



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 03:22 PM UTC

PDB ID : 3JCR / pdb_00003jcr
EMDB ID : EMD-6581
Title : 3D structure determination of the human*U4/U6.U5* tri-snRNP complex
Authors : Agafonov, D.E.; Kastner, B.; Dybkov, O.; Hofele, R.V.; Liu, W.T.; Urlaub, H.; Luhrmann, R.; Stark, H.
Deposited on : 2016-01-21
Resolution : 7.00 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:

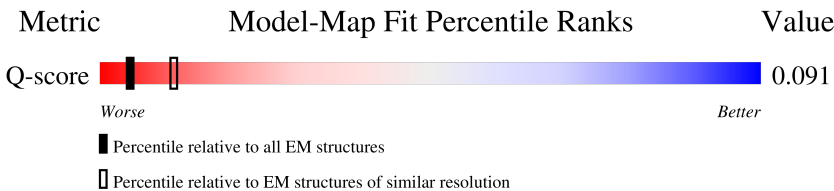
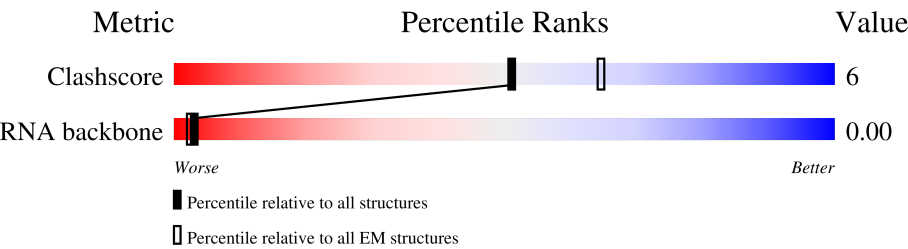
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.00 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	483 (6.50 - 7.50)

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	G	941	8% 43% 56%
2	D	357	78% 84% 15%
3	C	2136	17% 88% 12%
4	E	142	40% 94% 5%
5	A	2335	18% 94% 5%

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Mol	Chain	Length	Quality of chain
6	F	820	
7	B	972	
8	O	240	
8	o	240	
9	P	119	
9	p	119	
10	Q	118	
10	q	118	
11	R	126	
11	r	126	
12	S	92	
12	s	92	
13	T	86	
13	t	86	
14	U	76	
14	u	76	
15	8	96	
16	6	80	
17	5	91	
18	4	139	
19	3	102	
20	2	95	
21	7	103	
22	K	683	
23	L	521	

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Mol	Chain	Length	Quality of chain
24	J	499	
25	I	128	
26	V	565	
27	M	145	
28	N	106	
29	H	116	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 9403 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 hPrp6.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	G	418	Total	C	0	418
			418	418		

- Molecule 2 is a protein called U5-40K.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	D	302	Total	C	0	302
			302	302		

- Molecule 3 is a protein called hBrr2.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	1885	Total	C	0	1885
			1885	1885		

- Molecule 4 is a protein called hDim1.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	E	135	Total	C	0	135
			135	135		

- Molecule 5 is a protein called hPrp8.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	A	2222	Total	C	0	2222
			2222	2222		

- Molecule 6 is a protein called hPrp28.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	F	435	Total	C	0	435
			435	435		

- Molecule 7 is a protein called hSnu114.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	B	844	Total C 844 844	0	844

- Molecule 8 is a protein called SmB.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	O	89	Total C 89 89	0	89
8	o	89	Total C 89 89	0	89

- Molecule 9 is a protein called SmD1.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	P	93	Total C 93 93	0	93
9	p	94	Total C 94 94	0	94

- Molecule 10 is a protein called SmD2.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	Q	89	Total C 89 89	0	89
10	q	89	Total C 89 89	0	89

- Molecule 11 is a protein called SmD3.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	R	88	Total C 88 88	0	88
11	r	88	Total C 88 88	0	88

- Molecule 12 is a protein called SmE.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	S	78	Total C 78 78	0	78

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Mol	Chain	Residues	Atoms	AltConf	Trace
12	s	78	Total C 78 78	0	78

- Molecule 13 is a protein called SmF.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	T	73	Total C 73 73	0	73
13	t	83	Total C 83 83	0	83

- Molecule 14 is a protein called SmG.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	U	73	Total C 73 73	0	73
14	u	73	Total C 73 73	0	73

- Molecule 15 is a protein called LSm8.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	8	70	Total C 70 70	0	70

- Molecule 16 is a protein called LSm6.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	6	70	Total C 70 70	0	70

- Molecule 17 is a protein called LSm5.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	5	76	Total C 76 76	0	76

- Molecule 18 is a protein called LSm4.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	4	80	Total	C	0	80
			80	80		

- Molecule 19 is a protein called LSm3.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	3	83	Total	C	0	83
			83	83		

- Molecule 20 is a protein called LSm2.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	2	90	Total	C	0	90
			90	90		

- Molecule 21 is a protein called LSm7.

Mol	Chain	Residues	Atoms		AltConf	Trace
21	7	79	Total	C	0	79
			79	79		

- Molecule 22 is a protein called hPrp3.

Mol	Chain	Residues	Atoms		AltConf	Trace
22	K	131	Total	C	0	131
			131	131		

- Molecule 23 is a protein called hPrp4.

Mol	Chain	Residues	Atoms		AltConf	Trace
23	L	307	Total	C	0	307
			307	307		

- Molecule 24 is a protein called hPrp31.

Mol	Chain	Residues	Atoms		AltConf	Trace
24	J	239	Total	C	0	239
			239	239		

- Molecule 25 is a protein called hSnu13.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	I	126	Total	C	0	126
			126	126		

- Molecule 26 is a protein called hSad1.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	V	431	Total	C	0	431
			431	431		

- Molecule 27 is a RNA chain called U4 snRNA.

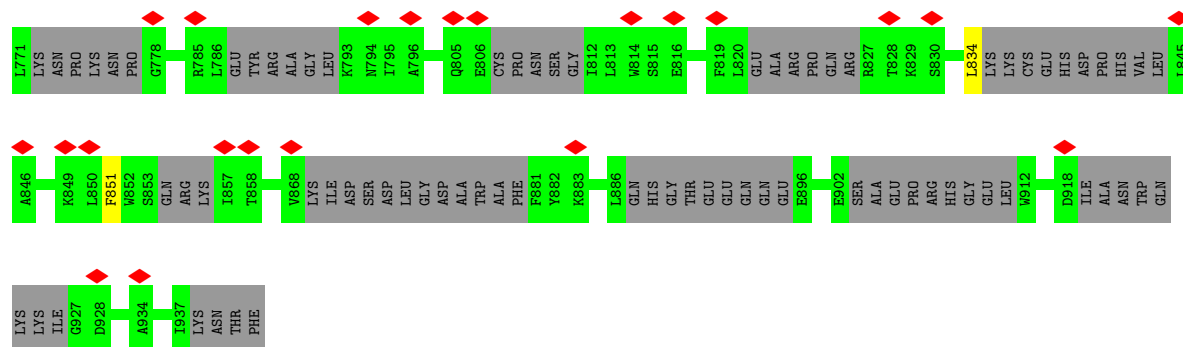
Mol	Chain	Residues	Atoms		AltConf	Trace
27	M	103	Total	P	0	103
			103	103		

- Molecule 28 is a RNA chain called U6 snRNA.

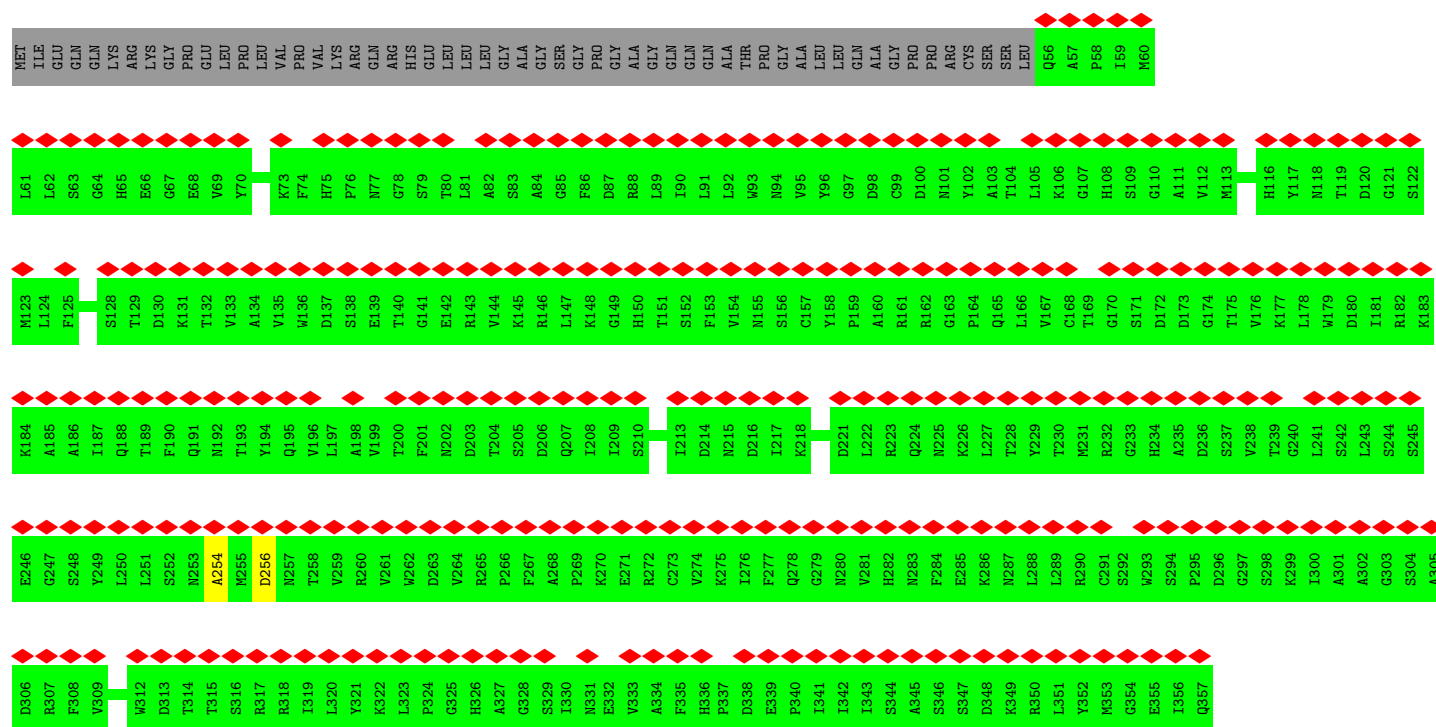
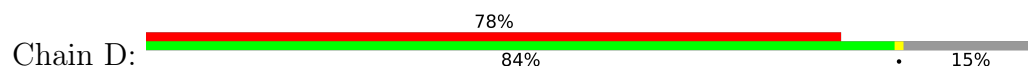
Mol	Chain	Residues	Atoms		AltConf	Trace
28	N	37	Total	P	0	37
			37	37		

- Molecule 29 is a RNA chain called U5 snRNA.

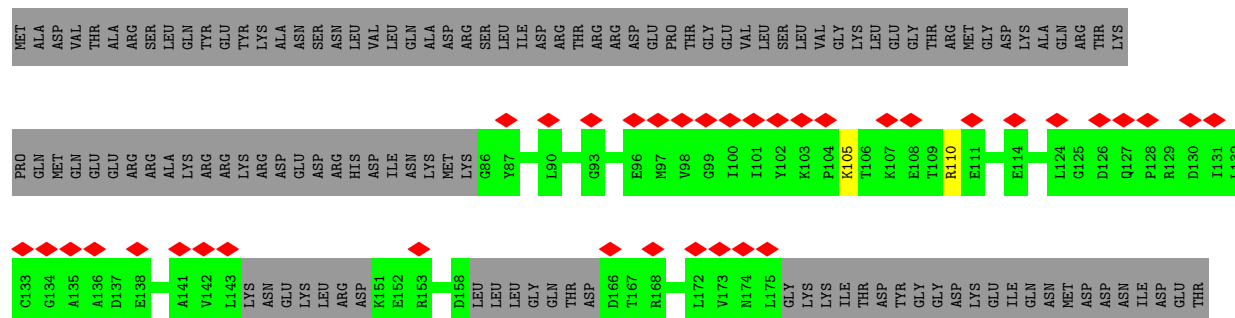
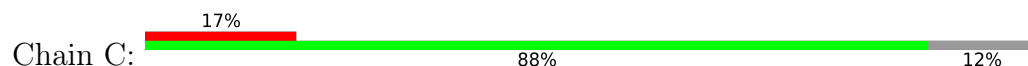
Mol	Chain	Residues	Atoms		AltConf	Trace
29	H	63	Total	P	0	63
			63	63		



• Molecule 2: U5-40K



• Molecule 3: hBrr2



Chain A: 18% 94% 5%



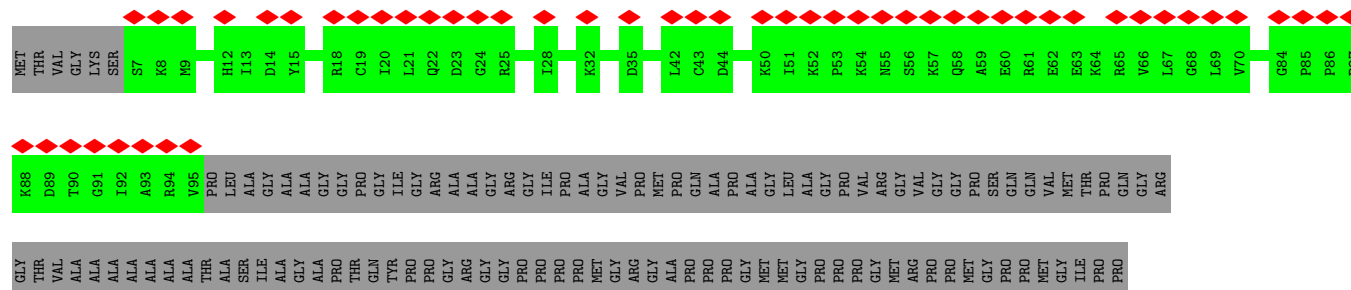
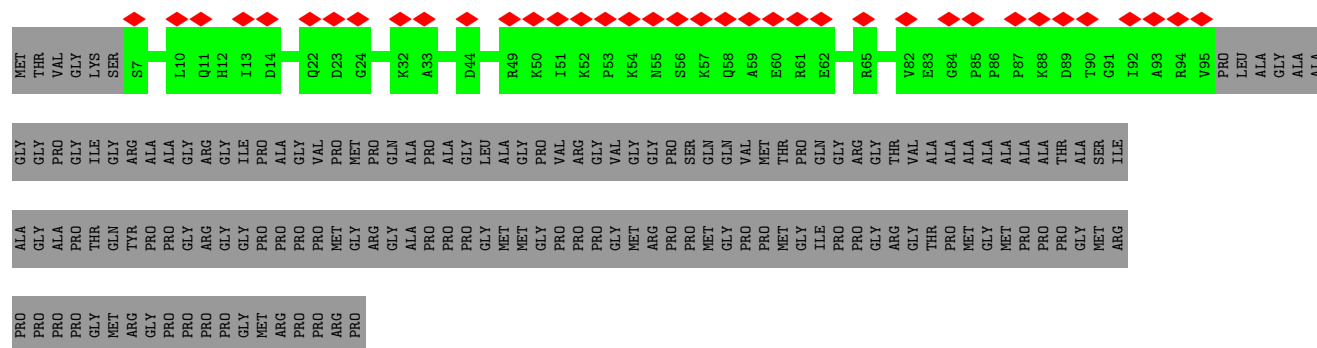
LEU
GLN
GLY
GLY
GLY
VAL
TYR
SER
ASP
ALA
ASP
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TYR
ALA

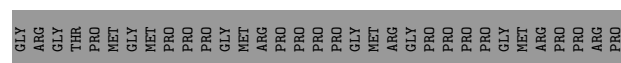
• Molecule 6: hPrp28

Chain F:  41% 52% 47%

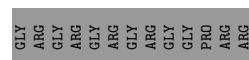
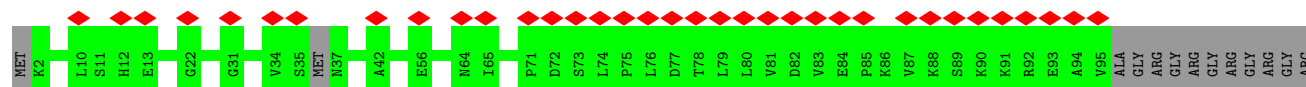
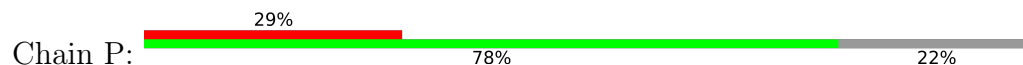
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SER	ARG	SER	ARG	SER	SER	LYS	LYS	ASP	GLY	GLY	ASP	GLY	ASP	GLY	ASP	GLY	ASP	GLY
ASP	ARG	ASP	SER	SER	LYS	LYS	ASP	GLY	GLY	GLY	ASP	GLY	ASP	GLY	ASP	GLY	ASP	GLY
VAL	GLU	ARG	GLN	ARG	MET	LEU	HIS	LEU	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LYS	ASP	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ARG	GLY	PHE	ILE	ALA	GLY	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E375	D376	T381	K382	G383	G384	R391	K394	D395	S396	S397	P399	H401	D407	K408	C409	G410	Y411	K412
P416	I417	P423	G425	L426	R429	T432	G433	V434	A435	E436	T437	G438	S439	G440	K441	T442	A444	P445
K458	T459	D460	R461	L462	E463	E464	S465	D466	D467	G468	L472	L473	L474	A475	P476	T477	R478	E479
L480	A481	Q482	Q483	L484	E485	E486	E487	T488	L489	K490	K493	P494	L495	G496	L497	R498	T499	V500
A501	V502	I503	G504	G505	L506	S507	R508	E509	D510	Q511	Q512	F513	R514	L515	R516	M517	CYS	E520
I521	V522	I523	A524	T525	P526	G527	A528	L529	I530	D531	V532	L533	E534	N535	A536	L538	V539	S541
R542	C543	T544	V545	V546	V547	L548	D549	E550	A551	D552	I555	D556	M557	G558	F559	E560	Q564	K565
L566	L567	E568	V572	S573	K576	P577	D578	T579	D580	E581	A582	E583	D584	P585	E586	K587	L588	L589
A590	N591	F592	E593	S594	G595	K596	H597	K598	Q601	T602	T606	A607	T608	M609	P610	P611	A612	V613
E614	R615	L616	A617	R618	S619	Y620	L621	R622	A625	V626	V627	V628	G630	SER	ALA	GLY	LYS	PRO
HIS	E637	R638	V639	E640	D641	K642	V643	P644	L645	M646	S647	E648	S649	E650	HIS	GLY	LYS	GLY
R651	R652	R653	R654	L655	L656	A657	T658	L659	E660	Q661	G662	F663	D664	P665	P666	I667	T668	I669
I670	V671	R672	Q673	M674	K675	G676	C677	D678	V679	L680	A681	K682	S683	L684	E685	K686	M687	G688
V689	N690	A691	C692	T693	L694	HIS	GLY	GLY	LYS	GLY	T698	D729	I730	Q731	D732	V733	S734	M735
V736	V737	N738	V739	D740	M741	A742	K743	N744	I745	E746	D747	V748	I749	H750	R751	I752	G753	R754
T755	G756	R757	A758	G759	S761	V762	V763	A764	T765	T766	F767	L768	T769	K770	E771	D772	S773	A774
V775	V776	V777	E778	L779	K780	Q781	A782	I783	L784	E785	S786	F787	V788	S789	CYS	F792	P793	E794
L795	A796	N797	H798	P799	D800	A801	Q802	H803	K804	P805	G806	THR	ILE	LEU	THR	LYS	LYS	ARG
ARG	GLU	GLU	THR	ILE	PHE	ALA												

• Molecule 7: hSnu114

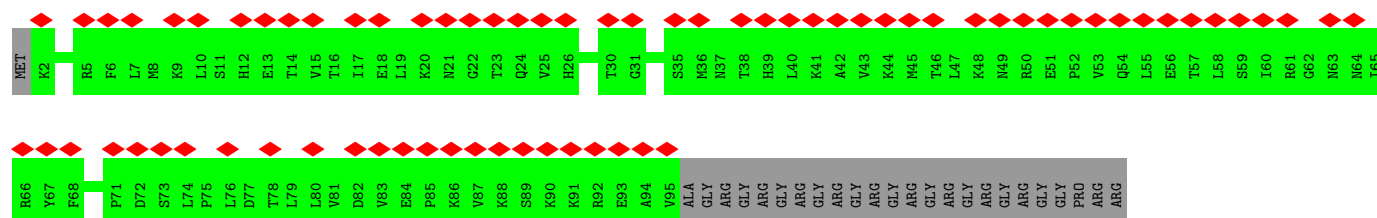
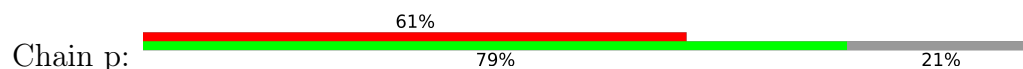
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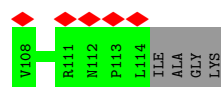
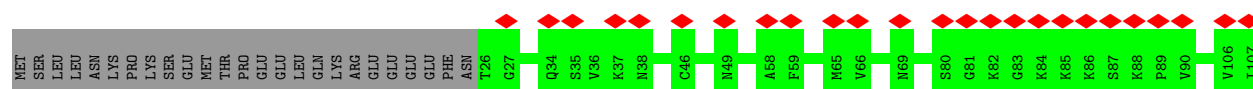
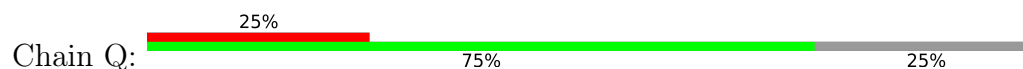
• Molecule 9: SmD1



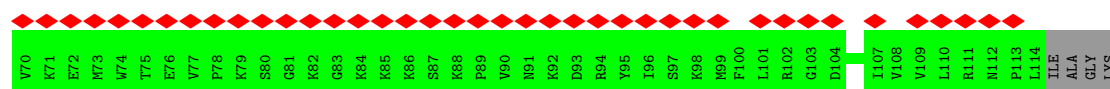
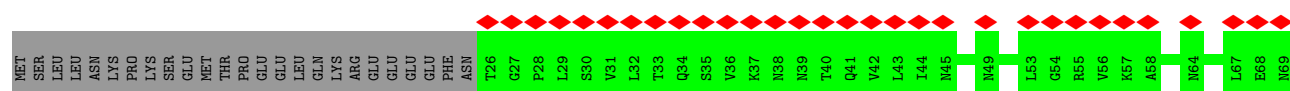
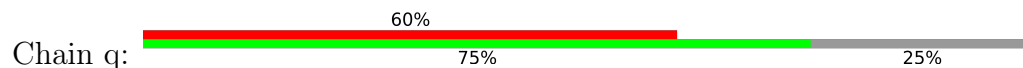
• Molecule 9: SmD1



• Molecule 10: SmD2

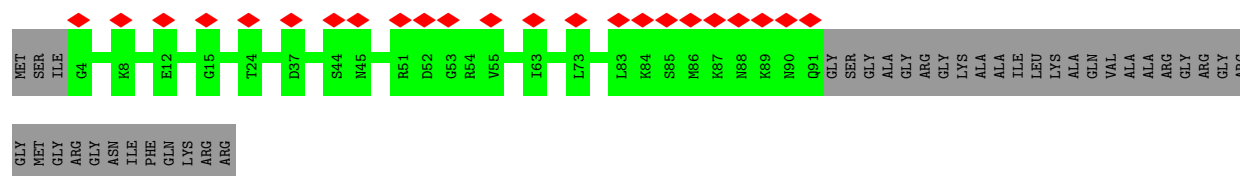


• Molecule 10: SmD2

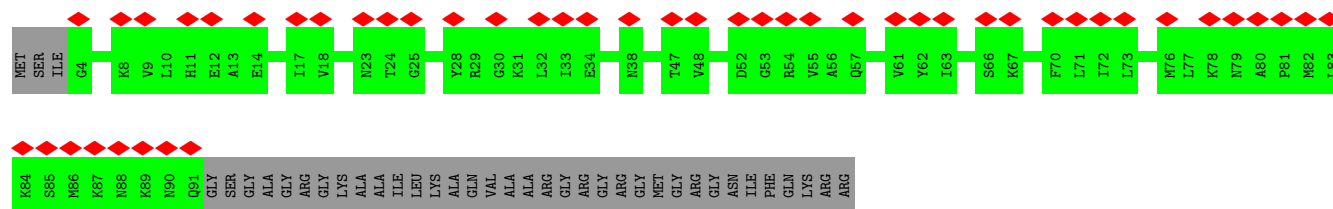
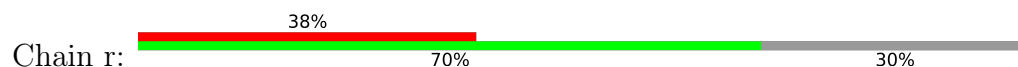


• Molecule 11: SmD3

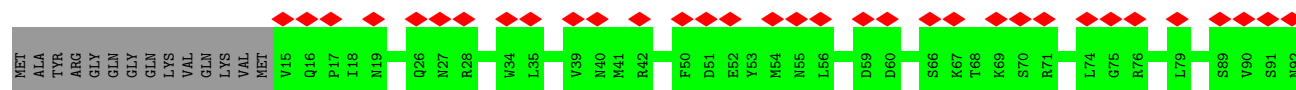
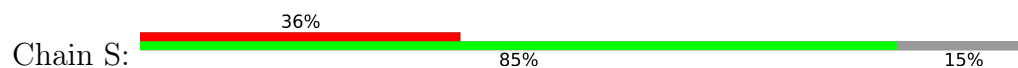




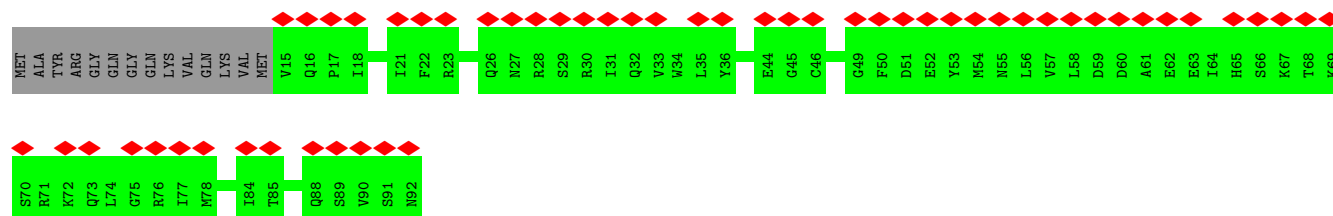
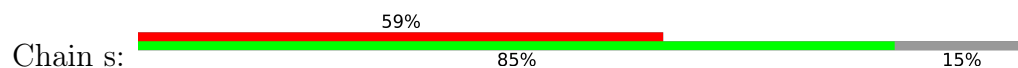
• Molecule 11: SmD3



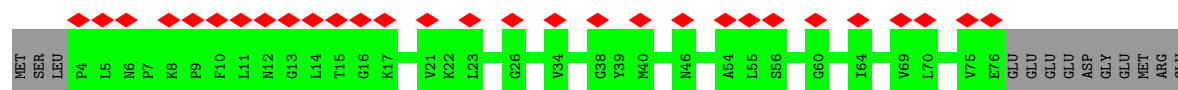
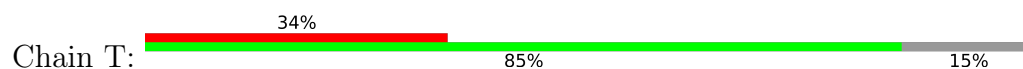
• Molecule 12: SmE



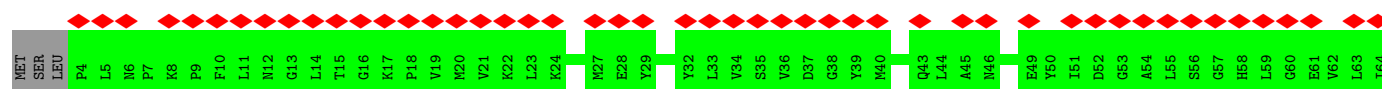
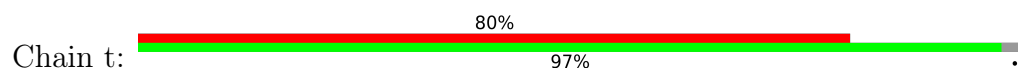
• Molecule 12: SmE

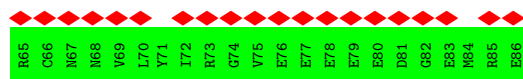


• Molecule 13: SmF

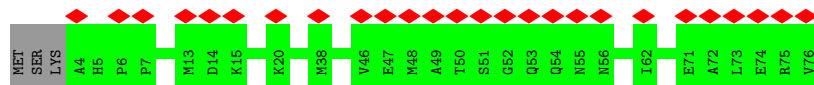


• Molecule 13: SmF

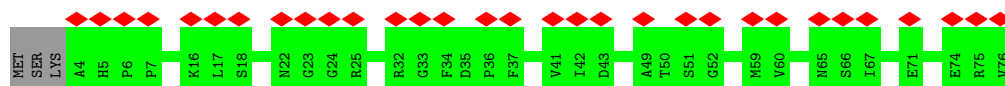




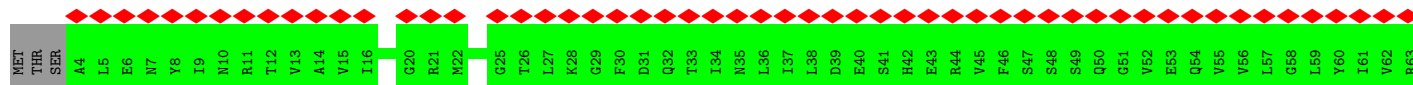
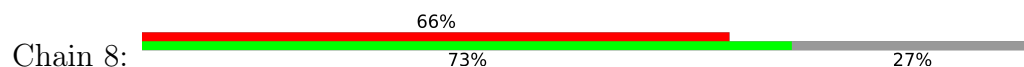
• Molecule 14: SmG



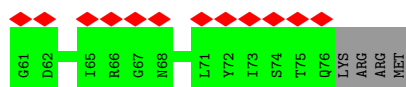
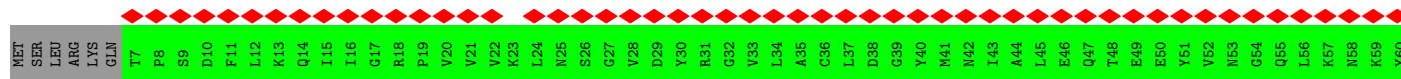
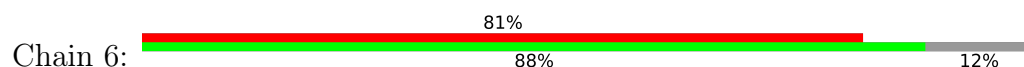
• Molecule 14: SmG



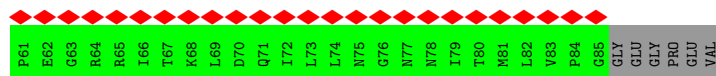
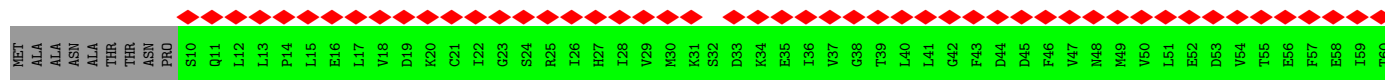
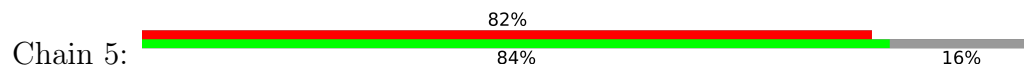
• Molecule 15: LSm8

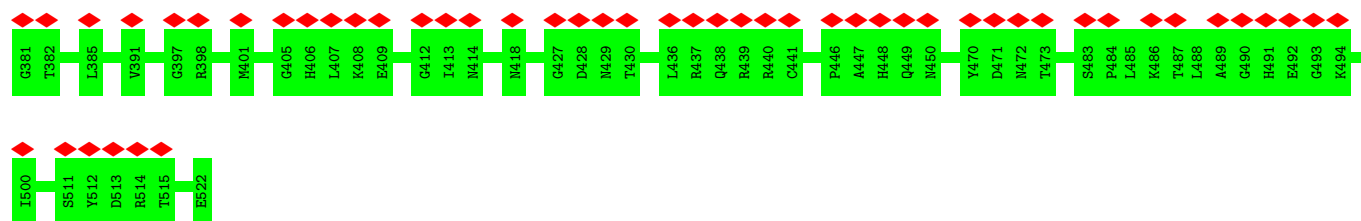


• Molecule 16: LSm6

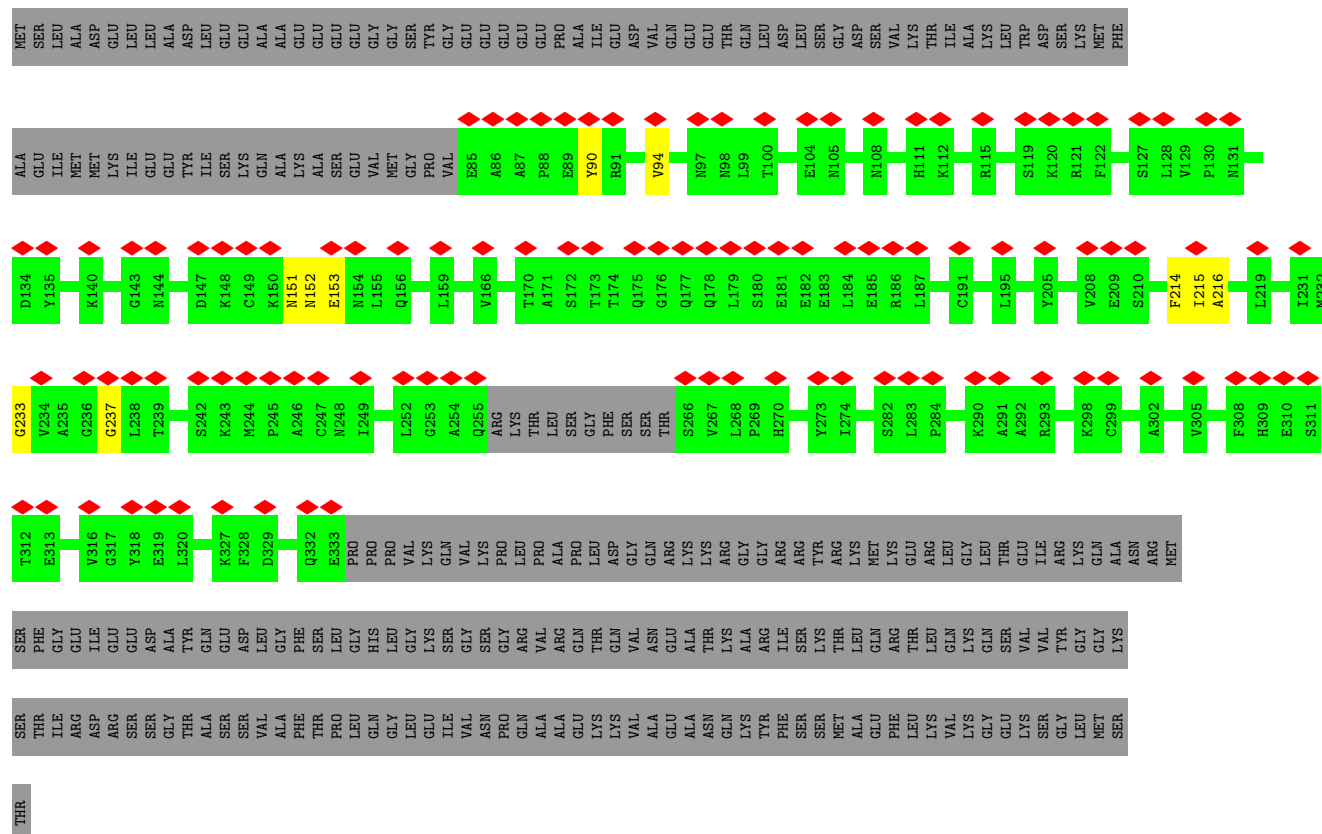


• Molecule 17: LSm5

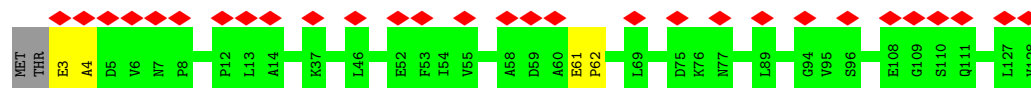




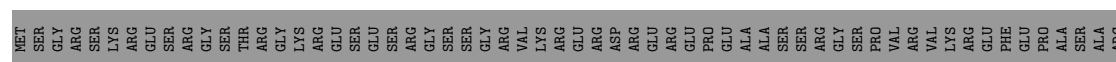
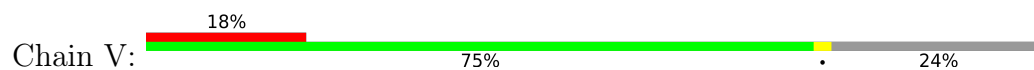
• Molecule 24: hPrp31



• Molecule 25: hSnu13



• Molecule 26: hSad1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141109	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5350	Depositor
Magnification	74000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.653	Depositor
Minimum map value	-0.382	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.0, 2.0, 2.0	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	G	418	0	0	6	0
2	D	302	0	0	3	0
3	C	1885	0	0	1	0
4	E	135	0	0	1	0
5	A	2222	0	0	20	0
6	F	435	0	0	6	0
7	B	844	0	0	4	0
8	O	89	0	0	0	0
8	o	89	0	0	0	0
9	P	93	0	0	0	0
9	p	94	0	0	0	0
10	Q	89	0	0	0	0
10	q	89	0	0	0	0
11	R	88	0	0	0	0
11	r	88	0	0	0	0
12	S	78	0	0	0	0
12	s	78	0	0	0	0
13	T	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	t	83	0	0	0	0
14	U	73	0	0	0	0
14	u	73	0	0	0	0
15	8	70	0	0	0	0
16	6	70	0	0	0	0
17	5	76	0	0	0	0
18	4	80	0	0	0	0
19	3	83	0	0	0	0
20	2	90	0	0	0	0
21	7	79	0	0	0	0
22	K	131	0	0	10	0
23	L	307	0	0	10	0
24	J	239	0	0	7	0
25	I	126	0	0	2	0
26	V	431	0	0	6	0
27	M	103	0	0	0	0
28	N	37	0	0	0	0
29	H	63	0	0	0	0
All	All	9403	0	0	52	0

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

The worst 5 of 52 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)
24:J:94:VAL:CA	24:J:233:GLY:CA	1.95	1.44
5:A:294:ASN:CA	5:A:1141:ARG:CA	1.96	1.43
4:E:95:GLY:CA	5:A:707:ARG:CA	1.95	1.42
22:K:669:TYR:CA	23:L:294:VAL:CA	1.98	1.39
24:J:215:ILE:CA	24:J:216:ALA:CA	2.03	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	M	0/145	-	-
28	N	0/106	-	-
29	H	0/116	-	-
All	All	0/367	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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.

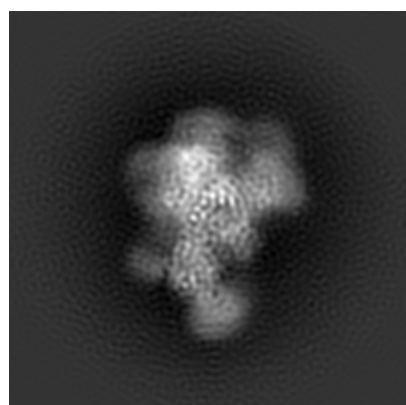
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6581. These allow visual inspection of the internal detail of the map and identification of artifacts.

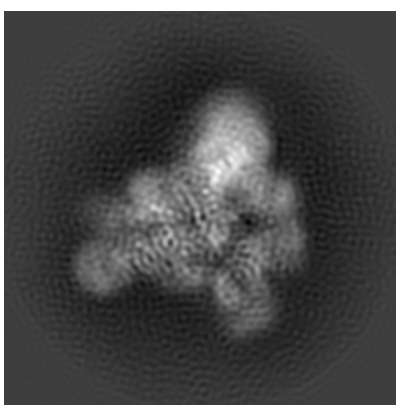
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

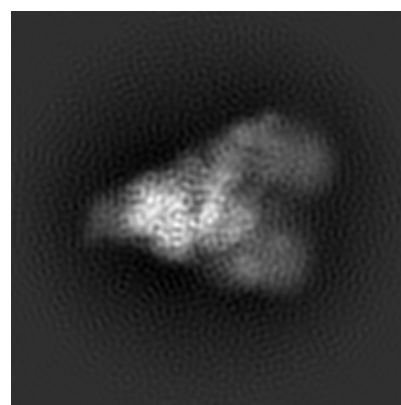
6.1.1 Primary map



X



Y

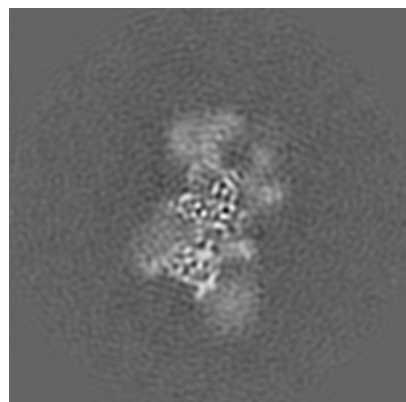


Z

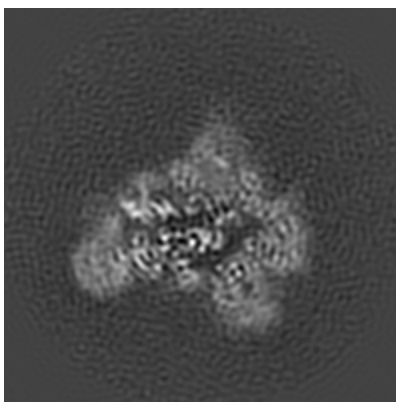
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

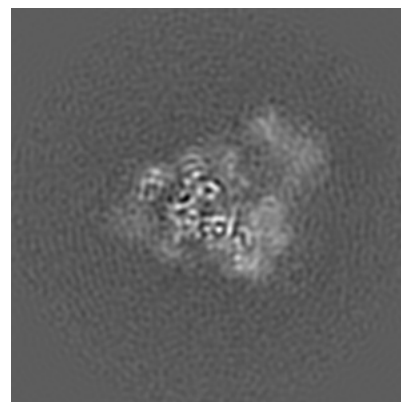
6.2.1 Primary map



X Index: 110



Y Index: 110

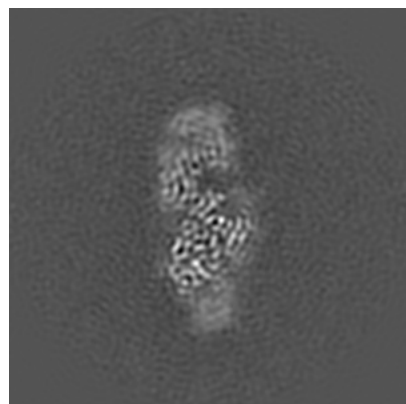


Z Index: 110

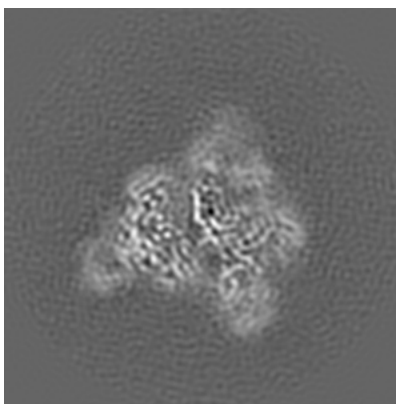
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

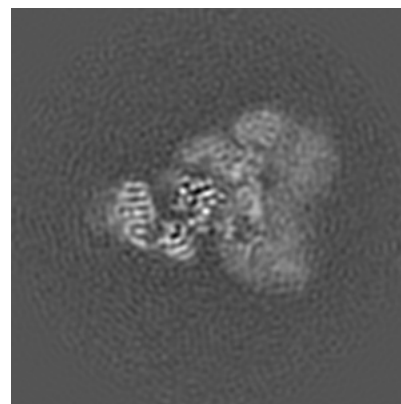
6.3.1 Primary map



X Index: 90



Y Index: 101

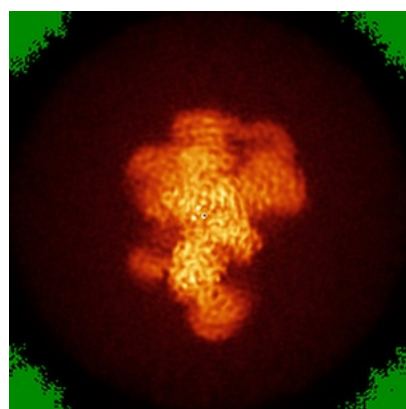


Z Index: 119

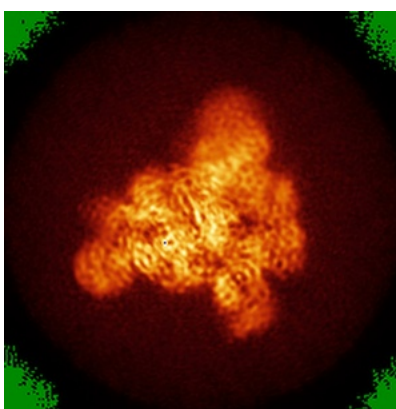
The images above show the largest variance slices of the map in three orthogonal directions.

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

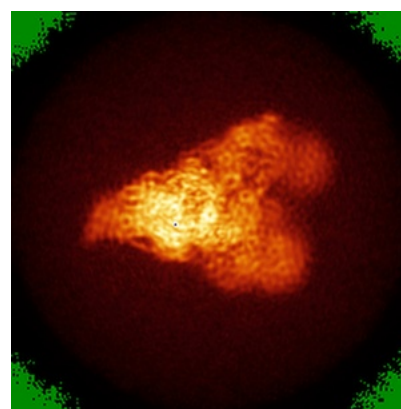
6.4.1 Primary map



X



Y

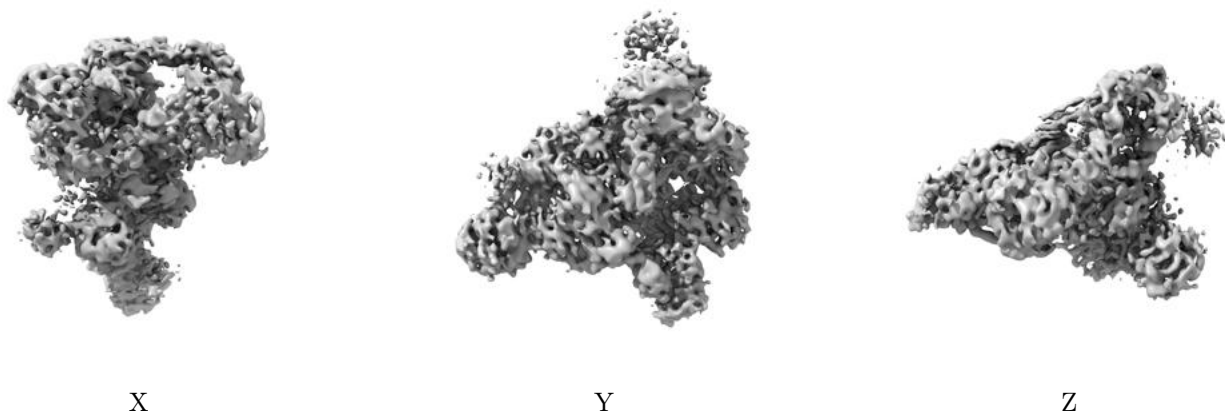


Z

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

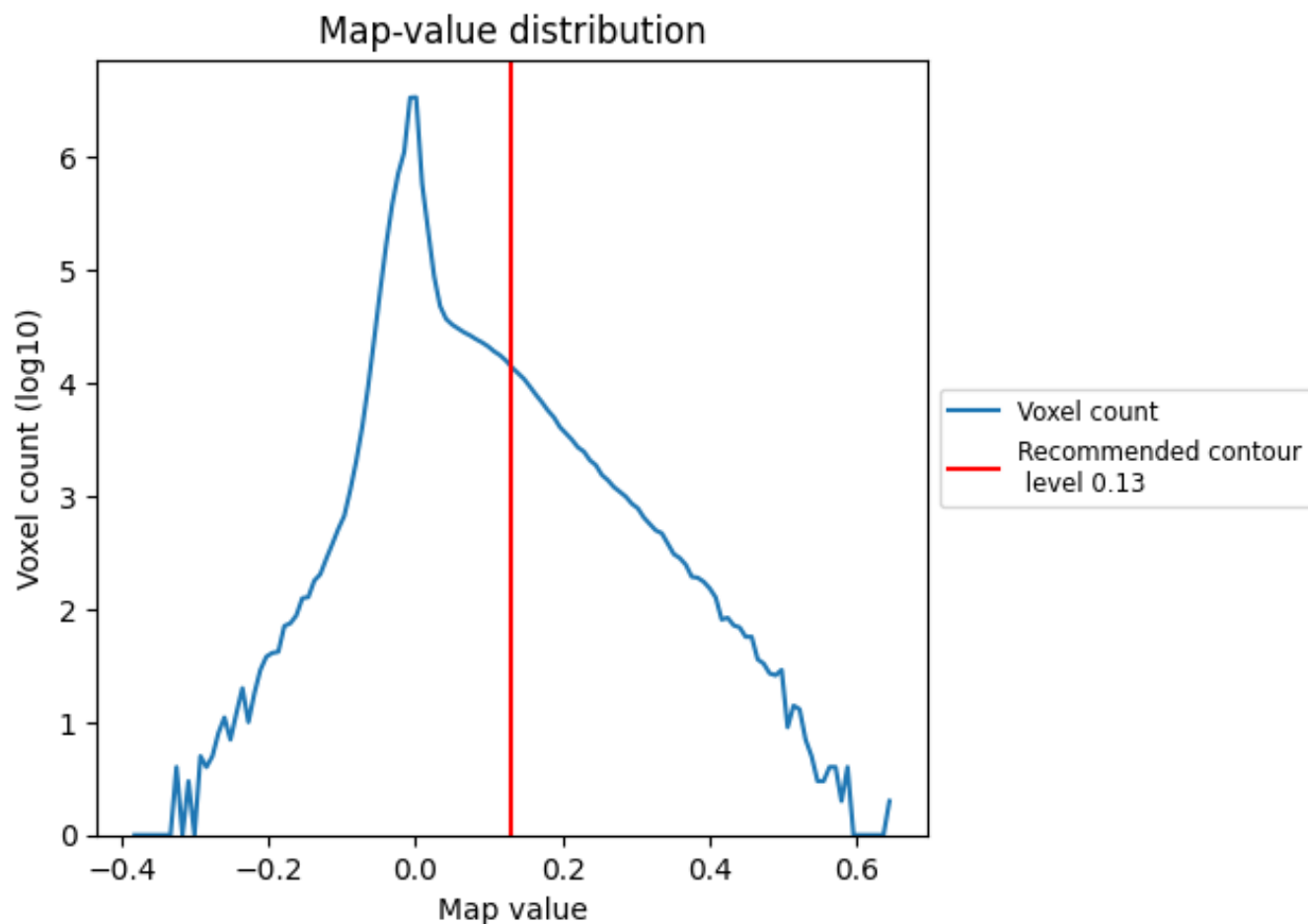
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

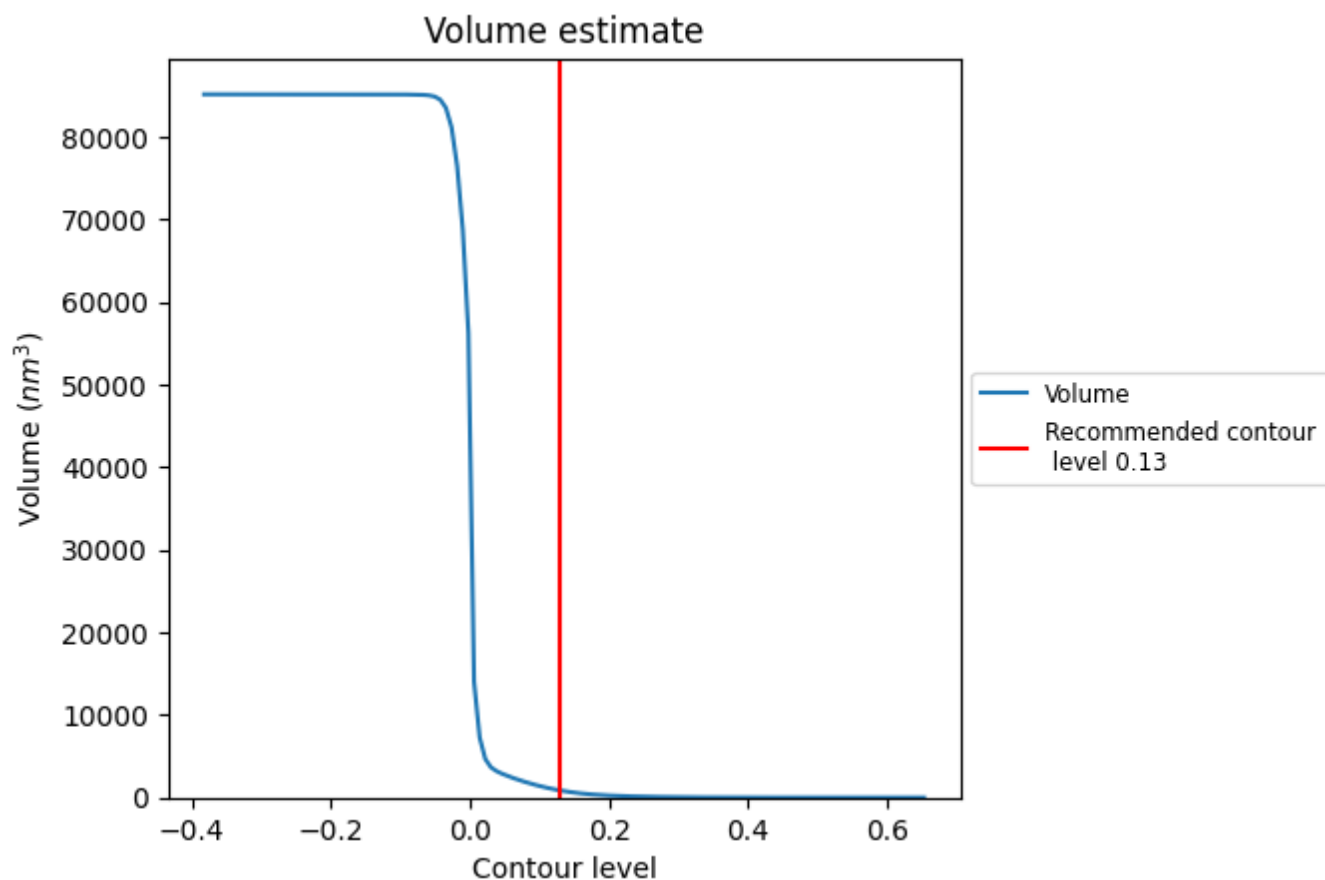
This section contains the results of statistical analysis of the map.

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.

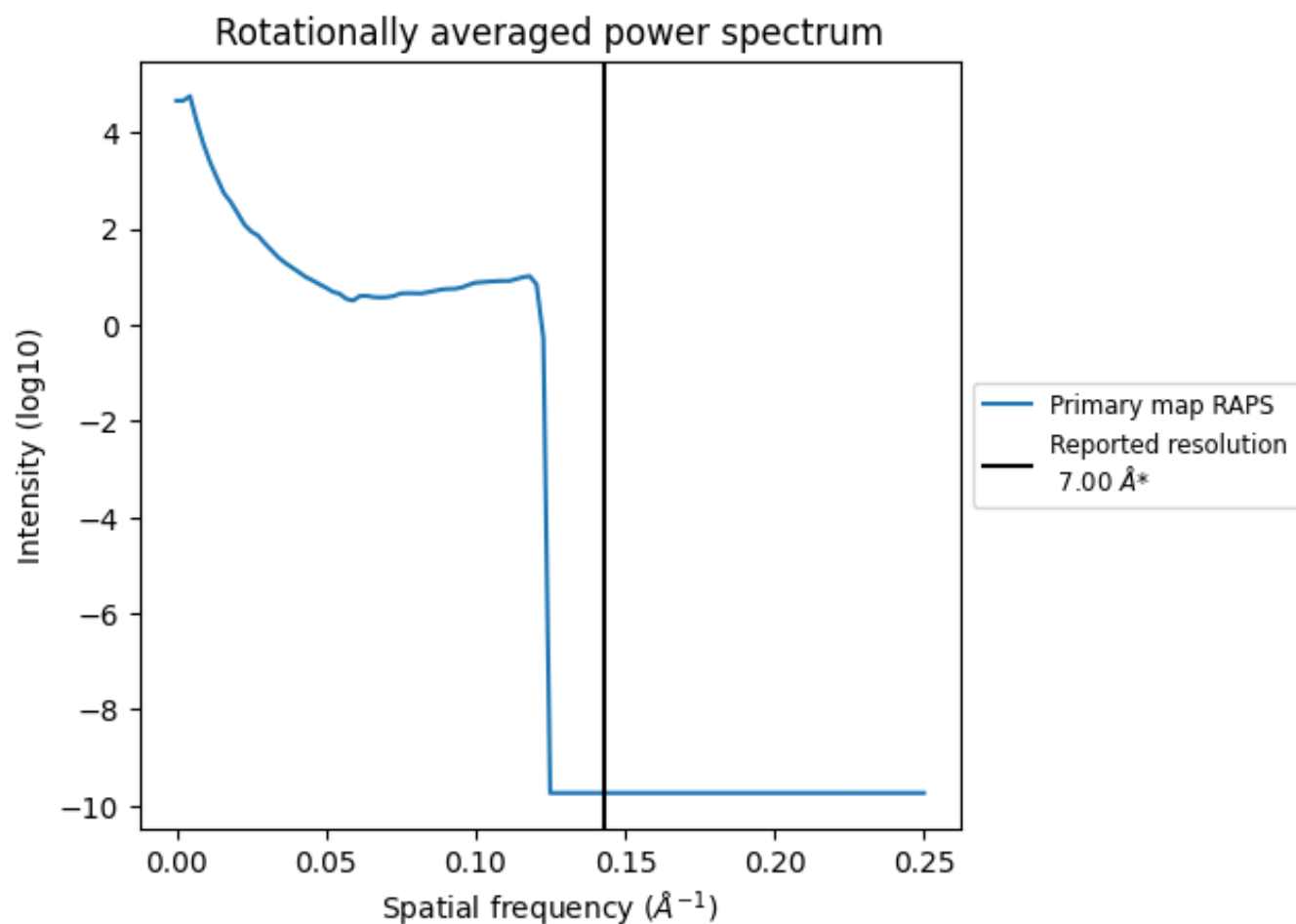
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860 nm³; this corresponds to an approximate mass of 777 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 0.143 Å⁻¹

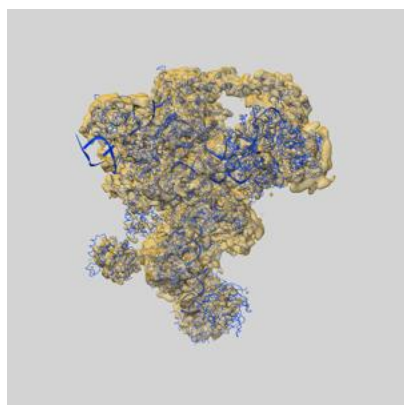
8 Fourier-Shell correlation

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

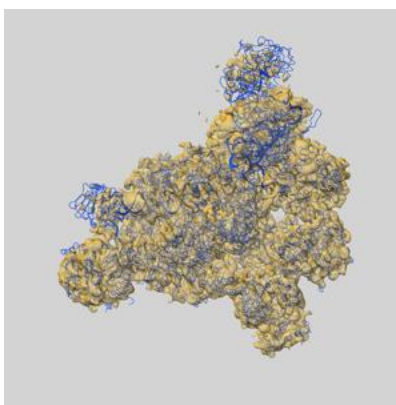
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6581 and PDB model 3JCR. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

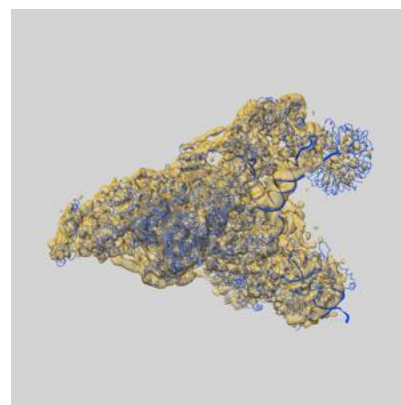
9.1 Map-model overlay [i](#)



X



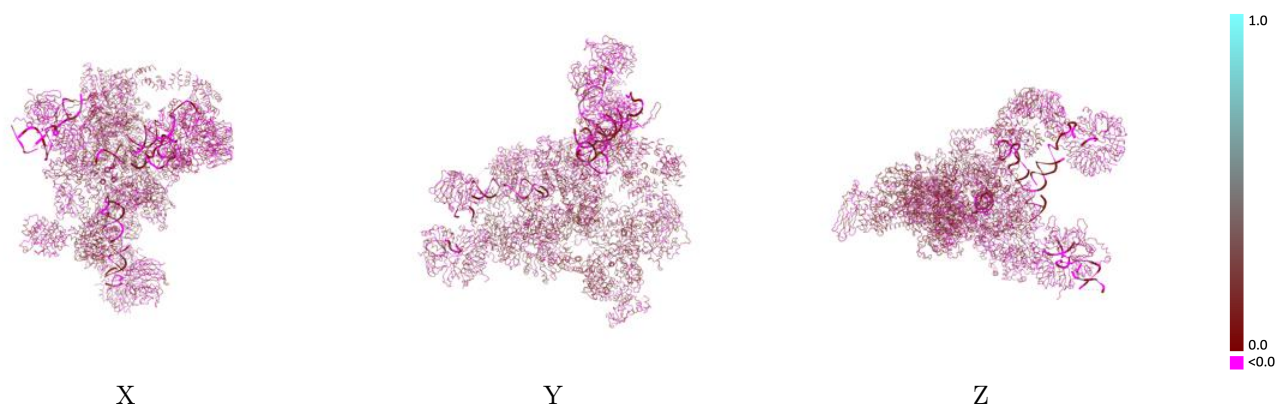
Y



Z

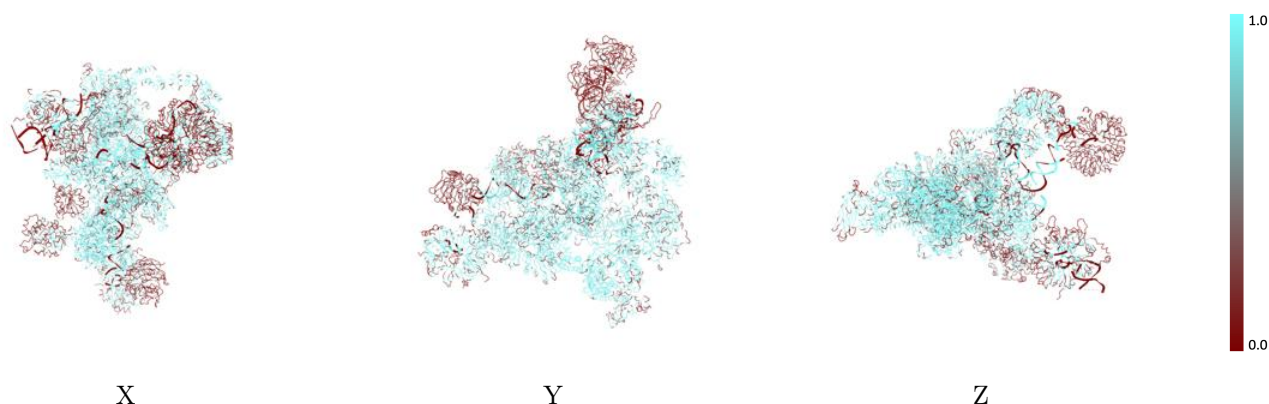
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



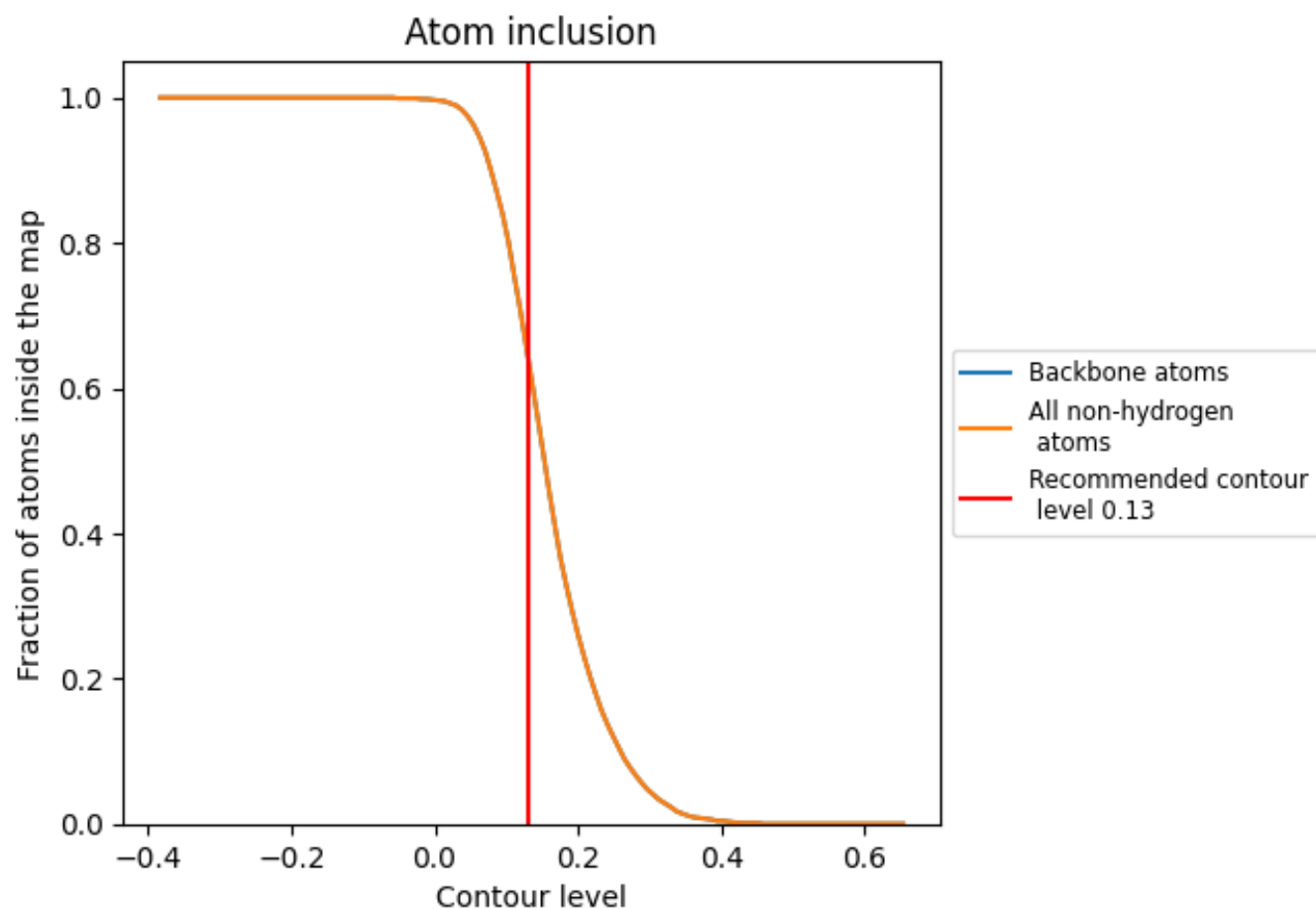
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.0910
2	 0.0110	 0.0190
3	 0.0840	 0.0170
4	 0.0370	 0.0140
5	 0.0130	 0.0110
6	 0.0710	 0.0210
7	 0.0380	 -0.0040
8	 0.1000	 0.0080
A	 0.8070	 0.1250
B	 0.8580	 0.1270
C	 0.8040	 0.1130
D	 0.0800	 0.0290
E	 0.5780	 0.0700
F	 0.2340	 0.0460
G	 0.8110	 0.0990
H	 0.5560	 0.0440
I	 0.7700	 0.1180
J	 0.5440	 0.0800
K	 0.3660	 0.0170
L	 0.6510	 0.0340
M	 0.3400	 0.0260
N	 0.5680	 0.0180
O	 0.5840	 0.0940
P	 0.6240	 0.0990
Q	 0.6630	 0.0960
R	 0.7390	 0.1090
S	 0.5770	 0.0660
T	 0.6030	 0.0890
U	 0.6440	 0.1020
V	 0.7680	 0.1080
o	 0.4160	 0.0430
p	 0.2340	 0.0330
q	 0.2020	 0.0130
r	 0.4550	 0.0020
s	 0.3080	 0.0390



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Chain	Atom inclusion	Q-score
t	 0.1690	 0.0160
u	 0.5750	 0.0900