG3	3:Ff:135:PHE:HB3	1.89	0.54
3:Fd:80:ILE:HD11	3:Fd:101:VAL:HG11	1.89	0.54
4:Ga:48:GLU:HG2	4:Ga:85:ALA:HA	1.88	0.54
4:Gj:89:VAL:HG13	4:Gj:142:VAL:HG13	1.89	0.54
5:Id:16:LEU:HD13	5:Id:138:LYS:HE3	1.90	0.54
2:EI:87:GLN:HG3	3:Fe:135:PHE:HB3	1.90	0.53
4:Gf:89:VAL:HG13	4:Gf:142:VAL:HG13	1.89	0.53
5:Id:264:LEU:HD12	5:Id:277:LYS:HE3	1.89	0.53
4:Hg:107:GLY:HA3	4:Hg:144:LEU:O	2.07	0.53
3:Fd:80:ILE:HB	3:Fd:144:VAL:HB	1.91	0.53
5:Ib:137:ALA:HA	5:Ib:160:ALA:HA	1.89	0.53
5:Ie:264:LEU:HD12	5:Ie:277:LYS:HE3	1.90	0.53
4:Gi:48:GLU:HG2	4:Gi:85:ALA:HA	1.89	0.52
4:Ga:89:VAL:HG13	4:Ga:142:VAL:HG13	1.92	0.52
4:Gi:89:VAL:HG13	4:Gi:142:VAL:HG13	1.91	0.52
5:If:16:LEU:HD13	5:If:138:LYS:HE3	1.91	0.52
3:Fb:80:ILE:HB	3:Fb:144:VAL:HB	1.92	0.52
5:If:264:LEU:HD12	5:If:277:LYS:HE3	1.91	0.52
2:Ee:87:GLN:HG3	3:Fc:135:PHE:HB3	1.90	0.52
4:Ge:89:VAL:HG13	4:Ge:142:VAL:HG13	1.91	0.52
2:Ej:38:ARG:HH12	4:Gi:29:ASP:HA	1.75	0.52
4:Gf:27:PRO:HD3	4:Gf:58:GLY:HA2	1.92	0.52
3:Fe:94:LEU:HD11	3:Fe:142:GLY:HA3	1.91	0.51
4:Gl:27:PRO:HD3	4:Gl:58:GLY:HA2	1.92	0.51
2:Ef:38:ARG:HH12	4:Ge:29:ASP:HA	1.75	0.51
2:Ed:38:ARG:HH12	4:Gc:29:ASP:HA	1.75	0.51
3:Fc:119:ASP:HB3	3:Fc:149:LYS:HB3	1.92	0.51
4:Hk:107:GLY:HA3	4:Hk:144:LEU:O	2.10	0.51
4:Gd:27:PRO:HD3	4:Gd:58:GLY:HA2	1.93	0.51
4:Gh:27:PRO:HD3	4:Gh:58:GLY:HA2	1.93	0.51
3:Fa:94:LEU:HD11	3:Fa:142:GLY:HA3	1.92	0.51
4:Gb:27:PRO:HD3	4:Gb:58:GLY:HA2	1.93	0.51
4:Gj:27:PRO:HD3	4:Gj:58:GLY:HA2	1.93	0.51
5:Id:22:LEU:HD22	5:Id:176:VAL:HG21	1.93	0.51
3:Fa:119:ASP:HB3	3:Fa:149:LYS:HB3	1.94	0.50
3:Fb:12:LYS:HD2	3:Fb:35:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ff:80:ILE:HB	3:Ff:144:VAL:HB	1.92	0.50
3:Fe:119:ASP:HB3	3:Fe:149:LYS:HB3	1.92	0.50
4:Hc:107:GLY:HA3	4:Hc:144:LEU:O	2.11	0.50
5:Ie:168:PRO:HA	5:Ie:173:TRP:CD1	2.47	0.50
3:Fb:4:ASP:HB3	3:Fb:74:ILE:HG21	1.94	0.50
4:Hh:2:VAL:HA	4:Hh:72:ARG:O	2.12	0.49
5:Ie:22:LEU:HD22	5:Ie:176:VAL:HG21	1.93	0.49
2:El:38:ARG:HH12	4:Gk:29:ASP:HA	1.77	0.49
5:If:22:LEU:HD22	5:If:176:VAL:HG21	1.95	0.49
4:Ha:59:HIS:HE1	4:Ha:61:TYR:CZ	2.30	0.49
4:Gi:107:GLY:HA3	4:Gi:144:LEU:O	2.12	0.49
5:Id:317:GLU:OE1	5:If:39:SER:HB2	2.13	0.49
2:Ee:15:PRO:HD2	2:Ee:18:VAL:HG21	1.95	0.49
2:Ei:9:GLU:HA	2:Ei:12:TYR:CD2	2.48	0.49
2:Ek:9:GLU:HA	2:Ek:12:TYR:CD2	2.48	0.49
3:Fa:68:LEU:HD23	5:Ia:257:ILE:HD12	1.95	0.49
3:Ff:12:LYS:HD2	3:Ff:35:VAL:HG23	1.95	0.49
4:Ga:107:GLY:HA3	4:Ga:144:LEU:O	2.12	0.48
4:Ge:107:GLY:HA3	4:Ge:144:LEU:O	2.12	0.48
5:If:168:PRO:HA	5:If:173:TRP:CD1	2.48	0.48
2:Ec:9:GLU:HA	2:Ec:12:TYR:CD2	2.48	0.48
5:Id:168:PRO:HA	5:Id:173:TRP:CD1	2.48	0.48
1:Dg:266:VAL:HG21	1:Dh:278:ILE:HG12	1.95	0.48
3:Fd:12:LYS:HD2	3:Fd:35:VAL:HG23	1.94	0.48
4:Ha:9:ARG:O	4:Ha:81:LEU:HB2	2.14	0.48
2:Eg:15:PRO:HD2	2:Eg:18:VAL:HG21	1.95	0.48
4:Ha:61:TYR:OH	4:Hl:79:GLY:HA2	2.14	0.48
4:He:9:ARG:O	4:He:81:LEU:HB2	2.13	0.48
5:Ia:133:ARG:HB3	5:Ia:164:ASP:OD1	2.13	0.48
2:Eb:38:ARG:HH12	4:Ga:29:ASP:HA	1.79	0.48
2:Ee:9:GLU:HA	2:Ee:12:TYR:CD2	2.49	0.48
2:Eg:9:GLU:HA	2:Eg:12:TYR:CD2	2.49	0.48
3:Fd:4:ASP:HB3	3:Fd:74:ILE:HG21	1.95	0.48
4:Hb:13:PHE:HB3	4:Hb:45:LEU:HB2	1.95	0.48
4:Hl:2:VAL:HA	4:Hl:72:ARG:O	2.12	0.48
5:Ic:133:ARG:HB3	5:Ic:164:ASP:OD1	2.13	0.48
4:Gj:92:LEU:HD12	4:Gj:105:LEU:HD11	1.95	0.48
5:Ib:133:ARG:HB3	5:Ib:164:ASP:OD1	2.13	0.48
5:Id:39:SER:HB2	5:Ie:317:GLU:OE1	2.13	0.48
5:Ie:39:SER:HB2	5:If:317:GLU:OE1	2.13	0.48
2:Ea:15:PRO:HD2	2:Ea:18:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: Ei:15: PRO: HD2	2: Ei:18: VAL: HG21	1.95	0.48
5: Id:2: ARG: HB2	5: Id:4: VAL: HG22	1.95	0.48
2: Ec:15: PRO: HD2	2: Ec:18: VAL: HG21	1.96	0.47
3: Fa:53: LYS: HG3	3: Fb:124: THR: HG22	1.95	0.47
4: Hd:2: VAL: HA	4: Hd:72: ARG: O	2.13	0.47
5: Ie:190: VAL: HG21	5: Ie:192: TYR: CZ	2.49	0.47
1: De:266: VAL: HG21	1: Df:278: ILE: HG12	1.96	0.47
4: Gi:92: LEU: HD12	4: Gi:105: LEU: HD11	1.96	0.47
5: Ib:52: ARG: HA	5: If:4: VAL: HB	1.96	0.47
5: If:190: VAL: HG21	5: If:192: TYR: CZ	2.50	0.47
2: Ea:9: GLU: HA	2: Ea:12: TYR: CD2	2.50	0.47
3: Fa:29: ARG: HD3	4: Ha:4: ASP: OD2	2.14	0.47
4: Gb:92: LEU: HD12	4: Gb:105: LEU: HD11	1.95	0.47
4: Hi:9: ARG: O	4: Hi:81: LEU: HB2	2.14	0.47
4: Hl:13: PHE: HB3	4: Hl:45: LEU: HB2	1.96	0.47
5: If:2: ARG: HB2	5: If:4: VAL: HG22	1.96	0.47
4: Gf:92: LEU: HD12	4: Gf:105: LEU: HD11	1.95	0.47
4: Hh:13: PHE: HB3	4: Hh:45: LEU: HB2	1.95	0.47
1: Dc:266: VAL: HG21	1: Dd:278: ILE: HG12	1.96	0.47
1: Di:266: VAL: HG21	1: Dj:278: ILE: HG12	1.96	0.47
1: Dj:279: LEU: HD11	1: Dj:285: PHE: HB2	1.97	0.47
4: Hd:13: PHE: HB3	4: Hd:45: LEU: HB2	1.96	0.47
5: Ic:1: MET: SD	5: Ic:123: PHE: HB3	2.55	0.47
5: Id:124: ASP: OD1	5: Id:129: LYS: HG2	2.15	0.47
5: Ie:124: ASP: OD1	5: Ie:129: LYS: HG2	2.14	0.47
1: Db:279: LEU: HD11	1: Db:285: PHE: HB2	1.96	0.47
1: Dc:237: GLU: OE2	2: Ec:126: ILE: HG22	2.15	0.47
3: Fc:29: ARG: HD3	4: He:4: ASP: OD2	2.14	0.47
4: Hf:13: PHE: HB3	4: Hf:45: LEU: HB2	1.96	0.47
5: Ia:168: PRO: HA	5: Ia:173: TRP: CD1	2.50	0.47
5: Id:190: VAL: HG21	5: Id:192: TYR: CZ	2.49	0.47
5: Ie:2: ARG: HB2	5: Ie:4: VAL: HG22	1.97	0.47
5: If:124: ASP: OD1	5: If:129: LYS: HG2	2.14	0.47
2: Ek:15: PRO: HD2	2: Ek:18: VAL: HG21	1.96	0.47
1: Da:237: GLU: OE2	2: Ea:126: ILE: HG22	2.15	0.47
1: Da:266: VAL: HG21	1: Db:278: ILE: HG12	1.95	0.47
3: Ff:94: LEU: HD11	3: Ff:142: GLY: HA3	1.97	0.47
1: Da:63: LEU: HD11	1: Da:130: ILE: HG21	1.96	0.46
1: Di:237: GLU: OE2	2: Ei:126: ILE: HG22	2.15	0.46
1: Dk:237: GLU: OE2	2: Ek:126: ILE: HG22	2.15	0.46
4: Hk:9: ARG: O	4: Hk:81: LEU: HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dg:237:GLU:OE2	2:Eg:126:ILE:HG22	2.16	0.46
4:Gh:13:PHE:HB3	4:Gh:45:LEU:HB2	1.96	0.46
3:Fc:53:LYS:HG3	3:Fd:124:THR:HG22	1.97	0.46
5:Ia:52:ARG:HA	5:Ie:4:VAL:HB	1.97	0.46
5:Ib:1:MET:SD	5:Ib:123:PHE:HB3	2.54	0.46
5:Ic:250:LEU:HD12	5:Ic:254:VAL:HG11	1.98	0.46
1:Dd:266:VAL:HG21	1:De:278:ILE:HG12	1.97	0.46
4:Gk:44:TYR:HE1	4:Gk:46:LYS:HG2	1.81	0.46
5:Ib:168:PRO:HA	5:Ib:173:TRP:CD1	2.51	0.46
3:Fc:109:ALA:HB1	3:Fc:118:THR:HG21	1.97	0.46
4:Gc:44:TYR:HE1	4:Gc:46:LYS:HG2	1.80	0.46
4:Hh:1:MET:HG3	4:Hh:71:GLN:HG3	1.97	0.46
1:Dh:266:VAL:HG21	1:Di:278:ILE:HG12	1.98	0.46
1:Di:63:LEU:HD11	1:Di:130:ILE:HG21	1.96	0.46
1:Dk:266:VAL:HG21	1:Di:278:ILE:HG12	1.97	0.46
3:Fa:109:ALA:HB1	3:Fa:118:THR:HG21	1.98	0.46
4:Ga:92:LEU:HD12	4:Ga:105:LEU:HD11	1.97	0.46
1:Dh:279:LEU:HD11	1:Dh:285:PHE:HB2	1.98	0.46
3:Fb:94:LEU:HD11	3:Fb:142:GLY:HA3	1.98	0.46
1:Dc:391:MET:HE2	1:Dc:423:LEU:HD22	1.98	0.46
4:Hi:1:MET:HG3	4:Hi:71:GLN:HG3	1.98	0.46
5:Ic:52:ARG:HA	5:Id:4:VAL:HB	1.97	0.46
1:Db:258:GLN:HG2	2:Ea:117:THR:OG1	2.16	0.46
1:De:391:MET:HE2	1:De:423:LEU:HD22	1.98	0.46
1:Dk:391:MET:HE2	1:Dk:423:LEU:HD22	1.98	0.46
4:Ge:92:LEU:HD12	4:Ge:105:LEU:HD11	1.97	0.46
1:Dd:279:LEU:HD11	1:Dd:285:PHE:HB2	1.98	0.45
1:De:237:GLU:OE2	2:Ee:126:ILE:HG22	2.16	0.45
3:Ff:4:ASP:HB3	3:Ff:74:ILE:HG21	1.97	0.45
1:Df:279:LEU:HD11	1:Df:285:PHE:HB2	1.98	0.45
4:Hg:9:ARG:O	4:Hg:81:LEU:HB2	2.16	0.45
5:Ic:168:PRO:HA	5:Ic:173:TRP:CD1	2.51	0.45
1:Df:266:VAL:HG21	1:Dg:278:ILE:HG12	1.98	0.45
4:Gg:44:TYR:HE1	4:Gg:46:LYS:HG2	1.82	0.45
4:He:13:PHE:HB3	4:He:45:LEU:HB2	1.98	0.45
4:Hj:13:PHE:HB3	4:Hj:45:LEU:HB2	1.97	0.45
3:Fe:53:LYS:HG3	3:Ff:124:THR:HG22	1.99	0.45
3:Fe:80:ILE:HD11	3:Fe:101:VAL:HG11	1.99	0.45
3:Fe:109:ALA:HB1	3:Fe:118:THR:HG21	1.98	0.45
4:Gj:48:GLU:HG2	4:Gj:85:ALA:HA	1.97	0.45
5:Ic:103:GLY:H	5:Ic:345:VAL:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:If:103:GLY:H	5:If:345:VAL:HG22	1.82	0.45
1:Df:86:VAL:HG23	1:Df:108:ILE:HG13	1.98	0.45
2:Ec:85:ALA:HB1	3:Fb:139:GLY:HA2	1.99	0.45
2:Ek:85:ALA:HB1	3:Ff:139:GLY:HA2	1.98	0.45
3:Fa:80:ILE:HD11	3:Fa:101:VAL:HG11	1.98	0.45
3:Fc:115:VAL:HG13	3:Fc:150:VAL:HG13	1.98	0.45
4:Gb:48:GLU:HG2	4:Gb:85:ALA:HA	1.97	0.45
4:Hd:44:TYR:HE2	4:Hd:46:LYS:HG2	1.81	0.45
5:Ie:214:PHE:CE1	5:Ie:289:LEU:HD13	2.52	0.45
5:If:122:GLY:HA2	5:If:131:VAL:HA	1.98	0.45
1:Df:258:GLN:HG2	2:Ee:117:THR:OG1	2.17	0.45
3:Fa:115:VAL:HG13	3:Fa:150:VAL:HG13	1.97	0.45
4:Hh:44:TYR:HE2	4:Hh:46:LYS:HG2	1.82	0.45
5:Id:122:GLY:HA2	5:Id:131:VAL:HA	1.98	0.45
1:Dg:391:MET:HE2	1:Dg:423:LEU:HD22	1.98	0.45
1:Dh:258:GLN:HG2	2:Eg:117:THR:OG1	2.16	0.45
1:Di:279:LEU:HD11	1:Di:285:PHE:HB2	1.99	0.45
3:Fd:105:LEU:O	3:Fd:109:ALA:HB2	2.17	0.45
4:Gd:13:PHE:HB3	4:Gd:45:LEU:HB2	1.98	0.45
5:Ia:1:MET:SD	5:Ia:123:PHE:HB3	2.57	0.45
5:Ib:250:LEU:HD12	5:Ib:254:VAL:HG11	1.99	0.45
5:Id:211:VAL:HG12	5:Id:250:LEU:HB3	1.99	0.45
4:Ga:13:PHE:HB3	4:Ga:45:LEU:HB2	1.99	0.45
4:Hi:13:PHE:HB3	4:Hi:45:LEU:HB2	1.99	0.45
4:Hi:44:TYR:HE2	4:Hi:46:LYS:HG2	1.81	0.45
5:Ia:103:GLY:H	5:Ia:345:VAL:HG22	1.82	0.45
1:Db:266:VAL:HG21	1:Dc:278:ILE:HG12	1.98	0.44
1:Dk:279:LEU:HD11	1:Dk:285:PHE:HB2	1.99	0.44
5:Ie:122:GLY:HA2	5:Ie:131:VAL:HA	1.98	0.44
1:Da:279:LEU:HD11	1:Da:285:PHE:HB2	1.99	0.44
1:Di:199:VAL:HG13	1:Di:355:TYR:HB2	1.99	0.44
4:Gk:20:SER:H	4:Gk:64:ASP:HA	1.82	0.44
4:Hc:9:ARG:O	4:Hc:81:LEU:HB2	2.17	0.44
5:Ie:103:GLY:HA3	5:Ie:345:VAL:HG22	2.00	0.44
1:Da:391:MET:HE2	1:Da:423:LEU:HD22	1.99	0.44
1:Df:63:LEU:HD11	1:Df:130:ILE:HG21	1.97	0.44
3:Fe:4:ASP:HB3	3:Fe:74:ILE:HG21	1.99	0.44
3:Fe:68:LEU:HD23	5:Ic:257:ILE:HD12	1.98	0.44
3:Fe:115:VAL:HG13	3:Fe:150:VAL:HG13	1.99	0.44
4:Gl:13:PHE:HB3	4:Gl:45:LEU:HB2	1.98	0.44
5:Id:214:PHE:CE1	5:Id:289:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dd:215:LEU:O	1:Dd:219:VAL:HG23	2.17	0.44
1:De:215:LEU:O	1:De:219:VAL:HG23	2.17	0.44
1:Dj:266:VAL:HG21	1:Dk:278:ILE:HG12	1.98	0.44
2:Eh:38:ARG:HH12	4:Gg:29:ASP:HA	1.82	0.44
3:Fe:29:ARG:HD3	4:Hi:4:ASP:OD2	2.17	0.44
3:Ff:105:LEU:O	3:Ff:109:ALA:HB2	2.18	0.44
4:Ha:13:PHE:HB3	4:Ha:45:LEU:HB2	1.99	0.44
5:Ib:103:GLY:H	5:Ib:345:VAL:HG22	1.82	0.44
1:Di:215:LEU:O	1:Di:219:VAL:HG23	2.17	0.44
3:Ff:119:ASP:HB3	3:Ff:149:LYS:HB3	1.99	0.44
5:Id:250:LEU:HD11	5:Id:275:LEU:HD11	2.00	0.44
5:If:214:PHE:CE1	5:If:289:LEU:HD13	2.52	0.44
1:De:279:LEU:HD11	1:De:285:PHE:HB2	1.99	0.44
1:Dg:279:LEU:HD11	1:Dg:285:PHE:HB2	1.99	0.44
1:Dh:199:VAL:HG13	1:Dh:355:TYR:HB2	1.99	0.44
1:Di:199:VAL:HG13	1:Di:355:TYR:HB2	2.00	0.44
5:Ic:199:LYS:HA	5:Ic:203:MET:HE2	1.99	0.44
5:Id:103:GLY:HA3	5:Id:345:VAL:HG22	2.00	0.44
3:Fc:80:ILE:HD11	3:Fc:101:VAL:HG11	1.99	0.44
3:Fd:94:LEU:HD11	3:Fd:142:GLY:HA3	2.00	0.44
1:Dd:391:MET:HE2	1:Dd:423:LEU:HD22	2.00	0.44
1:Df:215:LEU:O	1:Df:219:VAL:HG23	2.18	0.44
2:Eg:85:ALA:HB1	3:Fd:139:GLY:HA2	1.98	0.44
4:Hd:1:MET:HG3	4:Hd:71:GLN:HG3	1.99	0.44
1:Db:86:VAL:HG23	1:Db:108:ILE:HG13	2.00	0.44
1:Dg:215:LEU:O	1:Dg:219:VAL:HG23	2.18	0.44
1:Dh:215:LEU:O	1:Dh:219:VAL:HG23	2.17	0.44
3:Fa:4:ASP:HB3	3:Fa:74:ILE:HG21	2.00	0.44
5:Ia:250:LEU:HD12	5:Ia:254:VAL:HG11	2.00	0.44
1:Dj:391:MET:HA	1:Dj:394:LEU:HD12	2.00	0.43
1:Di:215:LEU:O	1:Di:219:VAL:HG23	2.17	0.43
4:Ge:13:PHE:HB3	4:Ge:45:LEU:HB2	1.99	0.43
5:Id:103:GLY:H	5:Id:345:VAL:HG22	1.83	0.43
1:Dh:391:MET:HE2	1:Dh:423:LEU:HD22	2.00	0.43
4:Hd:94:PHE:HB3	4:Hd:100:HIS:CD2	2.53	0.43
5:Ia:200:ALA:O	5:Ia:203:MET:HG3	2.19	0.43
5:Ie:250:LEU:HD11	5:Ie:275:LEU:HD11	2.00	0.43
1:Da:278:ILE:HG12	1:Di:266:VAL:HG21	1.98	0.43
1:Dd:258:GLN:HG2	2:Ec:117:THR:OG1	2.19	0.43
1:Di:391:MET:HE2	1:Di:423:LEU:HD22	1.99	0.43
5:If:211:VAL:HG12	5:If:250:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:If:250:LEU:HD11	5:If:275:LEU:HD11	2.00	0.43
1:De:355:TYR:O	1:De:359:LYS:HG2	2.19	0.43
1:Di:279:LEU:HD11	1:Di:285:PHE:HB2	2.00	0.43
1:Dk:215:LEU:O	1:Dk:219:VAL:HG23	2.18	0.43
1:Dl:258:GLN:HG2	2:Ek:117:THR:OG1	2.18	0.43
1:Dc:411:LEU:O	1:Dc:415:LEU:HG	2.19	0.43
1:Dj:62:MET:SD	1:Dj:219:VAL:HG22	2.59	0.43
1:Dk:411:LEU:O	1:Dk:415:LEU:HG	2.19	0.43
4:Gg:7:ILE:HG12	4:Gg:13:PHE:CD1	2.54	0.43
1:Da:215:LEU:O	1:Da:219:VAL:HG23	2.18	0.43
1:Db:215:LEU:O	1:Db:219:VAL:HG23	2.18	0.43
1:Dj:63:LEU:HD11	1:Dj:130:ILE:HG21	2.01	0.43
4:Hb:2:VAL:HA	4:Hb:72:ARG:O	2.19	0.43
1:Db:199:VAL:HG13	1:Db:355:TYR:HB2	2.00	0.43
3:Fb:105:LEU:O	3:Fb:109:ALA:HB2	2.17	0.43
3:Fc:68:LEU:HD23	5:Ib:257:ILE:HD12	2.01	0.43
4:Gf:20:SER:H	4:Gf:64:ASP:HA	1.84	0.43
4:Hj:2:VAL:HA	4:Hj:72:ARG:O	2.18	0.43
5:Ib:199:LYS:HA	5:Ib:203:MET:HE2	1.99	0.43
5:Ib:200:ALA:O	5:Ib:203:MET:HG3	2.18	0.43
1:Da:355:TYR:O	1:Da:359:LYS:HG2	2.19	0.43
1:Dc:215:LEU:O	1:Dc:219:VAL:HG23	2.18	0.43
1:Dd:62:MET:SD	1:Dd:219:VAL:HG22	2.59	0.43
1:Dg:86:VAL:HG23	1:Dg:108:ILE:HG13	2.01	0.43
1:Dl:63:LEU:HD11	1:Dl:130:ILE:HG21	1.99	0.43
3:Fb:16:GLU:HG3	3:Fb:33:ILE:HD12	2.01	0.43
4:Gj:20:SER:H	4:Gj:64:ASP:HA	1.84	0.43
1:Dj:394:LEU:HD21	1:Dj:415:LEU:HD11	2.00	0.43
2:Ea:14:MET:HE1	2:Ea:79:ILE:HB	2.01	0.43
1:Dd:391:MET:HA	1:Dd:394:LEU:HD12	2.01	0.43
4:Gi:13:PHE:HB3	4:Gi:45:LEU:HB2	2.01	0.43
5:Ic:200:ALA:O	5:Ic:203:MET:HG3	2.19	0.43
5:Ie:103:GLY:H	5:Ie:345:VAL:HG22	1.83	0.43
1:Db:62:MET:SD	1:Db:219:VAL:HG22	2.59	0.42
1:Dc:86:VAL:HG23	1:Dc:108:ILE:HG13	2.00	0.42
1:Dj:215:LEU:O	1:Dj:219:VAL:HG23	2.18	0.42
1:Dl:391:MET:HE2	1:Dl:423:LEU:HD22	2.01	0.42
4:Hh:94:PHE:HB3	4:Hh:100:HIS:CD2	2.53	0.42
5:Ie:211:VAL:HG12	5:Ie:250:LEU:HB3	2.00	0.42
5:Ie:308:ILE:HG12	5:Ie:342:VAL:HG22	2.01	0.42
1:Dc:279:LEU:HD11	1:Dc:285:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dj:199:VAL:HG13	1:Dj:355:TYR:HB2	2.01	0.42
1:Dj:258:GLN:HG2	2:Et:117:THR:OG1	2.18	0.42
4:Gk:7:ILE:HG12	4:Gk:13:PHE:CD1	2.53	0.42
5:If:103:GLY:HA3	5:If:345:VAL:HG22	2.01	0.42
1:Da:199:VAL:HG13	1:Da:355:TYR:HB2	2.01	0.42
1:Df:62:MET:SD	1:Df:219:VAL:HG22	2.59	0.42
1:Df:199:VAL:HG13	1:Df:355:TYR:HB2	2.00	0.42
1:Dl:76:PHE:CG	1:Dl:126:GLU:HG2	2.55	0.42
2:Ej:15:PRO:HG2	2:Ej:18:VAL:HG23	2.01	0.42
2:Ek:14:MET:HE1	2:Ek:79:ILE:HB	2.01	0.42
4:Gf:48:GLU:HG2	4:Gf:85:ALA:HA	2.00	0.42
3:Fd:62:GLY:HA2	5:Ib:6:THR:O	2.20	0.42
4:Hi:12:LEU:HD11	4:Hi:44:TYR:CZ	2.55	0.42
5:Ib:264:LEU:HD21	5:Ib:278:VAL:HG22	2.01	0.42
1:Dc:394:LEU:O	1:Dc:398:VAL:HG22	2.20	0.42
1:Dg:411:LEU:O	1:Dg:415:LEU:HG	2.19	0.42
2:Ef:15:PRO:HG2	2:Ef:18:VAL:HG23	2.01	0.42
4:Hl:94:PHE:HB3	4:Hl:100:HIS:CD2	2.54	0.42
1:Dj:86:VAL:HG23	1:Dj:108:ILE:HG13	2.01	0.42
1:Dk:340:THR:O	1:Dk:344:LEU:HG	2.20	0.42
4:Gc:20:SER:H	4:Gc:64:ASP:HA	1.84	0.42
4:Hb:9:ARG:O	4:Hb:81:LEU:HB2	2.20	0.42
5:If:308:ILE:HG12	5:If:342:VAL:HG22	2.01	0.42
1:Dd:199:VAL:HG13	1:Dd:355:TYR:HB2	2.00	0.42
1:De:63:LEU:HD11	1:De:130:ILE:HG21	2.01	0.42
1:De:199:VAL:HG13	1:De:355:TYR:HB2	2.00	0.42
1:Df:391:MET:HA	1:Df:394:LEU:HD12	2.02	0.42
1:Dk:199:VAL:HG13	1:Dk:355:TYR:HB2	2.02	0.42
1:Dl:62:MET:SD	1:Dl:219:VAL:HG22	2.60	0.42
3:Fc:37:TYR:CD1	3:Fd:128:VAL:HG11	2.55	0.42
4:Gb:20:SER:H	4:Gb:64:ASP:HA	1.84	0.42
4:Gc:7:ILE:HG12	4:Gc:13:PHE:CD1	2.54	0.42
4:Gg:13:PHE:HB3	4:Gg:45:LEU:HB2	2.01	0.42
5:Ic:245:THR:HG22	5:Ic:335:ASN:OD1	2.20	0.42
1:Dd:63:LEU:HD11	1:Dd:130:ILE:HG21	2.01	0.42
1:De:411:LEU:O	1:De:415:LEU:HG	2.20	0.42
2:Eh:52:LEU:HD13	2:Eh:62:TRP:CD1	2.55	0.42
1:Dg:394:LEU:O	1:Dg:398:VAL:HG22	2.20	0.42
1:Di:411:LEU:O	1:Di:415:LEU:HG	2.20	0.42
1:Dl:411:LEU:O	1:Dl:415:LEU:HG	2.20	0.42
2:Eg:14:MET:HE1	2:Eg:79:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Hd:79:GLY:HA2	4:He:61:TYR:OH	2.20	0.42
5:Ia:199:LYS:HA	5:Ia:203:MET:HE2	2.00	0.42
5:Ia:264:LEU:HD21	5:Ia:278:VAL:HG22	2.01	0.42
1:Da:62:MET:SD	1:Da:219:VAL:HG22	2.60	0.42
1:Dh:62:MET:SD	1:Dh:219:VAL:HG22	2.60	0.42
1:Dh:340:THR:O	1:Dh:344:LEU:HG	2.20	0.42
1:Dl:306:ALA:O	1:Dl:310:ARG:HG3	2.20	0.42
2:Eb:52:LEU:HD13	2:Eb:62:TRP:CD1	2.55	0.42
2:El:52:LEU:HD13	2:El:62:TRP:CD1	2.55	0.42
4:Gg:20:SER:H	4:Gg:64:ASP:HA	1.84	0.42
1:Dc:76:PHE:CG	1:Dc:126:GLU:HG2	2.55	0.41
1:Dd:306:ALA:O	1:Dd:310:ARG:HG3	2.20	0.41
1:Dk:394:LEU:O	1:Dk:398:VAL:HG22	2.20	0.41
1:Dl:427:ASP:HB3	1:Dl:430:ARG:HB3	2.02	0.41
4:Hj:9:ARG:O	4:Hj:81:LEU:HB2	2.20	0.41
1:Da:411:LEU:O	1:Da:415:LEU:HG	2.20	0.41
1:Db:340:THR:O	1:Db:344:LEU:HG	2.21	0.41
1:Db:391:MET:HE2	1:Db:423:LEU:HD22	2.02	0.41
3:Fe:60:ARG:HD3	5:Ic:210:PRO:HB2	2.01	0.41
4:He:59:HIS:HE1	4:He:61:TYR:CZ	2.38	0.41
4:Hh:79:GLY:HA2	4:Hi:61:TYR:OH	2.19	0.41
1:Dc:199:VAL:HG13	1:Dc:355:TYR:HB2	2.01	0.41
1:Dd:411:LEU:O	1:Dd:415:LEU:HG	2.20	0.41
1:De:340:THR:O	1:De:344:LEU:HG	2.20	0.41
1:Df:76:PHE:CG	1:Df:126:GLU:HG2	2.55	0.41
1:Df:306:ALA:O	1:Df:310:ARG:HG3	2.20	0.41
2:Ef:52:LEU:HD13	2:Ef:62:TRP:CD1	2.56	0.41
4:Hi:88:GLN:HG3	4:Hi:146:GLY:HA3	2.02	0.41
1:Dd:340:THR:O	1:Dd:344:LEU:HG	2.20	0.41
1:Dh:394:LEU:O	1:Dh:398:VAL:HG22	2.21	0.41
1:Di:427:ASP:HB3	1:Di:430:ARG:HB3	2.02	0.41
1:Dj:391:MET:HE2	1:Dj:423:LEU:HD22	2.01	0.41
4:Ha:12:LEU:HD11	4:Ha:44:TYR:CZ	2.55	0.41
5:Ib:317:GLU:HA	5:Ib:318:PRO:HD3	1.94	0.41
1:Db:306:ALA:O	1:Db:310:ARG:HG3	2.21	0.41
1:Db:394:LEU:HD21	1:Db:415:LEU:HD11	2.03	0.41
1:Dd:76:PHE:CG	1:Dd:126:GLU:HG2	2.55	0.41
1:Dj:254:GLN:HG2	1:Dj:259:TRP:CE2	2.56	0.41
1:Dj:306:ALA:O	1:Dj:310:ARG:HG3	2.20	0.41
4:He:12:LEU:HD11	4:He:44:TYR:CZ	2.56	0.41
4:He:90:GLU:HB2	4:He:143:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:If:311:PRO:HD2	5:If:339:THR:O	2.20	0.41
1:Dd:394:LEU:O	1:Dd:398:VAL:HG22	2.21	0.41
1:Df:394:LEU:O	1:Df:398:VAL:HG22	2.21	0.41
1:Dg:62:MET:SD	1:Dg:219:VAL:HG22	2.61	0.41
1:Dg:355:TYR:O	1:Dg:359:LYS:HG2	2.21	0.41
1:Dj:411:LEU:O	1:Dj:415:LEU:HG	2.20	0.41
2:El:15:PRO:HG2	2:El:18:VAL:HG23	2.02	0.41
1:Da:340:THR:O	1:Da:344:LEU:HG	2.21	0.41
1:Db:394:LEU:O	1:Db:398:VAL:HG22	2.21	0.41
1:Dd:394:LEU:HD21	1:Dd:415:LEU:HD11	2.03	0.41
2:Ed:84:ARG:HD3	3:Fb:138:TRP:CG	2.56	0.41
3:Ff:62:GLY:HA2	5:Ic:6:THR:O	2.20	0.41
5:Ib:7:PHE:CE2	5:Ib:122:GLY:HA3	2.56	0.41
5:Ie:311:PRO:HD2	5:Ie:339:THR:O	2.21	0.41
1:Da:306:ALA:O	1:Da:310:ARG:HG3	2.21	0.41
1:Db:411:LEU:O	1:Db:415:LEU:HG	2.20	0.41
1:Dc:63:LEU:HD11	1:Dc:130:ILE:HG21	2.02	0.41
1:Dc:306:ALA:O	1:Dc:310:ARG:HG3	2.21	0.41
1:Dd:86:VAL:HG23	1:Dd:108:ILE:HG13	2.03	0.41
1:Dh:306:ALA:O	1:Dh:310:ARG:HG3	2.21	0.41
1:Dh:411:LEU:O	1:Dh:415:LEU:HG	2.20	0.41
1:Dj:340:THR:O	1:Dj:344:LEU:HG	2.21	0.41
2:Ed:52:LEU:HD13	2:Ed:62:TRP:CD1	2.56	0.41
4:Hf:2:VAL:HA	4:Hf:72:ARG:O	2.20	0.41
5:Id:308:ILE:HG12	5:Id:342:VAL:HG22	2.02	0.41
1:Da:391:MET:HA	1:Da:394:LEU:HD12	2.03	0.41
1:Db:355:TYR:O	1:Db:359:LYS:HG2	2.21	0.41
1:Db:391:MET:HA	1:Db:394:LEU:HD12	2.02	0.41
1:Df:391:MET:HE2	1:Df:423:LEU:HD22	2.03	0.41
1:Df:427:ASP:HB3	1:Df:430:ARG:HB3	2.03	0.41
1:Dg:306:ALA:O	1:Dg:310:ARG:HG3	2.20	0.41
1:Dg:394:LEU:HD21	1:Dg:415:LEU:HD11	2.03	0.41
1:Di:62:MET:SD	1:Di:219:VAL:HG22	2.61	0.41
1:Di:394:LEU:O	1:Di:398:VAL:HG22	2.21	0.41
1:Dj:355:TYR:O	1:Dj:359:LYS:HG2	2.21	0.41
1:Dk:86:VAL:HG23	1:Dk:108:ILE:HG13	2.02	0.41
1:Dk:427:ASP:HB3	1:Dk:430:ARG:HB3	2.03	0.41
1:Dl:340:THR:O	1:Dl:344:LEU:HG	2.21	0.41
2:Ed:15:PRO:HG2	2:Ed:18:VAL:HG23	2.03	0.41
2:Ei:14:MET:HE1	2:Ei:79:ILE:HB	2.03	0.41
2:El:84:ARG:HD3	3:Ff:138:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Fb:155:GLN:HG3	3:Fc:99:TRP:HH2	1.86	0.41
4:He:88:GLN:HG3	4:He:146:GLY:HA3	2.03	0.41
1:Dc:427:ASP:HB3	1:Dc:430:ARG:HB3	2.03	0.41
1:Dd:232:ILE:HG23	1:Dd:294:MET:SD	2.61	0.41
1:Dd:355:TYR:O	1:Dd:359:LYS:HG2	2.21	0.41
1:Dd:427:ASP:HB3	1:Dd:430:ARG:HB3	2.03	0.41
1:Df:411:LEU:O	1:Df:415:LEU:HG	2.20	0.41
1:Dg:340:THR:O	1:Dg:344:LEU:HG	2.20	0.41
1:Dh:76:PHE:CG	1:Dh:126:GLU:HG2	2.56	0.41
1:Di:355:TYR:O	1:Di:359:LYS:HG2	2.20	0.41
1:Dj:394:LEU:O	1:Dj:398:VAL:HG22	2.21	0.41
1:Dk:355:TYR:O	1:Dk:359:LYS:HG2	2.20	0.41
2:Ee:14:MET:HE1	2:Ee:79:ILE:HB	2.02	0.41
4:Hf:9:ARG:O	4:Hf:81:LEU:HB2	2.21	0.41
5:Ia:244:VAL:HB	5:Ia:336:ALA:HB3	2.03	0.41
5:Ib:245:THR:HG22	5:Ib:335:ASN:OD1	2.21	0.41
5:Ic:57:GLN:HB2	5:Ic:60:TYR:CD2	2.56	0.41
5:Ic:264:LEU:HD21	5:Ic:278:VAL:HG22	2.01	0.41
1:Di:76:PHE:CG	1:Di:126:GLU:HG2	2.56	0.40
1:Dl:391:MET:HA	1:Dl:394:LEU:HD12	2.03	0.40
1:Dl:394:LEU:O	1:Dl:398:VAL:HG22	2.20	0.40
4:Gk:48:GLU:HG2	4:Gk:85:ALA:HA	2.03	0.40
4:Gl:44:TYR:HE1	4:Gl:46:LYS:HG2	1.87	0.40
5:Ic:244:VAL:HB	5:Ic:336:ALA:HB3	2.02	0.40
1:Dg:76:PHE:CG	1:Dg:126:GLU:HG2	2.56	0.40
2:Ej:52:LEU:HD13	2:Ej:62:TRP:CD1	2.56	0.40
3:Ff:129:THR:HB	3:Ff:141:TYR:H	1.87	0.40
4:Gc:13:PHE:HB3	4:Gc:45:LEU:HB2	2.03	0.40
4:Gi:91:LEU:HD12	4:Gi:142:VAL:HG22	2.03	0.40
4:Hb:94:PHE:HB3	4:Hb:100:HIS:CD2	2.56	0.40
5:Ia:245:THR:HG22	5:Ia:335:ASN:OD1	2.21	0.40
1:Dc:340:THR:O	1:Dc:344:LEU:HG	2.21	0.40
1:Df:394:LEU:HD21	1:Df:415:LEU:HD11	2.03	0.40
1:Dg:427:ASP:HB3	1:Dg:430:ARG:HB3	2.03	0.40
1:Dj:51:GLN:HB3	1:Dj:52:GLY:H	1.74	0.40
1:Dk:76:PHE:CG	1:Dk:126:GLU:HG2	2.57	0.40
1:Dl:86:VAL:HG23	1:Dl:108:ILE:HG13	2.02	0.40
5:Ib:294:PRO:HA	5:Ib:303:PRO:HB3	2.03	0.40
5:Id:311:PRO:HD2	5:Id:339:THR:O	2.21	0.40
1:Dg:391:MET:HA	1:Dg:394:LEU:HD12	2.04	0.40
4:Gd:44:TYR:HE1	4:Gd:46:LYS:HG2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Gh:44:TYR:HE1	4:Gh:46:LYS:HG2	1.87	0.40
4:Gk:13:PHE:HB3	4:Gk:45:LEU:HB2	2.02	0.40
4:Hj:94:PHE:HB3	4:Hj:100:HIS:CD2	2.57	0.40
1:De:62:MET:SD	1:De:219:VAL:HG22	2.61	0.40
1:Dh:86:VAL:HG23	1:Dh:108:ILE:HG13	2.04	0.40
1:Di:86:VAL:HG23	1:Di:108:ILE:HG13	2.03	0.40
1:Di:306:ALA:O	1:Di:310:ARG:HG3	2.21	0.40
1:Di:340:THR:O	1:Di:344:LEU:HG	2.22	0.40
2:Eh:15:PRO:HG2	2:Eh:18:VAL:HG23	2.04	0.40
3:Fd:64:GLY:HA2	5:Ib:4:VAL:O	2.22	0.40
4:Hc:44:TYR:HE1	4:Hc:46:LYS:HG2	1.87	0.40
5:Ia:7:PHE:CE2	5:Ia:122:GLY:HA3	2.56	0.40
5:Ic:7:PHE:CE2	5:Ic:122:GLY:HA3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Da	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Db	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dc	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dd	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	De	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Df	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dg	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dh	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Di	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dj	421/448 (94%)	417 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Dk	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
1	Dl	421/448 (94%)	417 (99%)	4 (1%)	0	100	100
2	Ea	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	Eb	128/130 (98%)	128 (100%)	0	0	100	100
2	Ec	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	Ed	128/130 (98%)	128 (100%)	0	0	100	100
2	Ee	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	Ef	128/130 (98%)	128 (100%)	0	0	100	100
2	Eg	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	Eh	128/130 (98%)	128 (100%)	0	0	100	100
2	Ei	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	Ej	128/130 (98%)	128 (100%)	0	0	100	100
2	Ek	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
2	El	128/130 (98%)	128 (100%)	0	0	100	100
3	Fa	153/155 (99%)	153 (100%)	0	0	100	100
3	Fb	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
3	Fc	153/155 (99%)	153 (100%)	0	0	100	100
3	Fd	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
3	Fe	153/155 (99%)	153 (100%)	0	0	100	100
3	Ff	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
4	Ga	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gb	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gc	85/146 (58%)	85 (100%)	0	0	100	100
4	Gd	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
4	Ge	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gf	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gg	85/146 (58%)	85 (100%)	0	0	100	100
4	Gh	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
4	Gi	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gj	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
4	Gk	85/146 (58%)	85 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Gl	85/146 (58%)	84 (99%)	1 (1%)	0	100	100
4	Ha	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
4	Hb	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hc	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hd	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	He	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
4	Hf	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hg	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hh	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hi	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
4	Hj	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hk	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
4	Hl	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
5	Ia	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	Ib	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	Ic	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
5	Id	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
5	Ie	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
5	If	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
All	All	12684/13458 (94%)	12527 (99%)	157 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	Da	352/374 (94%)	352 (100%)	0	100	100
1	Db	352/374 (94%)	352 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Dc	352/374 (94%)	352 (100%)	0	100	100
1	Dd	352/374 (94%)	352 (100%)	0	100	100
1	De	352/374 (94%)	352 (100%)	0	100	100
1	Df	352/374 (94%)	352 (100%)	0	100	100
1	Dg	352/374 (94%)	352 (100%)	0	100	100
1	Dh	352/374 (94%)	352 (100%)	0	100	100
1	Di	352/374 (94%)	352 (100%)	0	100	100
1	Dj	352/374 (94%)	352 (100%)	0	100	100
1	Dk	352/374 (94%)	352 (100%)	0	100	100
1	Dl	352/374 (94%)	352 (100%)	0	100	100
2	Ea	105/105 (100%)	105 (100%)	0	100	100
2	Eb	105/105 (100%)	105 (100%)	0	100	100
2	Ec	105/105 (100%)	105 (100%)	0	100	100
2	Ed	105/105 (100%)	105 (100%)	0	100	100
2	Ee	105/105 (100%)	105 (100%)	0	100	100
2	Ef	105/105 (100%)	105 (100%)	0	100	100
2	Eg	105/105 (100%)	105 (100%)	0	100	100
2	Uh	105/105 (100%)	105 (100%)	0	100	100
2	Ei	105/105 (100%)	105 (100%)	0	100	100
2	Ej	105/105 (100%)	105 (100%)	0	100	100
2	Ek	105/105 (100%)	105 (100%)	0	100	100
2	El	105/105 (100%)	105 (100%)	0	100	100
3	Fa	129/129 (100%)	129 (100%)	0	100	100
3	Fb	129/129 (100%)	129 (100%)	0	100	100
3	Fc	129/129 (100%)	129 (100%)	0	100	100
3	Fd	129/129 (100%)	129 (100%)	0	100	100
3	Fe	129/129 (100%)	129 (100%)	0	100	100
3	Ff	129/129 (100%)	129 (100%)	0	100	100
4	Ga	124/124 (100%)	124 (100%)	0	100	100
4	Gb	124/124 (100%)	124 (100%)	0	100	100
4	Gc	75/124 (60%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Gd	75/124 (60%)	75 (100%)	0	100	100
4	Ge	124/124 (100%)	124 (100%)	0	100	100
4	Gf	124/124 (100%)	124 (100%)	0	100	100
4	Gg	75/124 (60%)	75 (100%)	0	100	100
4	Gh	75/124 (60%)	75 (100%)	0	100	100
4	Gi	124/124 (100%)	124 (100%)	0	100	100
4	Gj	124/124 (100%)	124 (100%)	0	100	100
4	Gk	75/124 (60%)	75 (100%)	0	100	100
4	Gl	75/124 (60%)	75 (100%)	0	100	100
4	Ha	124/124 (100%)	124 (100%)	0	100	100
4	Hb	124/124 (100%)	124 (100%)	0	100	100
4	Hc	124/124 (100%)	124 (100%)	0	100	100
4	Hd	124/124 (100%)	124 (100%)	0	100	100
4	He	124/124 (100%)	124 (100%)	0	100	100
4	Hf	124/124 (100%)	124 (100%)	0	100	100
4	Hg	124/124 (100%)	124 (100%)	0	100	100
4	Hh	124/124 (100%)	124 (100%)	0	100	100
4	Hi	124/124 (100%)	124 (100%)	0	100	100
4	Hj	124/124 (100%)	124 (100%)	0	100	100
4	Hk	124/124 (100%)	124 (100%)	0	100	100
4	Hi	124/124 (100%)	124 (100%)	0	100	100
5	Ia	282/282 (100%)	282 (100%)	0	100	100
5	Ib	282/282 (100%)	282 (100%)	0	100	100
5	Ic	282/282 (100%)	282 (100%)	0	100	100
5	Id	282/282 (100%)	282 (100%)	0	100	100
5	Ie	282/282 (100%)	282 (100%)	0	100	100
5	If	282/282 (100%)	282 (100%)	0	100	100
All	All	10632/11190 (95%)	10632 (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 (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	Da	345	GLN
1	Db	268	ASN
1	Db	345	GLN
1	Db	396	ASN
1	Dc	345	GLN
1	Dc	396	ASN
1	Dd	275	HIS
1	De	345	GLN
1	Df	275	HIS
1	Df	345	GLN
1	Df	396	ASN
1	Dg	345	GLN
1	Dg	396	ASN
1	Dh	268	ASN
1	Dh	275	HIS
1	Dj	345	GLN
1	Dj	396	ASN
1	Dk	345	GLN
1	Di	268	ASN
1	Di	275	HIS
2	Eg	55	ASN
2	Ek	55	ASN
3	Fa	50	HIS
3	Fc	50	HIS
3	Fd	10	HIS
3	Fe	50	HIS
4	Gb	108	GLN
4	Gc	71	GLN
4	Gf	108	GLN
4	Gg	71	GLN
4	Gj	28	GLN
4	Gj	108	GLN
4	Gk	71	GLN
4	Ha	59	HIS
4	Hc	66	ASN
4	Hd	38	GLN
4	He	38	GLN
4	Hf	66	ASN
4	Hg	66	ASN
4	Hh	38	GLN
4	Hk	66	ASN
4	Hi	38	GLN
5	Ia	42	GLN

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Mol	Chain	Res	Type
5	Ia	149	ASN
5	Ia	155	ASN
5	Ib	42	GLN
5	Ib	149	ASN
5	Ib	155	ASN
5	Ic	42	GLN
5	Ic	149	ASN
5	Ic	155	ASN
5	Id	57	GLN
5	Id	63	ASN
5	Ie	34	ASN
5	Ie	63	ASN
5	Ie	270	HIS
5	If	34	ASN
5	If	63	ASN
5	If	270	HIS

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 ⓘ

There are no chain breaks in this entry.

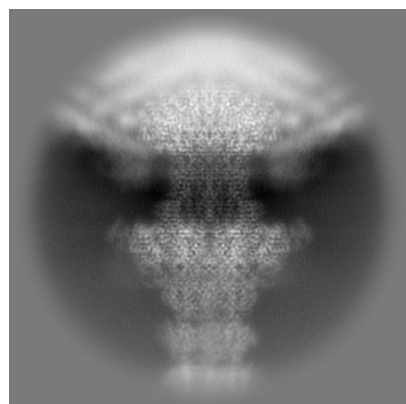
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70278. These allow visual inspection of the internal detail of the map and identification of artifacts.

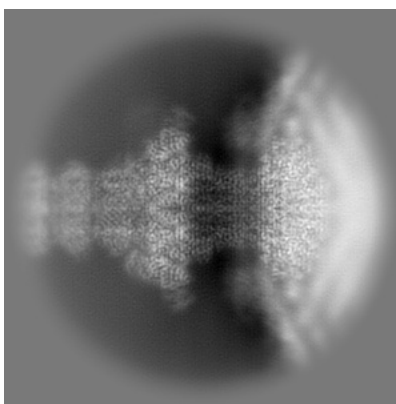
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

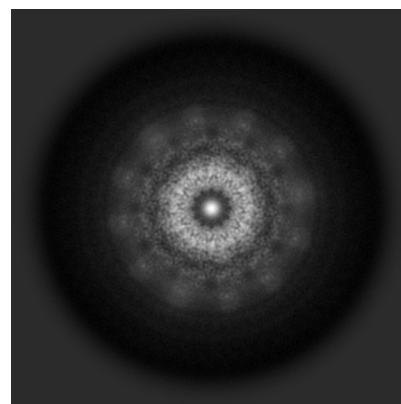
6.1.1 Primary map



X

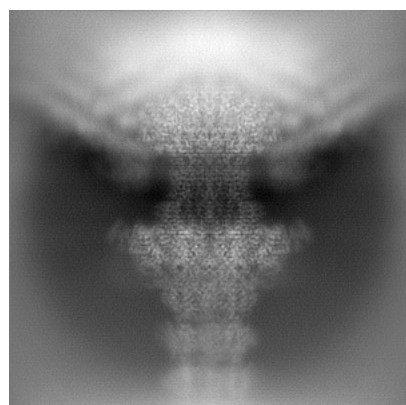


Y

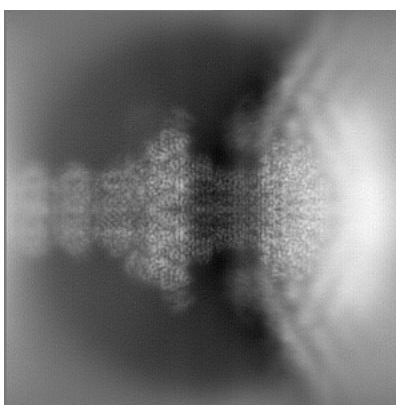


Z

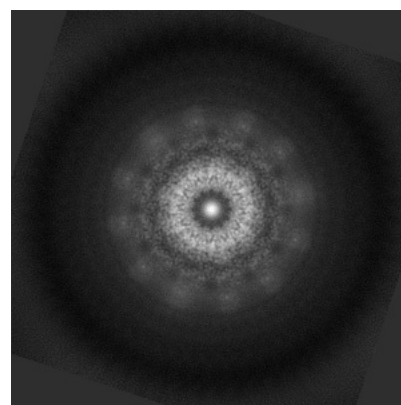
6.1.2 Raw map



X



Y

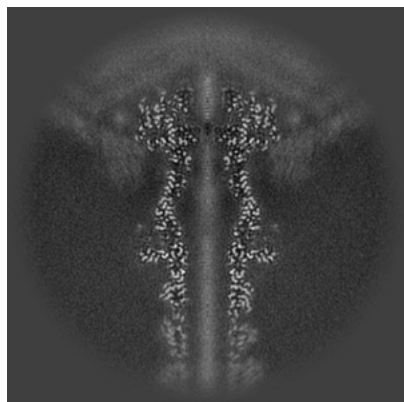


Z

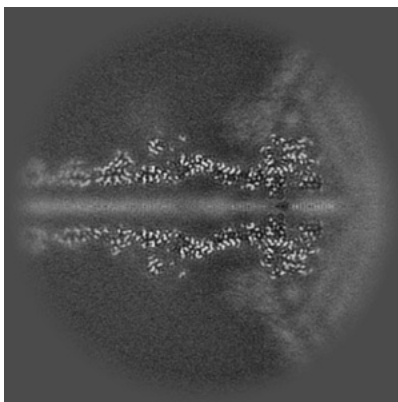
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

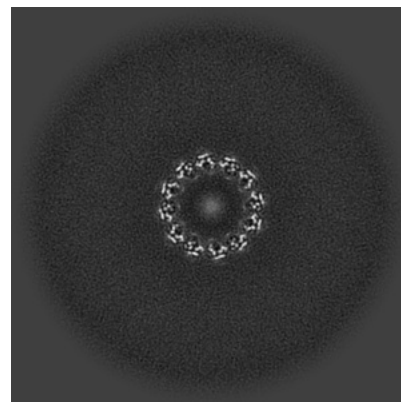
6.2.1 Primary map



X Index: 180

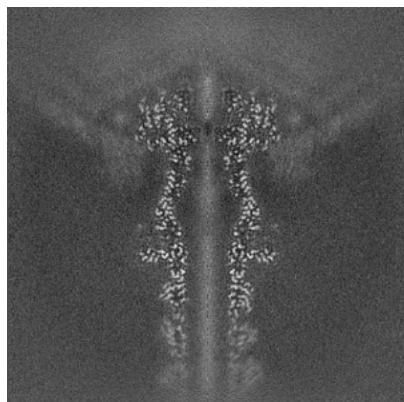


Y Index: 180

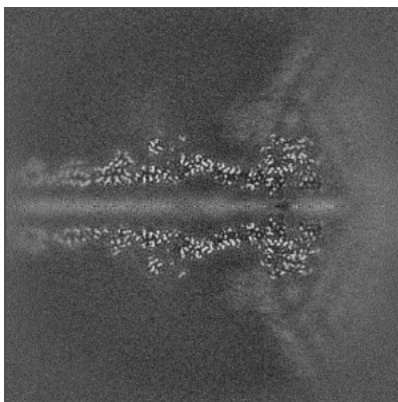


Z Index: 180

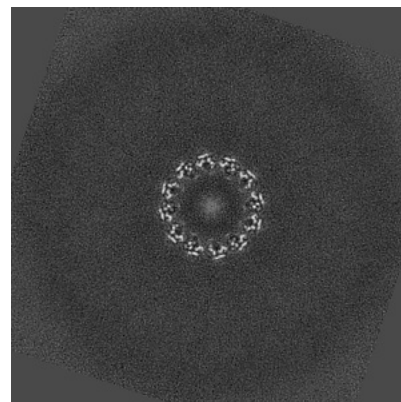
6.2.2 Raw map



X Index: 180



Y Index: 180

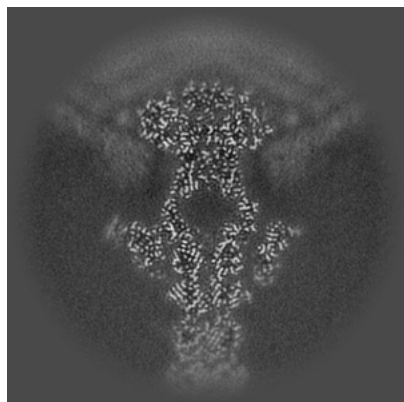


Z Index: 180

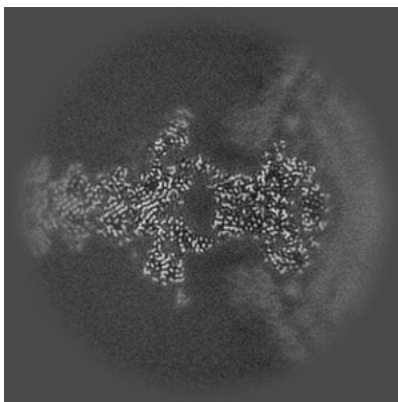
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

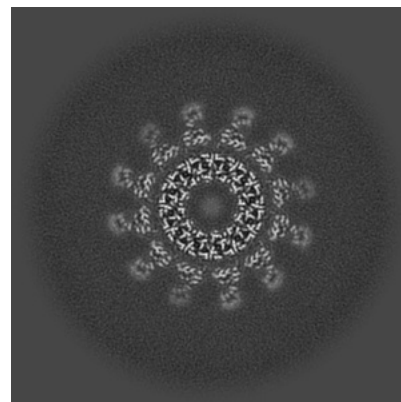
6.3.1 Primary map



X Index: 200

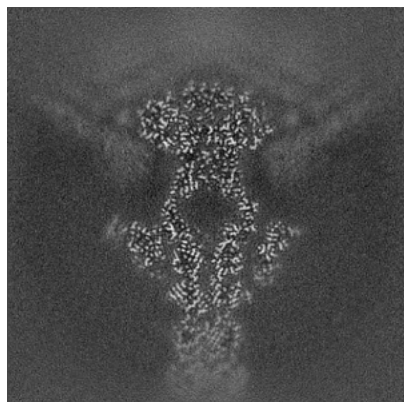


Y Index: 158

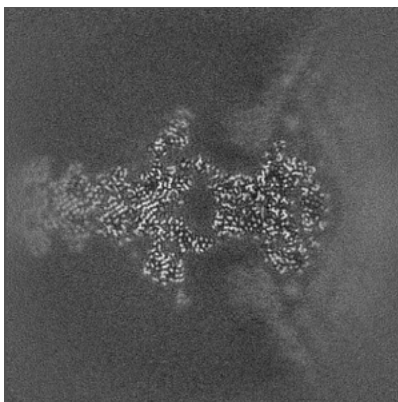


Z Index: 160

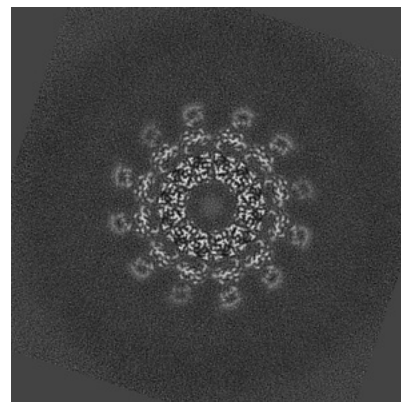
6.3.2 Raw map



X Index: 200



Y Index: 158

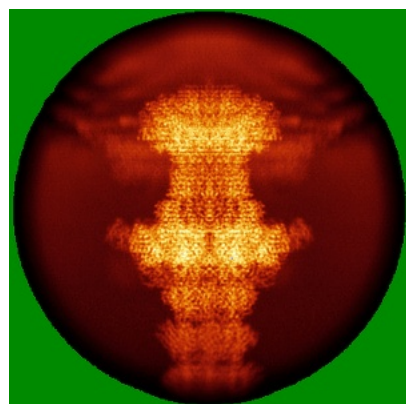


Z Index: 159

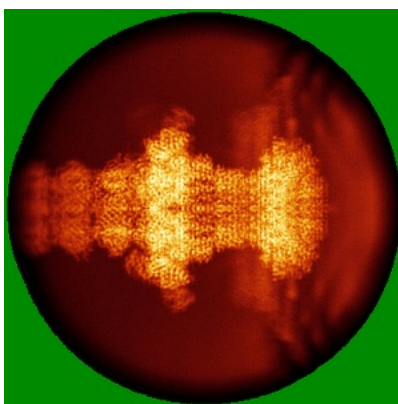
The images above show the largest variance slices of the map in three orthogonal directions.

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

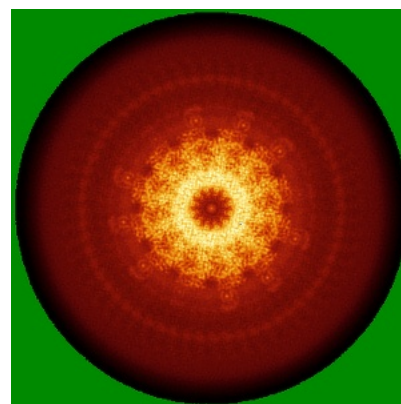
6.4.1 Primary map



X

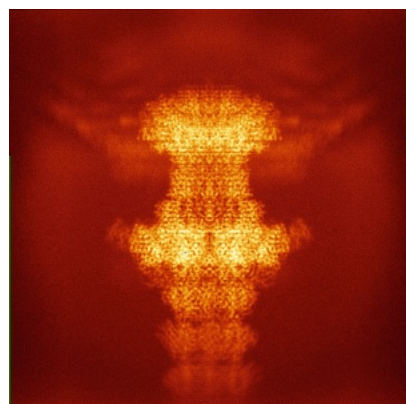


Y

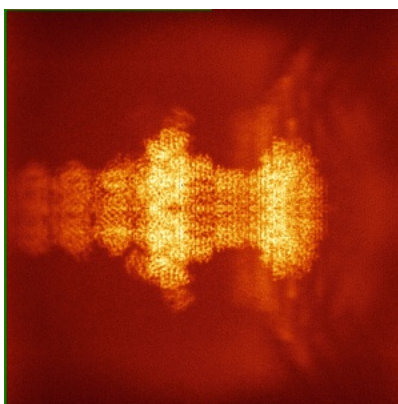


Z

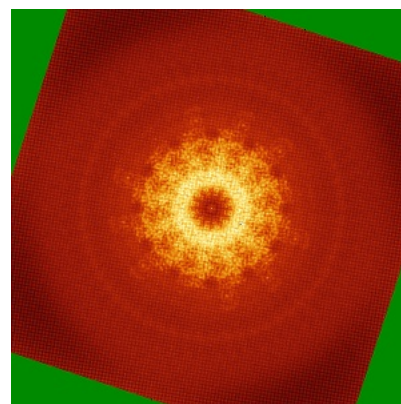
6.4.2 Raw map



X



Y



Z

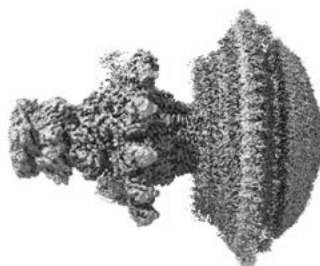
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

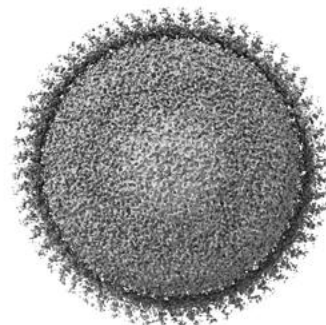
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

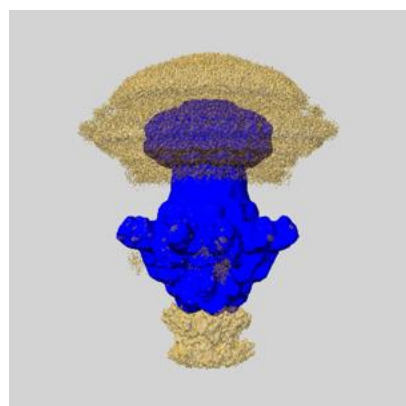
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

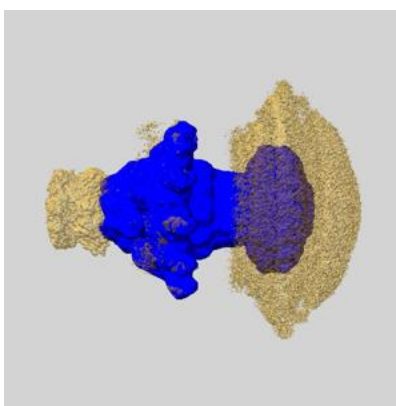
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

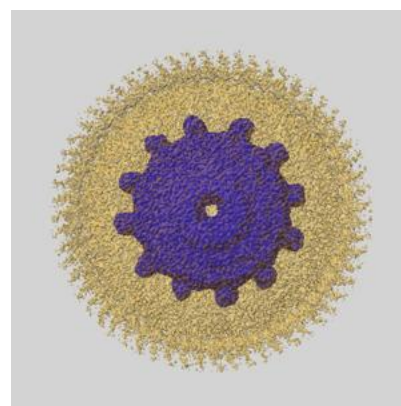
6.6.1 emd_70278_msk_1.map [i](#)



X



Y

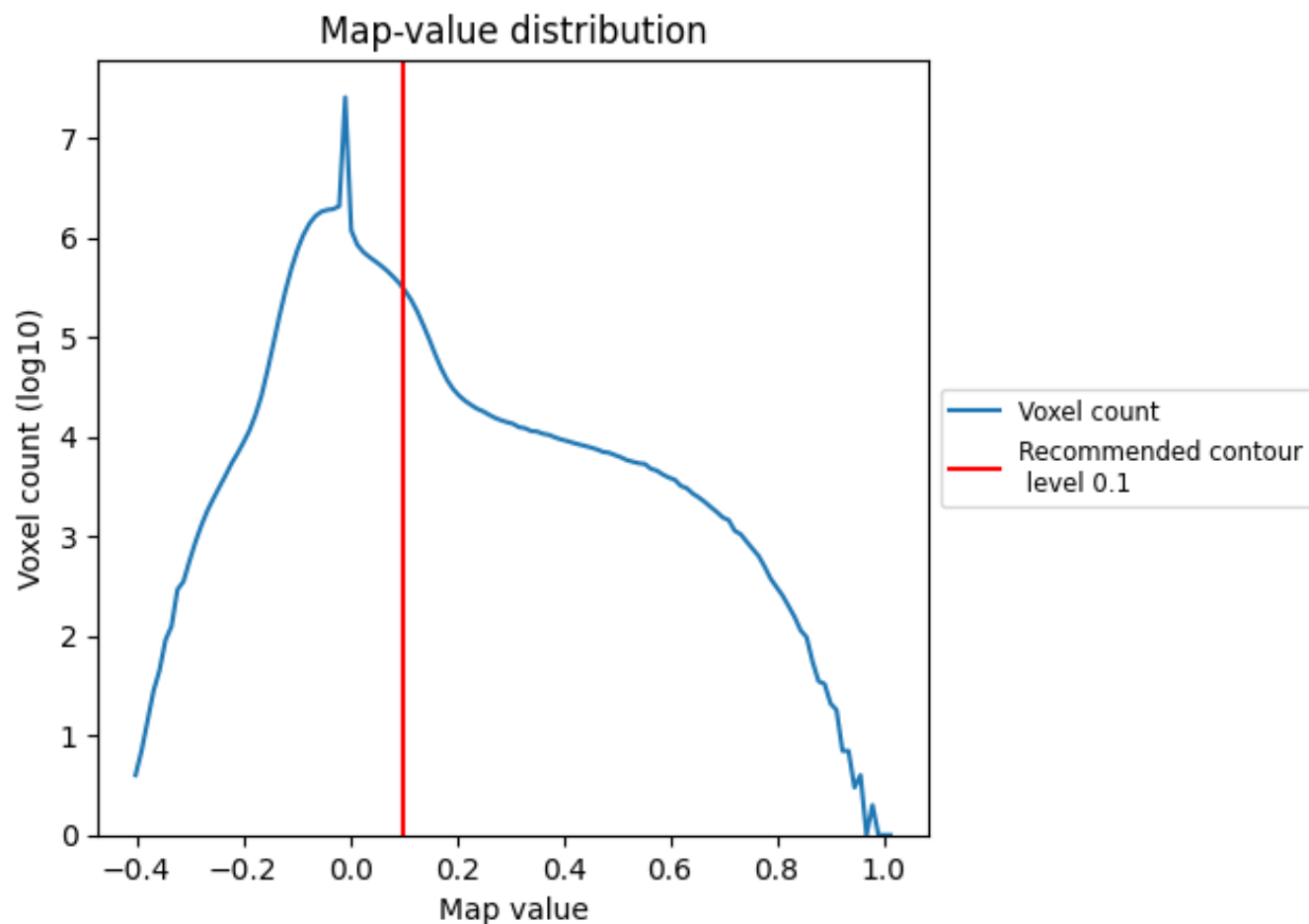


Z

7 Map analysis [i](#)

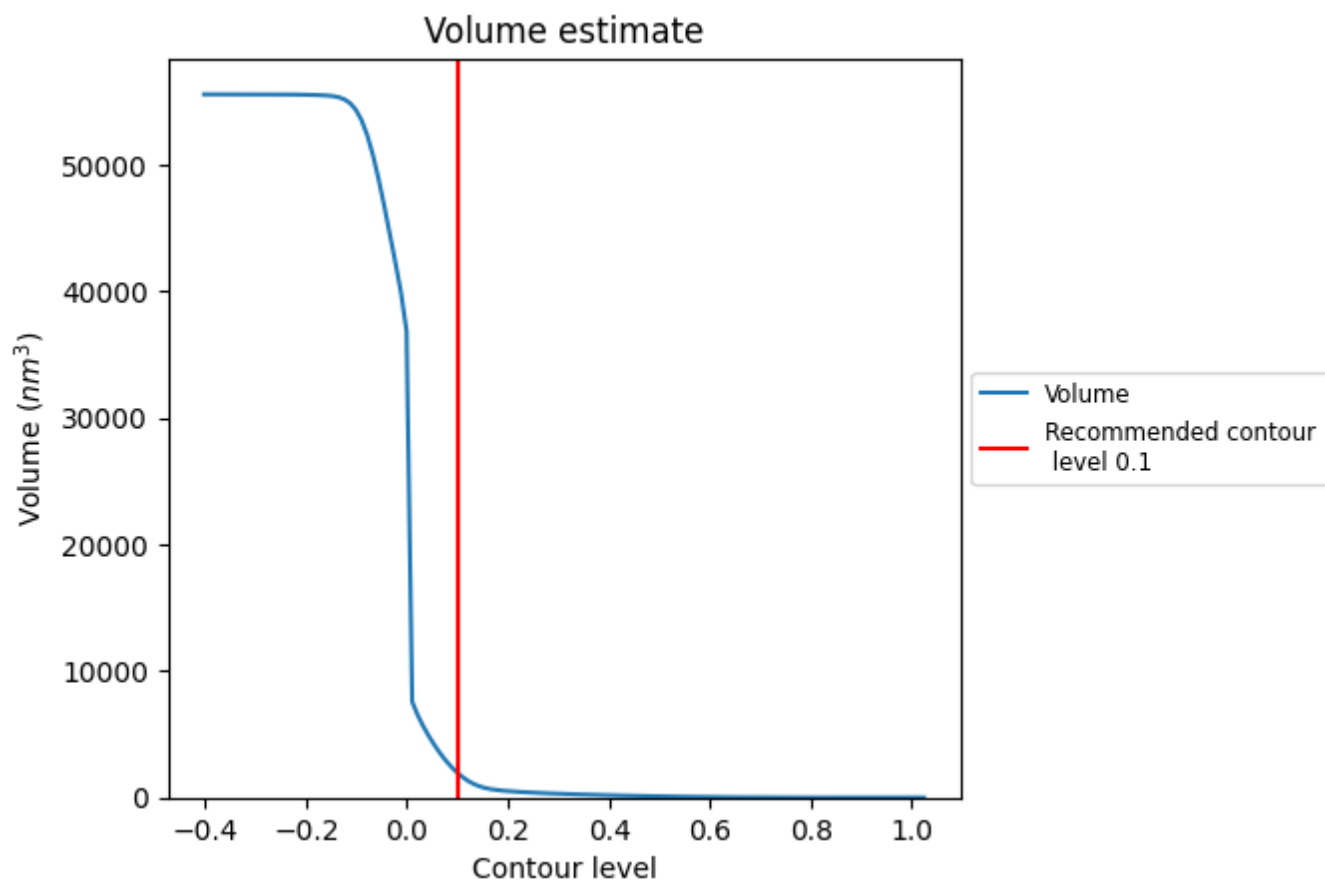
This section contains the results of statistical analysis of the map.

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.

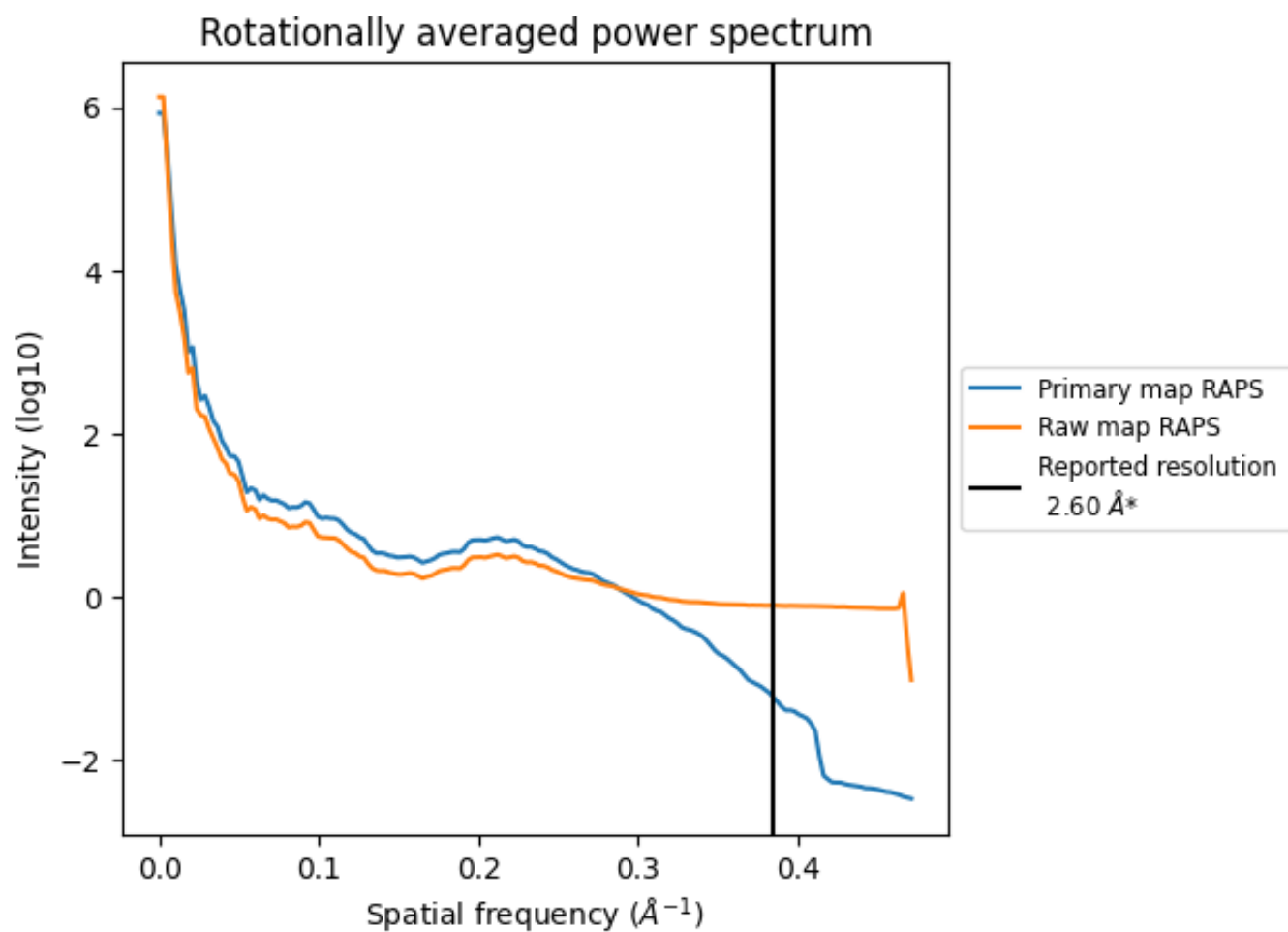
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1963 nm³; this corresponds to an approximate mass of 1774 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 ⓘ

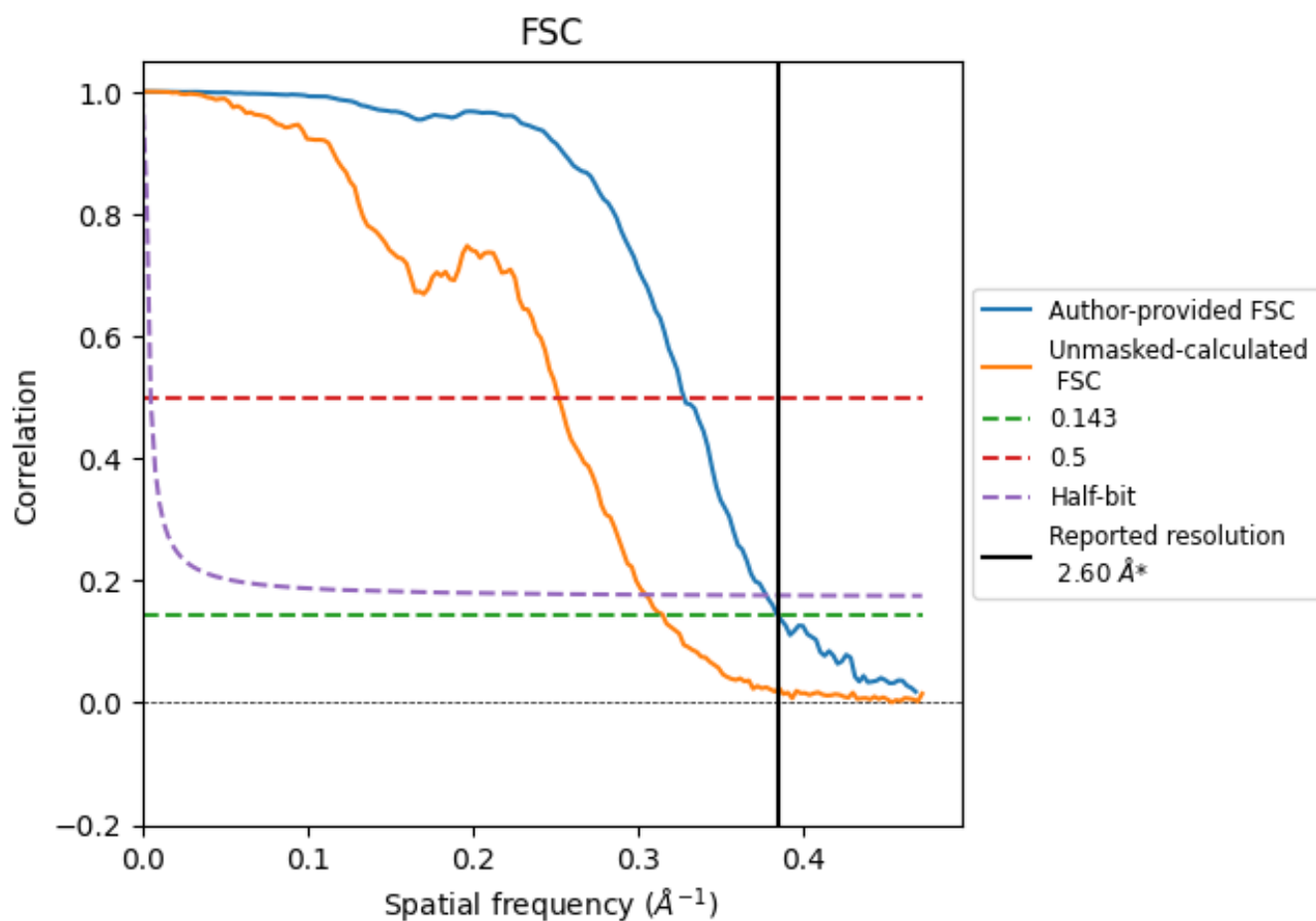


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

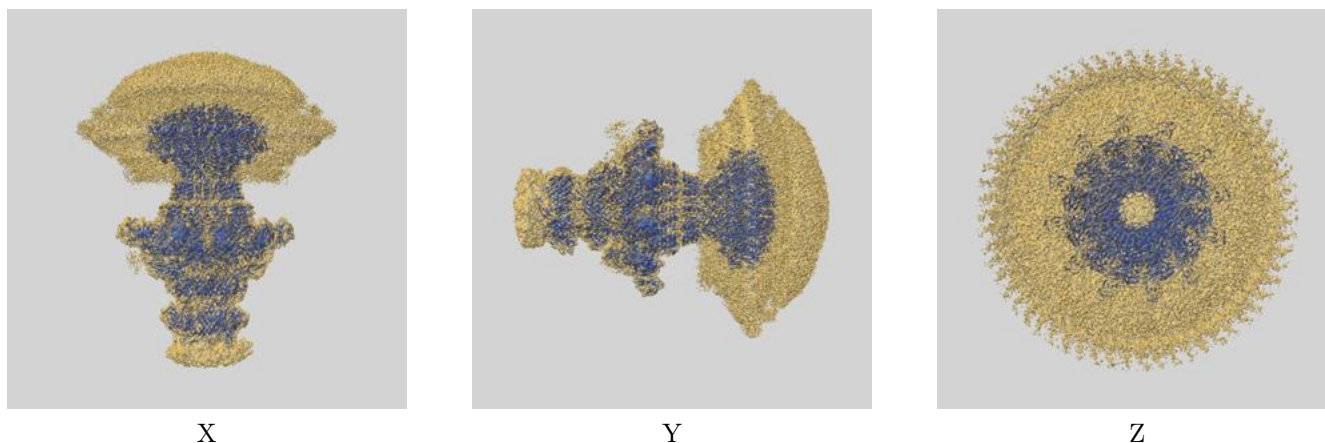
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.05	2.65
Unmasked-calculated*	3.18	3.97	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

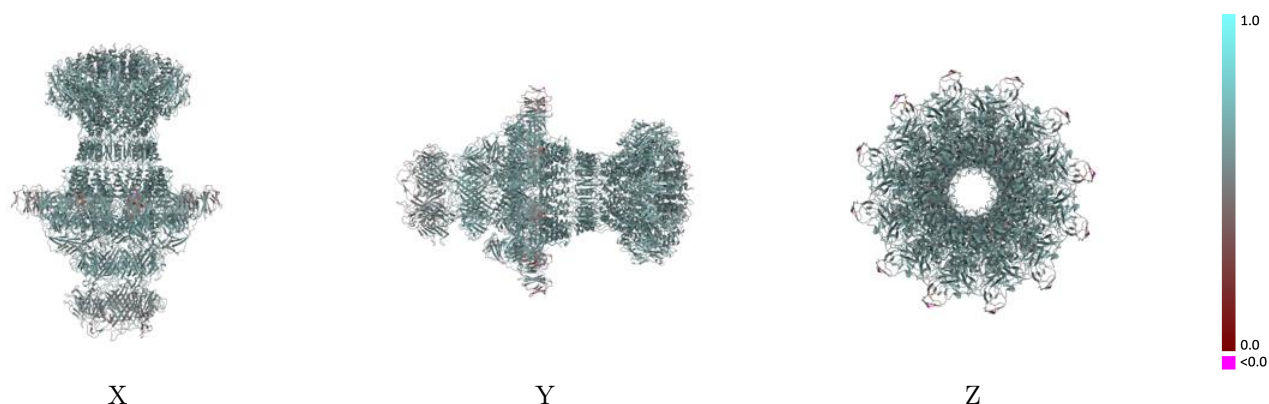
This section contains information regarding the fit between EMDB map EMD-70278 and PDB model 9OAB. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

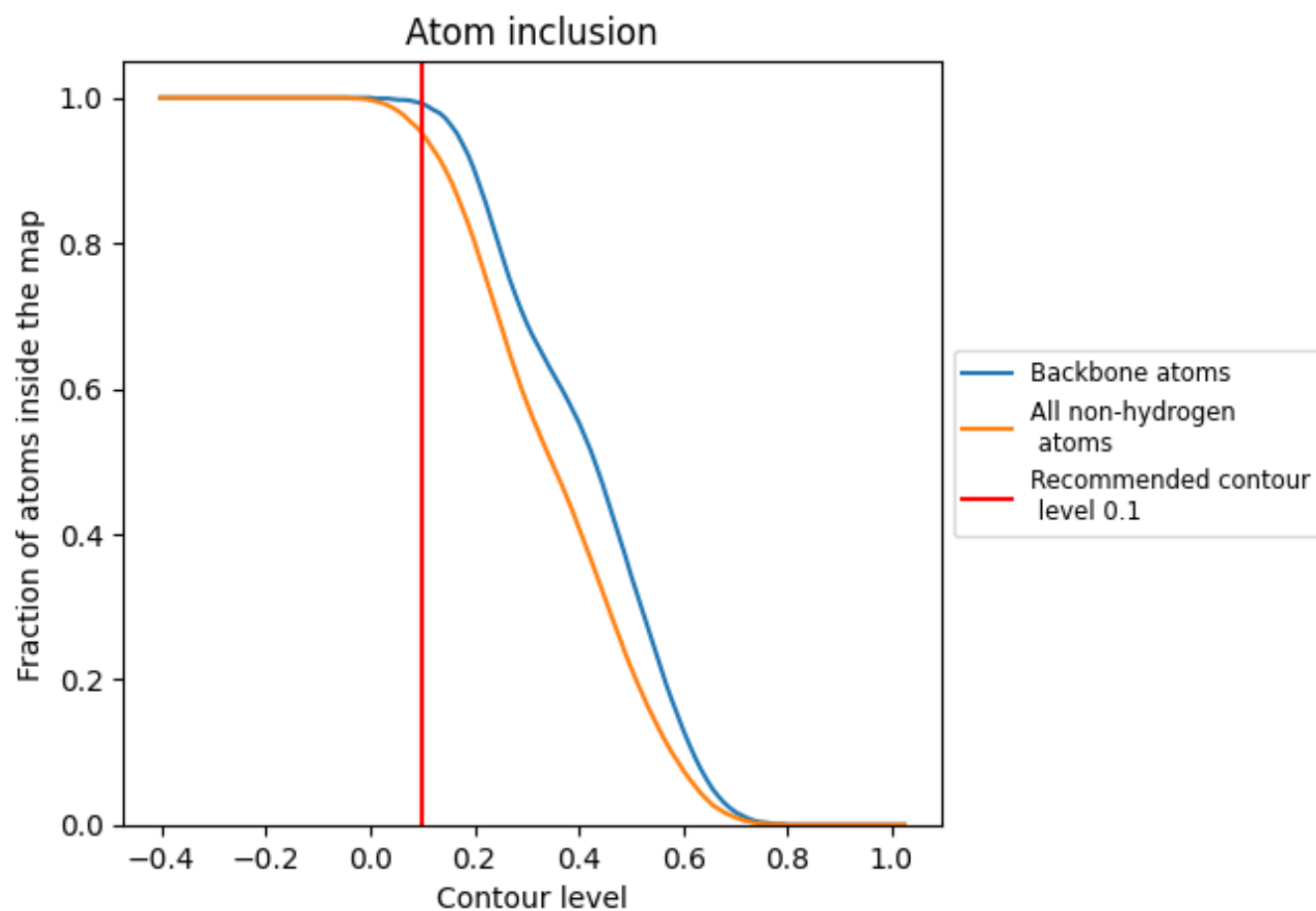


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.5840
Da	 0.9530	 0.5970
Db	 0.9510	 0.5930
Dc	 0.9540	 0.5950
Dd	 0.9530	 0.5940
De	 0.9520	 0.5960
Df	 0.9510	 0.5930
Dg	 0.9530	 0.5960
Dh	 0.9520	 0.5940
Di	 0.9530	 0.5970
Dj	 0.9520	 0.5930
Dk	 0.9530	 0.5960
Dl	 0.9520	 0.5950
Ea	 0.9580	 0.6060
Eb	 0.9570	 0.6090
Ec	 0.9560	 0.6050
Ed	 0.9500	 0.6030
Ee	 0.9570	 0.6060
Ef	 0.9590	 0.6110
Eg	 0.9600	 0.6060
Uh	 0.9500	 0.6080
Ei	 0.9590	 0.6110
Ej	 0.9570	 0.6110
Ek	 0.9580	 0.6070
El	 0.9500	 0.6040
Fa	 0.9700	 0.6230
Fb	 0.9750	 0.6150
Fc	 0.9710	 0.6200
Fd	 0.9700	 0.6150
Fe	 0.9730	 0.6200
Ff	 0.9760	 0.6180
Ga	 0.9510	 0.5760
Gb	 0.9460	 0.5770
Gc	 0.9660	 0.5950
Gd	 0.9320	 0.5830



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Chain	Atom inclusion	Q-score
Ge	 0.9500	 0.5750
Gf	 0.9460	 0.5790
Gg	 0.9690	 0.5970
Gh	 0.9260	 0.5880
Gi	 0.9510	 0.5770
Gj	 0.9470	 0.5800
Gk	 0.9690	 0.5950
Gl	 0.9290	 0.5870
Ha	 0.9390	 0.5660
Hb	 0.9380	 0.5560
Hc	 0.8420	 0.5380
Hd	 0.9140	 0.5460
He	 0.9390	 0.5680
Hf	 0.9370	 0.5560
Hg	 0.8470	 0.5410
Hh	 0.9190	 0.5440
Hi	 0.9380	 0.5680
Hj	 0.9380	 0.5560
Hk	 0.8460	 0.5380
Hl	 0.9200	 0.5450
Ia	 0.9770	 0.6000
Ib	 0.9770	 0.5990
Ic	 0.9780	 0.6010
Id	 0.9600	 0.4970
Ie	 0.9600	 0.4980
If	 0.9610	 0.4990