



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:23 PM UTC

PDB ID : 8QPE / pdb_00008qpe
EMDB ID : EMD-18548
Title : Cryo-EM Structure of Pre-B-like Complex (core part)
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-01
Resolution : 3.10 Å(reported)

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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:

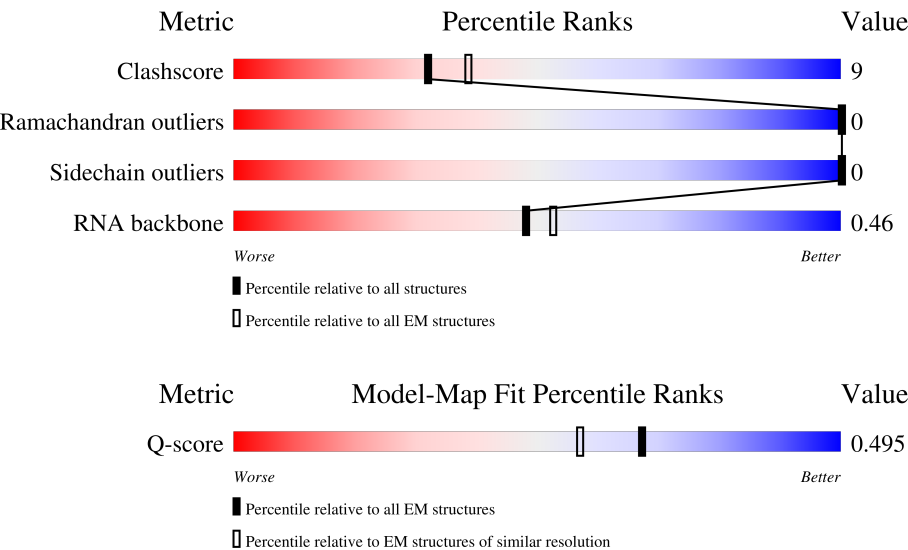
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



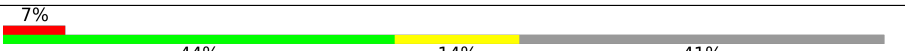
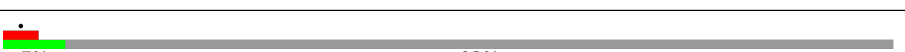
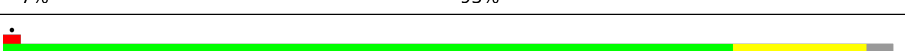
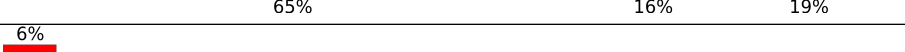
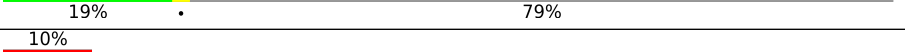
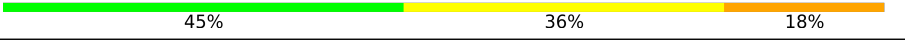
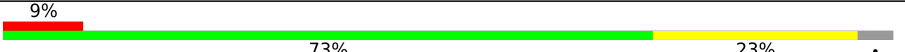
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	4	144	26%17%56%
2	5	117	37% 57%33%8%
3	6	106	14%21%6%59%

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Mol	Chain	Length	Quality of chain
4	7	793	
5	C	972	
6	D	142	
7	I	312	
8	K	439	
9	M	128	
10	U	565	
11	X	376	
12	r	199	
13	z1	11	
14	z2	4	
15	J	683	
16	L	499	
17	F	522	
18	N	941	
19	A	2335	
20	S	800	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 54566 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 RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	63	Total	C	N	O	P	0	0
			1342	599	235	445	63		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	115	Total	C	N	O	P	0	0
			2420	1084	403	818	115		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	43	Total	C	N	O	P	0	0
			926	414	177	292	43		

- Molecule 4 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	81	Total	C	N	O	S	0	0
			650	405	115	128	2		

- Molecule 5 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	836	Total	C	N	O	S	0	0
			6592	4211	1110	1238	33		

- Molecule 6 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	141	Total	C	N	O	S	0	0
			1170	751	194	215	10		

- Molecule 7 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	183	Total	C	N	O	S	0	0
			1513	973	255	276	9		

- Molecule 8 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	31	Total	C	N	O		0	0
			159	96	32	31			

- Molecule 9 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 10 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	456	Total	C	N	O	S	0	0
			3742	2421	635	672	14		

- Molecule 11 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	80	Total	C	N	O	S	0	0
			657	413	116	124	4		

- Molecule 12 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	89	Total	C	N	O	S	0	0
			728	452	137	132	7		

- Molecule 13 is a RNA chain called oligo1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	z1	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 14 is a RNA chain called oligo2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z2	4	Total	C	N	O	P	0	0
			90	40	20	26	4		

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	224	Total	C	N	O	S	0	0
			1806	1135	345	318	8		

- Molecule 16 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	376	Total	C	N	O	S	0	0
			2871	1785	522	551	13		

- Molecule 17 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	404	Total	C	N	O	S	0	0
			3194	2005	582	587	20		

- Molecule 18 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	831	Total	C	N	O	S	0	0
			6071	3787	1132	1128	24		

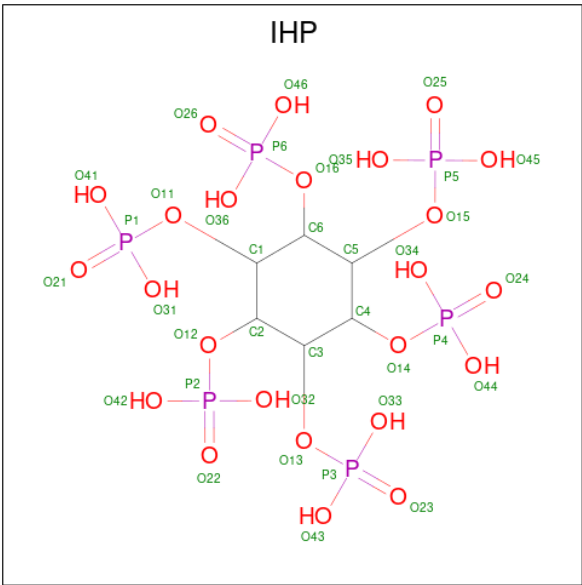
- Molecule 19 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	2247	Total	C	N	O	S	0	0
			18231	11711	3189	3258	73		

- Molecule 20 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	148	Total	C	N	O	S	0	0
			1167	727	216	222	2		

- Molecule 21 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).

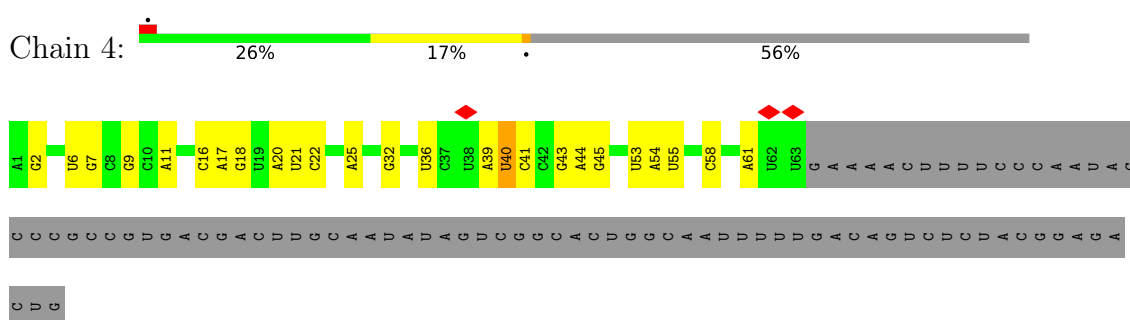


Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			36	6	24	6	

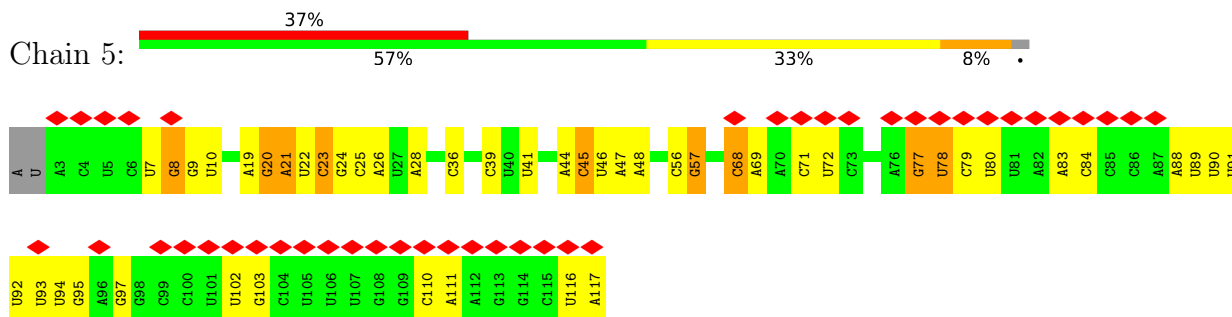
3 Residue-property plots [i](#)

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.

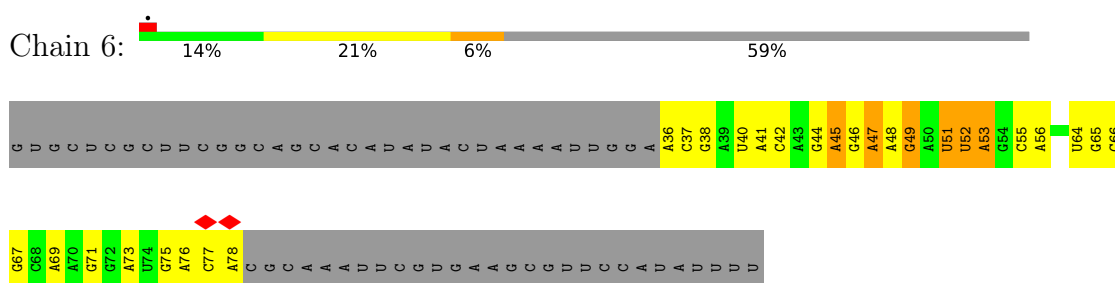
• Molecule 1: U4 snRNA



• Molecule 2: U5 snRNA



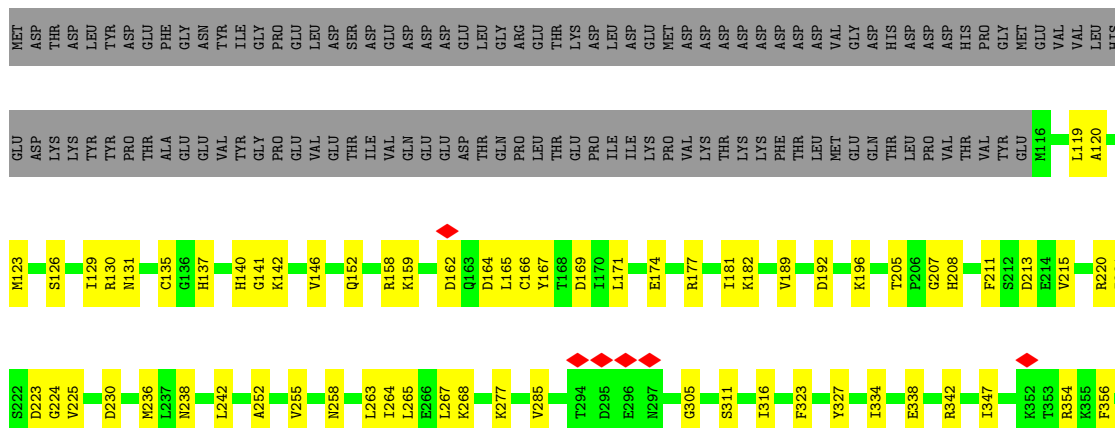
• Molecule 3: U6 snRNA



• Molecule 4: Splicing factor 3A subunit 1



- Molecule 5: 116 kDa U5 small nuclear ribonucleoprotein component



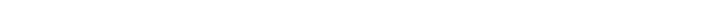
[illegible]

- Molecule 9: NHP2-like protein 1, N-terminally processed

Chain M: 82% 15%

MET	THR	GLU	ALA
D6	V6	Y11	P12
L13	A14	L18	L22
N40	K44	V55	M56
E64	N77	Y80	V81
F82	R91	C102	I123
L126	L127	V128	

- Molecule 10: Ubiquitin carboxyl-terminal hydrolase 39

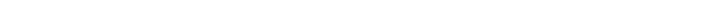
Chain U: 

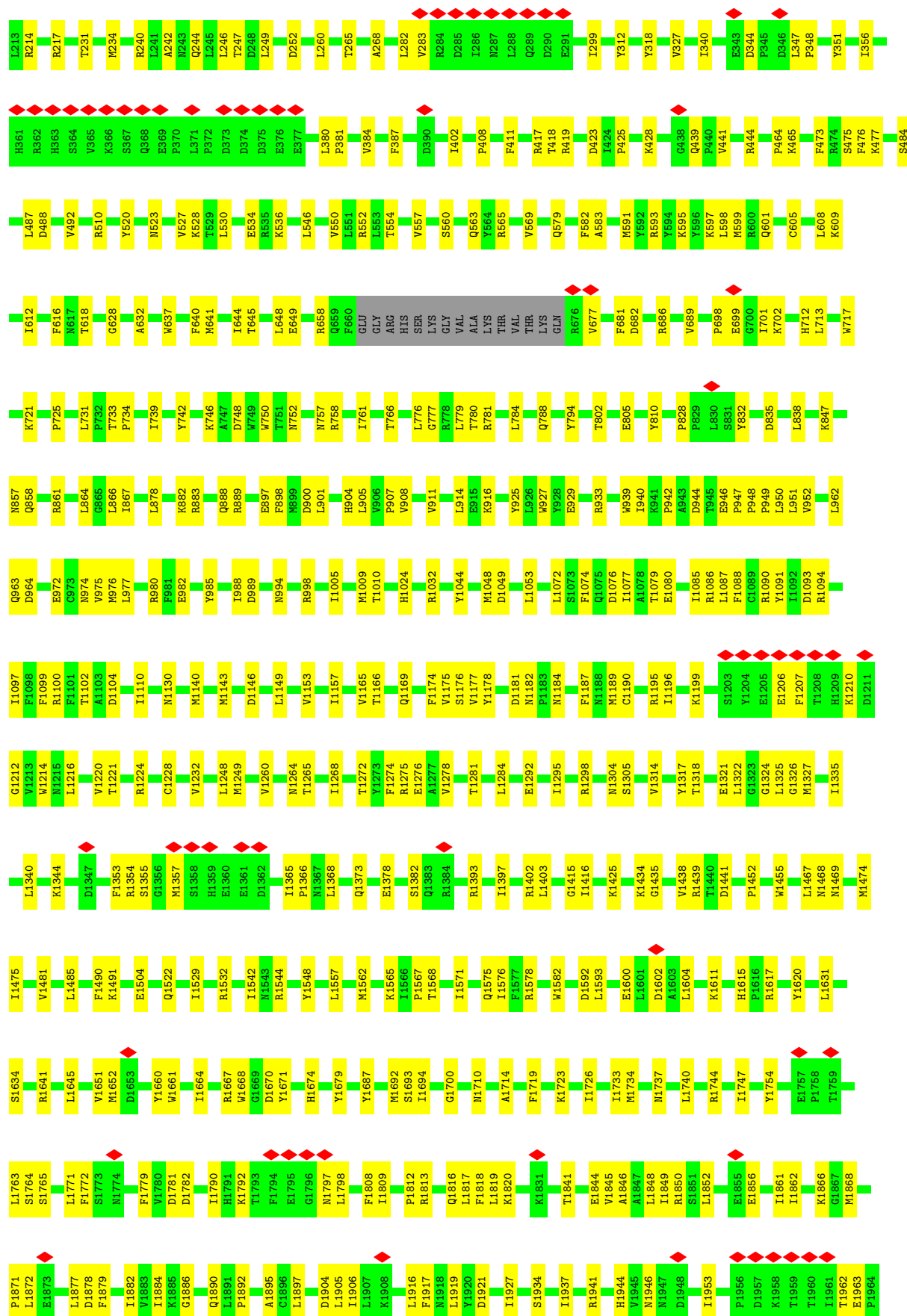
V303	L243	D183	E121	GLU	MET
V304	S244	S184	K122	ALA	SER
L305	N245	S185	L123	PRO	GLY
C306	N246	L186	C124	SER	SER
S307	P247	E187	S125	VAL	LYS
K308	P248	D188	I126	VAL	ARG
K309	L249	T189	I127	PRO	GLU
T310	R250	T190	S128	PHE	SER
F311	N251	T191	S129	VAL	ARG
Q312	Y252	V192	H130	VAL	GLY
I313	F253	L193	I131	LYS	THR
T314	L254	K194	M132	ARG	GLY
K315	E255	P195	A133	ARG	LYS
Q316	E256	T196	Y134	GLU	ARG
Q317	D257	F197	A135	VAL	GLU
D318	N258	T198	C136	ASP	SER
G319	Y259	K199	L137	ASP	SER
V320	K260	Q200	V138	SER	ARG
D321	N261	Q201	C139	GLU	GLY
F322	I262	I202	G140	PRO	SER
L323	K263	A203	K141	GLU	SER
F326	R264	N204	Y142	ARG	GLY
L327	P265	L205	F143	VAL	VAL
N328	P266	D206	Q144	ARG	LYS
N329	G267	K207	G145	ALA	ARG
L330	D268	Q208	R146	LYS	GLU
H331	I269	A209	G147	ASN	ARG
S332	M270	K210	L148	GLY	ASP
A333	F271	L211	K149	ARG	ARG
L334	L272	S212	S150	VAL	GLU
G335	V273	R213	H151	ASP	GLU
G336	Q275	A214	I154	ASP	GLU
K337	R276	Y215	I157	R100	ALA
K338	P277	D216	Q158	R101	ALA
K339	G278	G217	F159	S102	SER
K340	E279	T218	S160	R103	SER
K341	L280	T219	H161	H104	GLY
K342	M281	Y220	H162	C105	SER
T343	R282	L221	V163	P106	PRO
I344	K283	P222	F164	Y107	VAL
V345	L284	G223	L165	L108	ARG
T346	W285	I224	M166	D109	LYS
D347	N286	V225	L167	T110	ARG
V348	P287	G226	H168	I111	GLU
F349	R288	L227	T169	M112	PHE
Q350	N289	N228	L170	R113	GLU
G351	F290	M229	K171	S114	PRO
S352	K291	T230	F172	V115	ALA
M353	A292	K231	Y173	L116	SER
R354	H293	A232	C174	D117	ALA
I355	V294	N233	L175	F118	ALA
F356	S295	D234	P176	D119	ARG
T357	P296	Y235	D177	F120	
K358	H297	A236	M178		
K359	E298	N237	Y179		
L360	M299	K238	I180		
P361	L300	V239	I181		
H362	Q301	L240	I182		
P363	A302	Q241			
		A242			

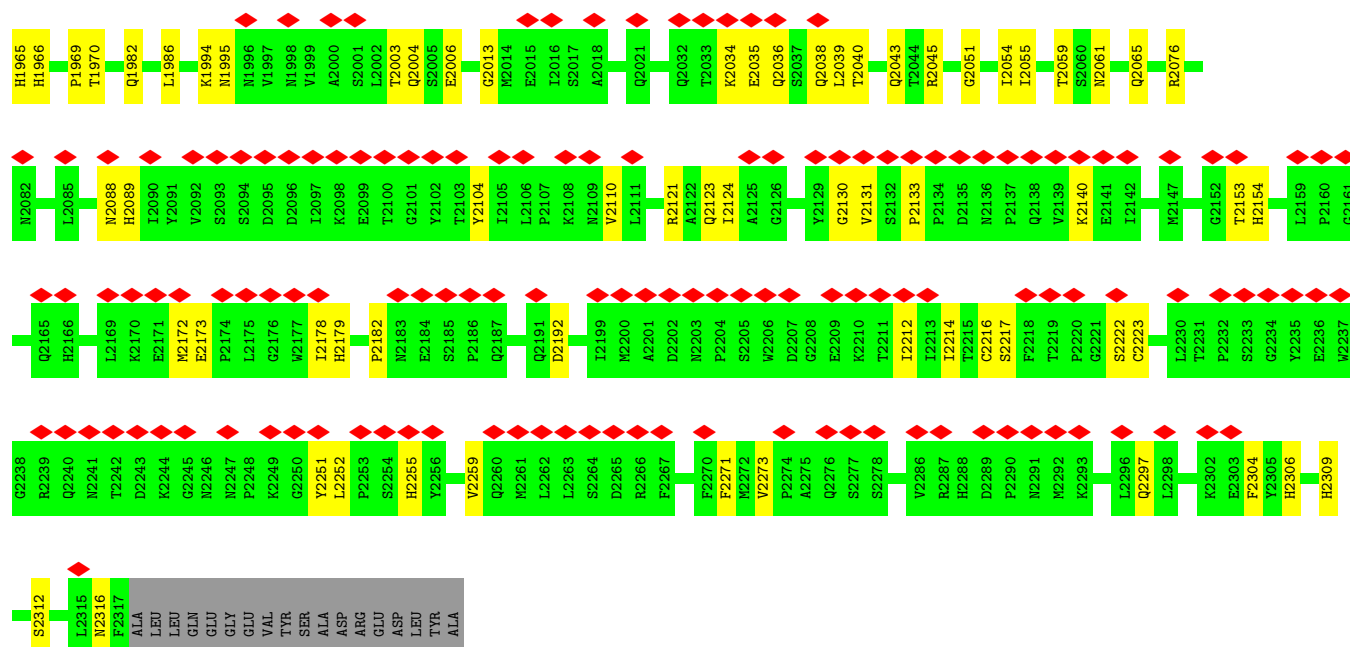
A-3	A-2	G-1	G1	U2	A3	A4	G5		U8
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- A-3 G1

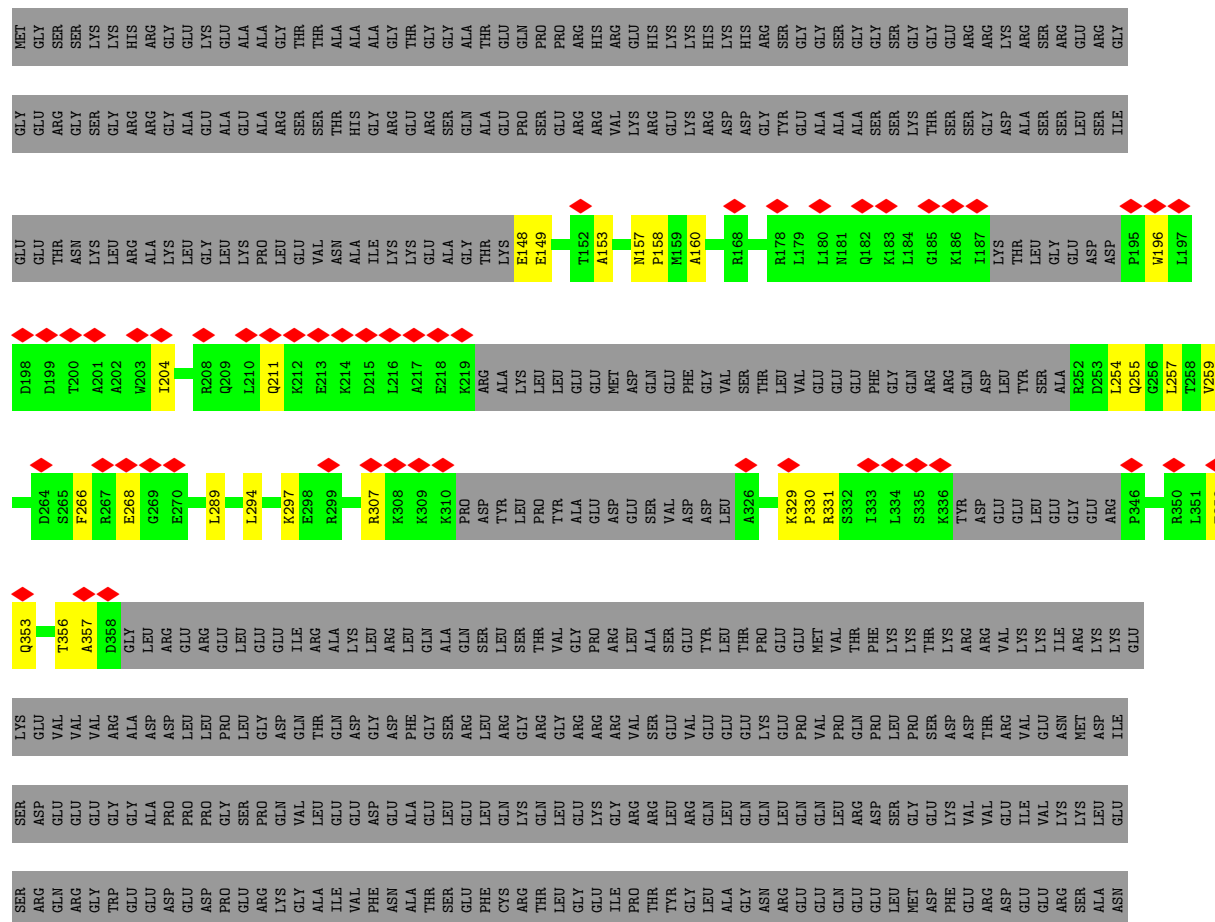
- [illegible]

- Chain L:  9% 60% 16% 25%





• Molecule 20: U4/U6.U5 tri-snRNP-associated protein 1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.414	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	675.0, 675.0, 675.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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	4	0.09	0/1499	0.14	0/2334
2	5	0.08	0/2698	0.17	0/4195
3	6	0.12	0/1038	0.28	0/1617
4	7	0.11	0/659	0.27	0/884
5	C	0.10	0/6739	0.25	0/9151
6	D	0.12	0/1199	0.25	0/1620
7	I	0.08	0/1543	0.23	0/2080
8	K	0.05	0/158	0.16	0/218
9	M	0.11	0/974	0.25	0/1316
10	U	0.08	0/3837	0.24	0/5197
11	X	0.08	0/670	0.19	0/892
12	r	0.13	0/736	0.32	0/978
13	z1	0.12	0/268	0.21	0/416
14	z2	0.09	0/101	0.25	0/156
15	J	0.14	0/1833	0.28	0/2447
16	L	0.10	0/2909	0.25	0/3922
17	F	0.10	0/3271	0.27	0/4430
18	N	0.10	0/6168	0.27	0/8371
19	A	0.12	0/18724	0.27	0/25448
20	S	0.09	0/1175	0.24	0/1571
All	All	0.11	0/56199	0.25	0/77243

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	4	1342	0	676	14	0
2	5	2420	0	1226	18	0
3	6	926	0	468	30	0
4	7	650	0	655	11	0
5	C	6592	0	6615	120	0
6	D	1170	0	1141	17	0
7	I	1513	0	1532	32	0
8	K	159	0	78	1	0
9	M	962	0	1012	15	0
10	U	3742	0	3762	58	0
11	X	657	0	645	6	0
12	r	728	0	759	16	0
13	z1	239	0	119	3	0
14	z2	90	0	45	1	0
15	J	1806	0	1896	46	0
16	L	2871	0	2848	59	0
17	F	3194	0	3125	61	0
18	N	6071	0	5694	112	0
19	A	18231	0	17841	381	0
20	S	1167	0	1182	23	0
21	A	36	0	6	1	0
All	All	54566	0	51325	895	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 9.

The worst 5 of 895 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)
19:A:1146:ASP:HB2	19:A:1177:VAL:HG21	1.55	0.87
16:L:383:ILE:HA	19:A:1321:GLU:HG3	1.64	0.80
18:N:818:ILE:HG22	18:N:830:SER:OG	1.83	0.79
7:I:114:ILE:HG23	7:I:177:LEU:HD21	1.64	0.79
19:A:2110:VAL:HG23	19:A:2271:PHE:HE1	1.47	0.78

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	
4	7	79/793 (10%)	77 (98%)	2 (2%)	0	100	100
5	C	834/972 (86%)	815 (98%)	19 (2%)	0	100	100
6	D	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
7	I	181/312 (58%)	176 (97%)	5 (3%)	0	100	100
8	K	29/439 (7%)	29 (100%)	0	0	100	100
9	M	122/128 (95%)	122 (100%)	0	0	100	100
10	U	454/565 (80%)	447 (98%)	7 (2%)	0	100	100
11	X	78/376 (21%)	78 (100%)	0	0	100	100
12	r	87/199 (44%)	86 (99%)	1 (1%)	0	100	100
15	J	220/683 (32%)	217 (99%)	3 (1%)	0	100	100
16	L	372/499 (74%)	365 (98%)	7 (2%)	0	100	100
17	F	400/522 (77%)	387 (97%)	13 (3%)	0	100	100
18	N	823/941 (88%)	799 (97%)	24 (3%)	0	100	100
19	A	2243/2335 (96%)	2208 (98%)	35 (2%)	0	100	100
20	S	138/800 (17%)	137 (99%)	1 (1%)	0	100	100
All	All	6199/9706 (64%)	6081 (98%)	118 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7	71/709 (10%)	71 (100%)	0	100	100
5	C	738/866 (85%)	738 (100%)	0	100	100
6	D	129/130 (99%)	129 (100%)	0	100	100
7	I	166/293 (57%)	166 (100%)	0	100	100
8	K	1/395 (0%)	1 (100%)	0	100	100
9	M	108/111 (97%)	108 (100%)	0	100	100
10	U	417/511 (82%)	417 (100%)	0	100	100
11	X	68/333 (20%)	68 (100%)	0	100	100
12	r	84/181 (46%)	84 (100%)	0	100	100
15	J	193/599 (32%)	193 (100%)	0	100	100
16	L	299/424 (70%)	299 (100%)	0	100	100
17	F	344/442 (78%)	344 (100%)	0	100	100
18	N	547/792 (69%)	547 (100%)	0	100	100
19	A	1942/2108 (92%)	1942 (100%)	0	100	100
20	S	121/681 (18%)	121 (100%)	0	100	100
All	All	5228/8575 (61%)	5228 (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. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
18	N	308	HIS
19	A	368	GLN
19	A	2255	HIS
19	A	105	ASN
19	A	326	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	4	62/144 (43%)	14 (22%)	0
13	z1	10/11 (90%)	5 (50%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	z2	3/4 (75%)	0	0
2	5	114/117 (97%)	32 (28%)	2 (1%)
3	6	42/106 (39%)	10 (23%)	3 (7%)
All	All	231/382 (60%)	61 (26%)	5 (2%)

5 of 61 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	4	9	G
1	4	11	A
1	4	22	C
1	4	25	A
1	4	36	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	77	G
2	5	78	U
3	6	45	A
3	6	51	U
3	6	77	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	IHP	A	2401	-	36,36,36	0.74	0	60,60,60	1.15	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	IHP	A	2401	-	-	1/30/54/54	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2401	IHP	C3-C2-C1	2.79	116.54	110.43
21	A	2401	IHP	P3-O13-C3	-2.30	117.29	123.43
21	A	2401	IHP	P1-O11-C1	-2.09	117.84	123.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	2401	IHP	C4-O14-P4-O44

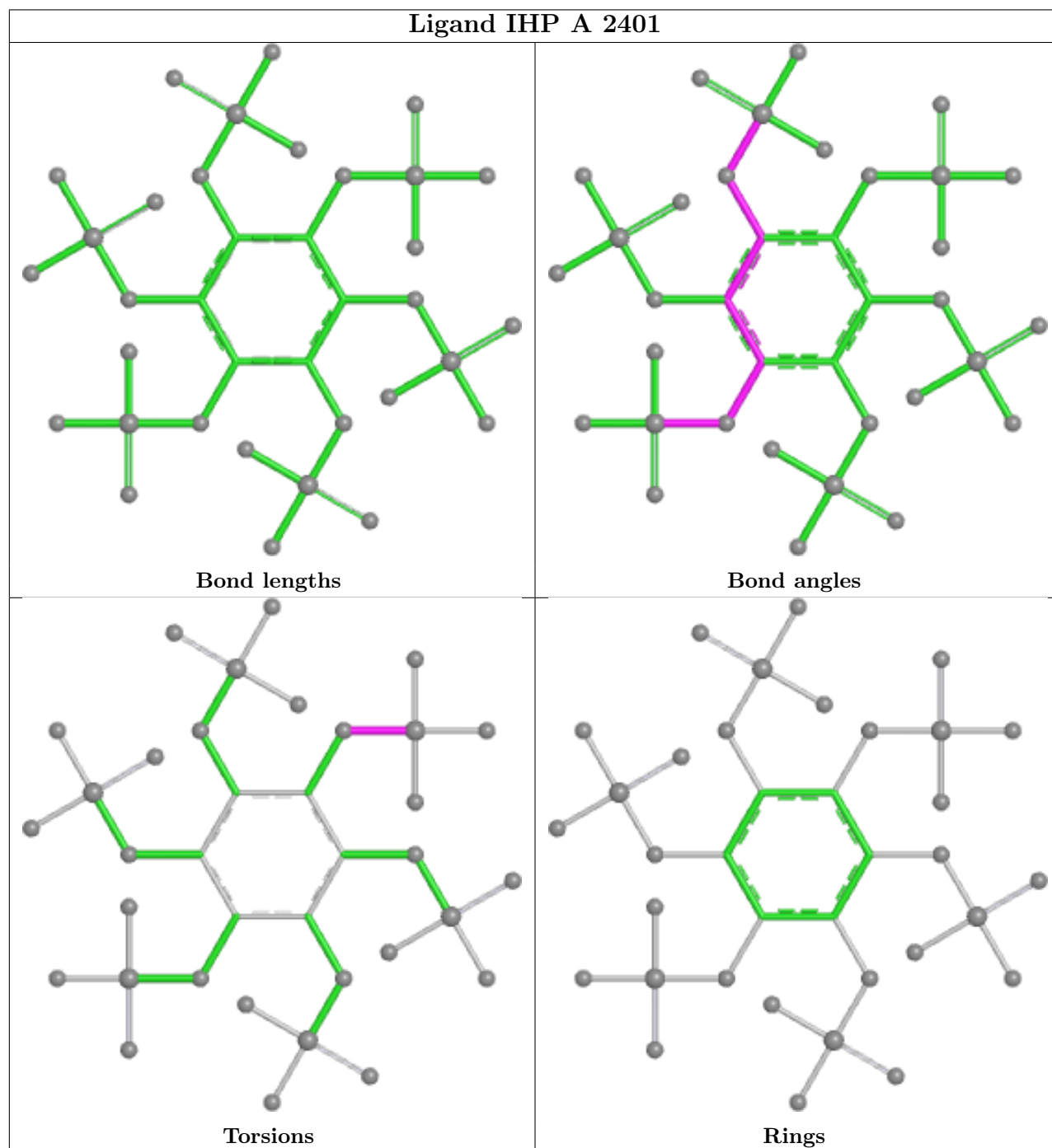
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	2401	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

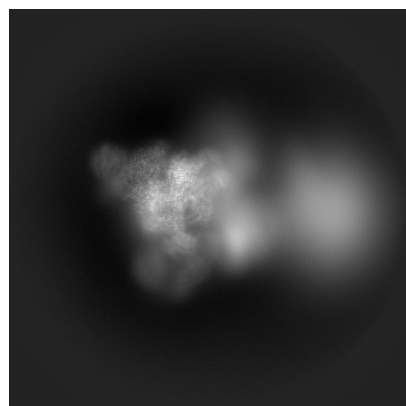
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18548. These allow visual inspection of the internal detail of the map and identification of artifacts.

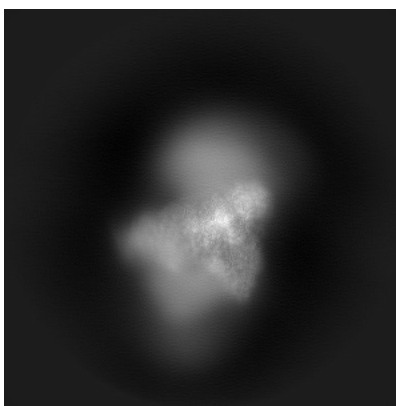
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

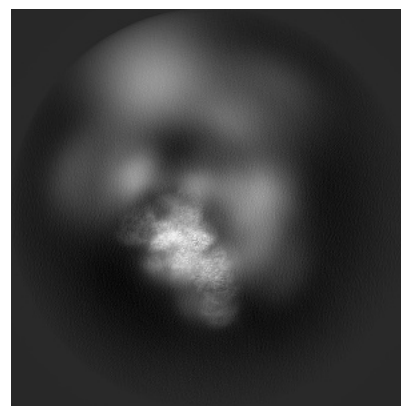
6.1.1 Primary map



X

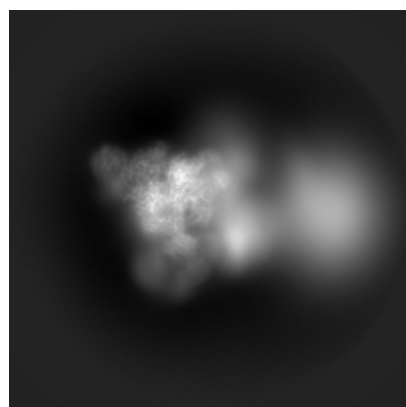


Y

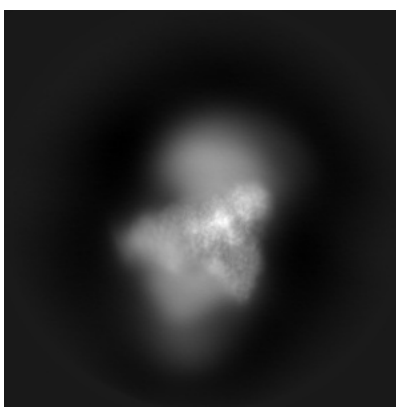


Z

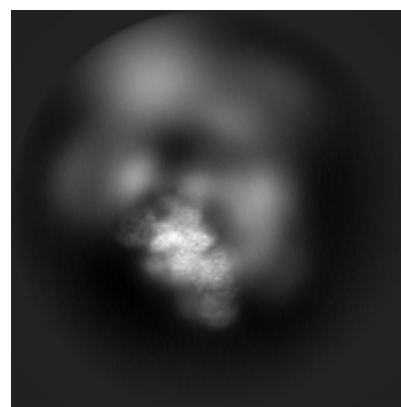
6.1.2 Raw map



X



Y



Z

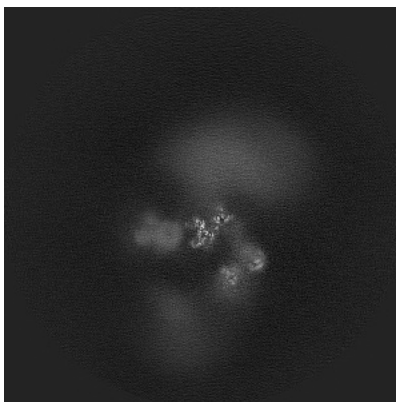
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

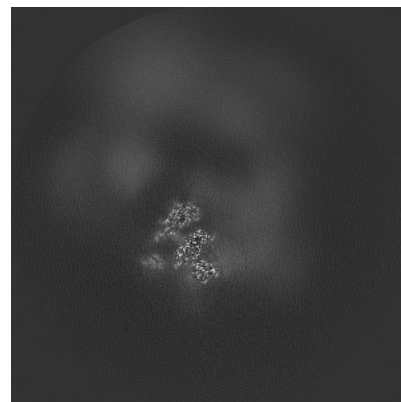
6.2.1 Primary map



X Index: 250

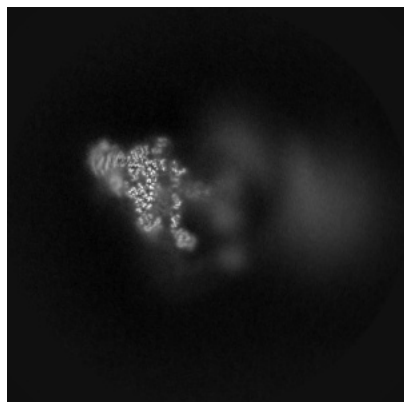


Y Index: 250

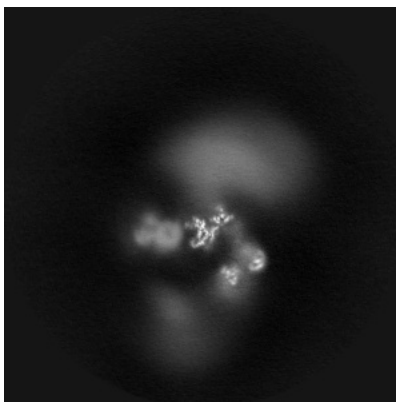


Z Index: 250

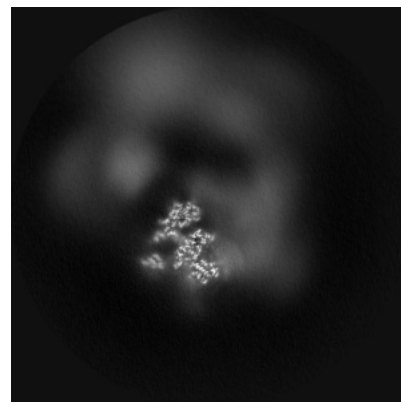
6.2.2 Raw map



X Index: 250



Y Index: 250

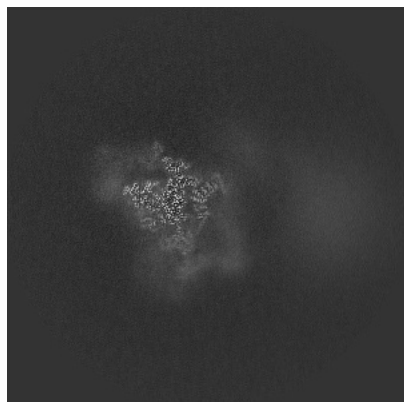


Z Index: 250

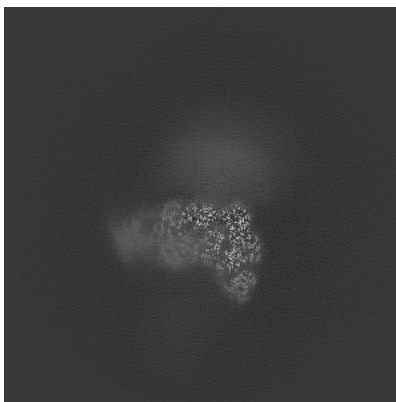
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

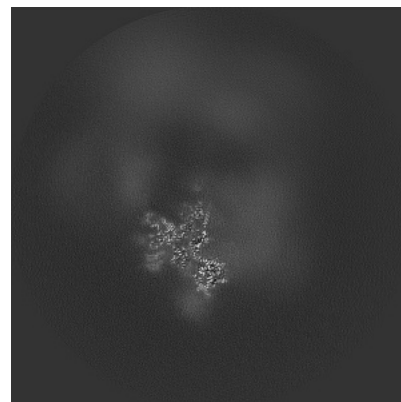
6.3.1 Primary map



X Index: 233

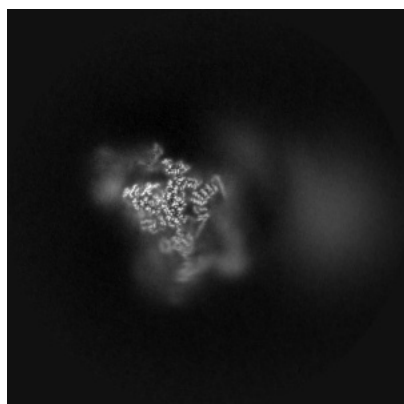


Y Index: 213

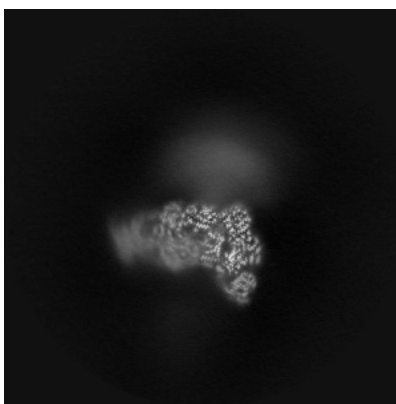


Z Index: 266

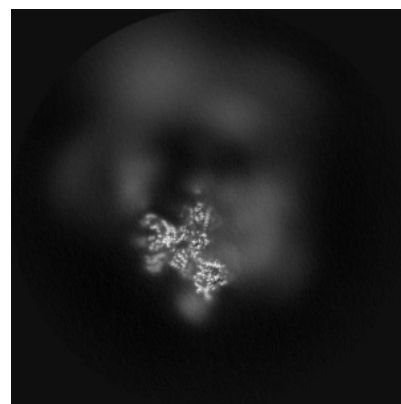
6.3.2 Raw map



X Index: 233



Y Index: 213

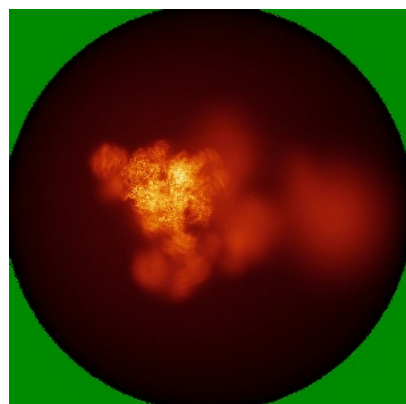


Z Index: 267

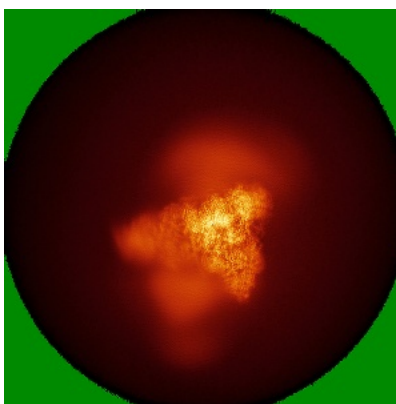
The images above show the largest variance slices of the map in three orthogonal directions.

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

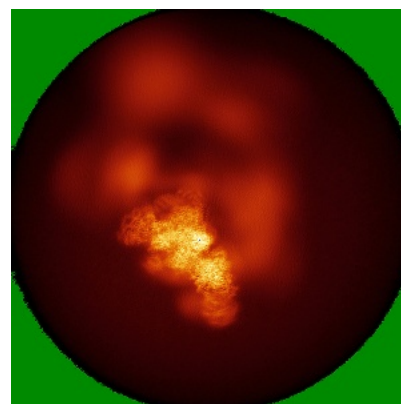
6.4.1 Primary map



X

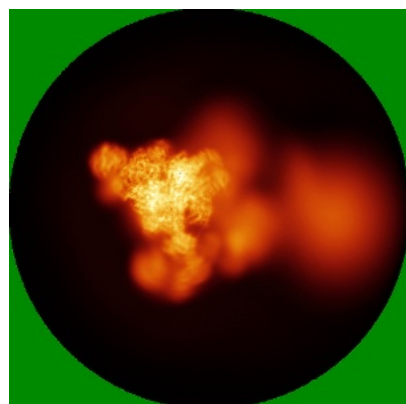


Y

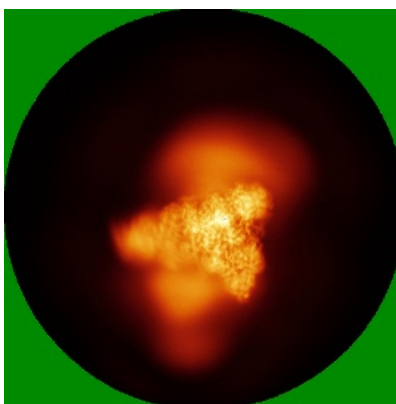


Z

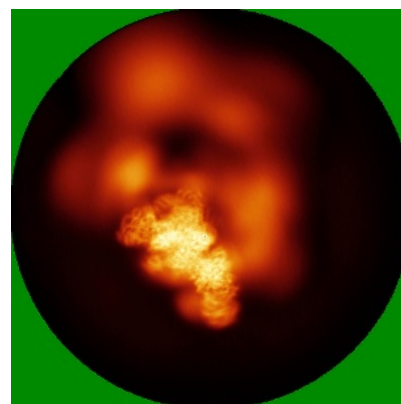
6.4.2 Raw map



X



Y

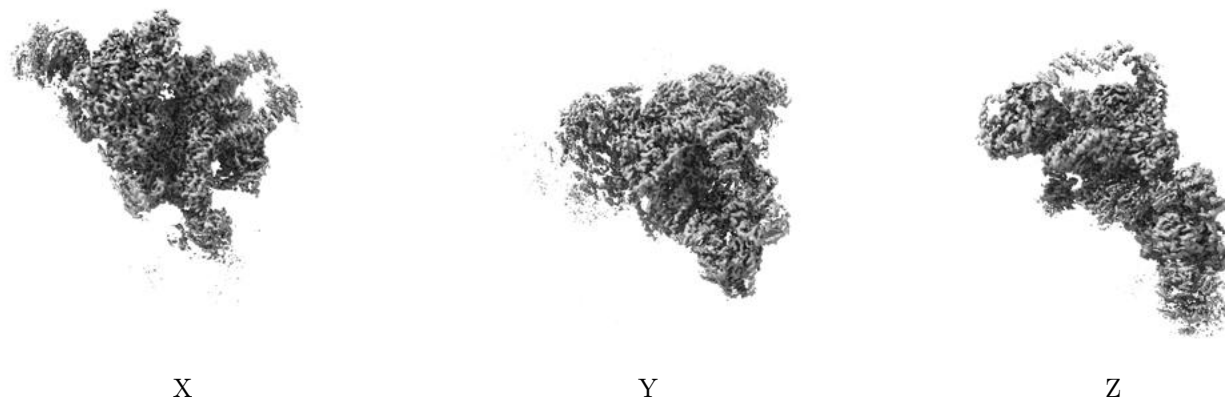


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

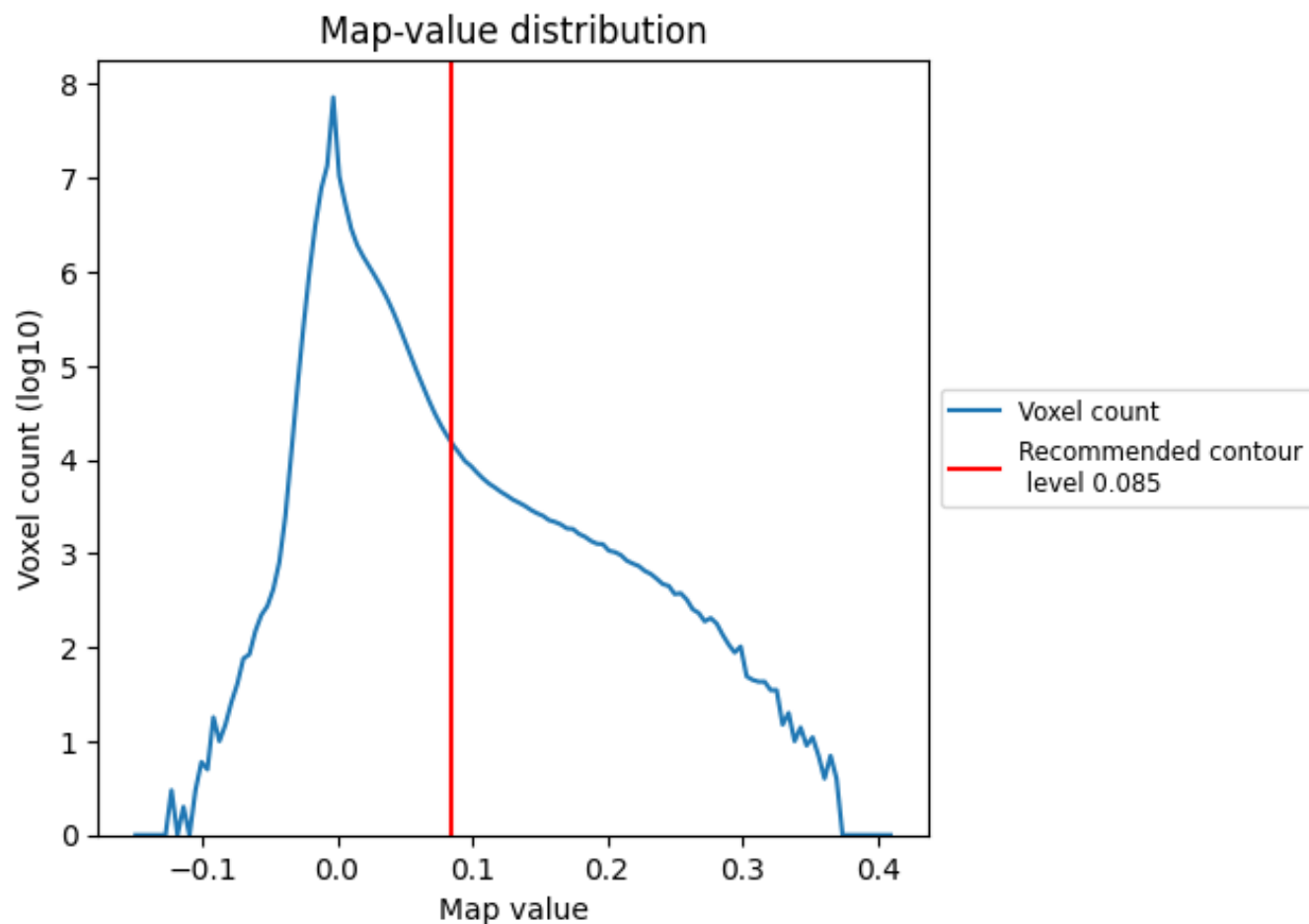
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

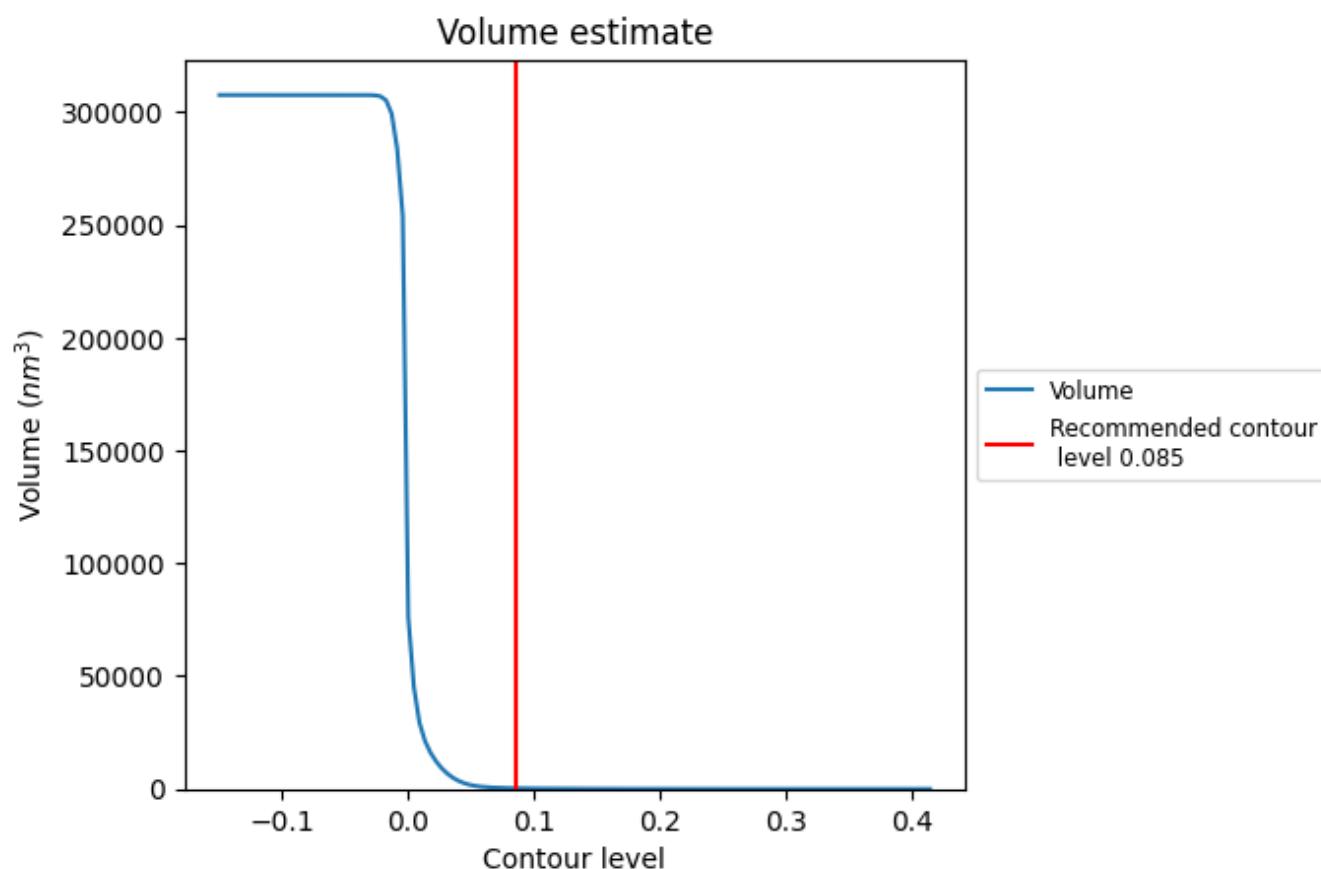
This section contains the results of statistical analysis of the map.

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.

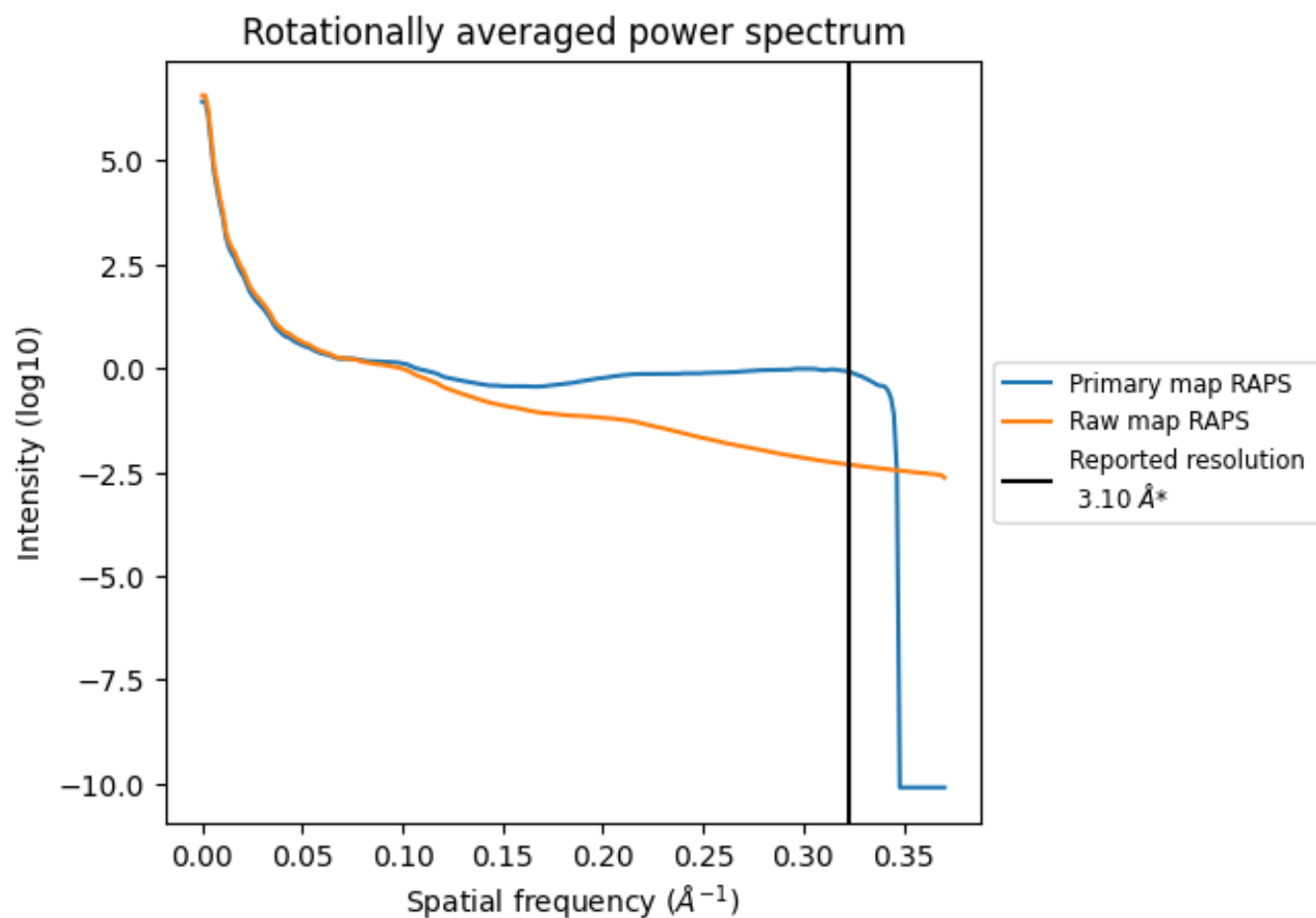
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 313 nm³; this corresponds to an approximate mass of 283 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 ⓘ

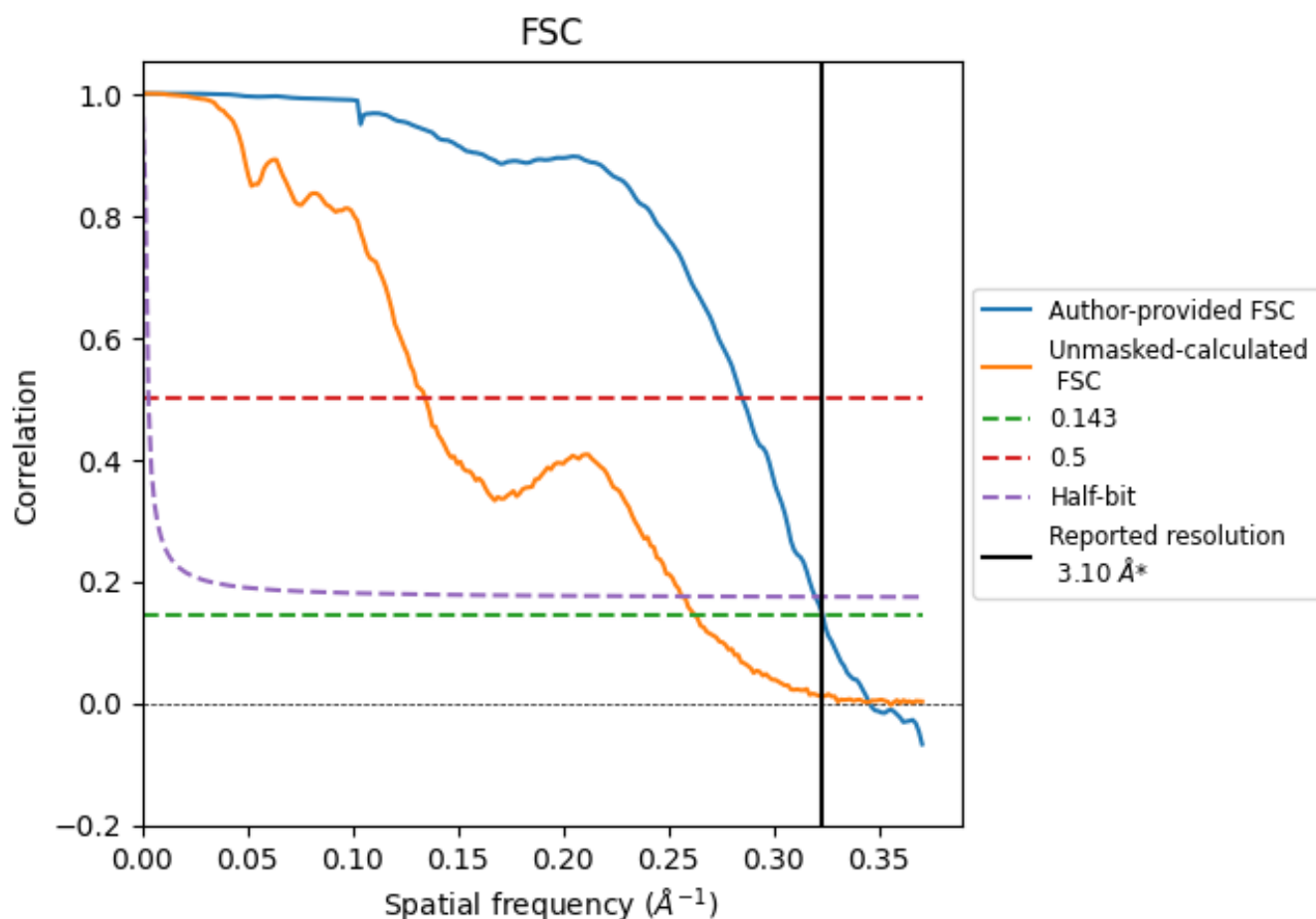


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

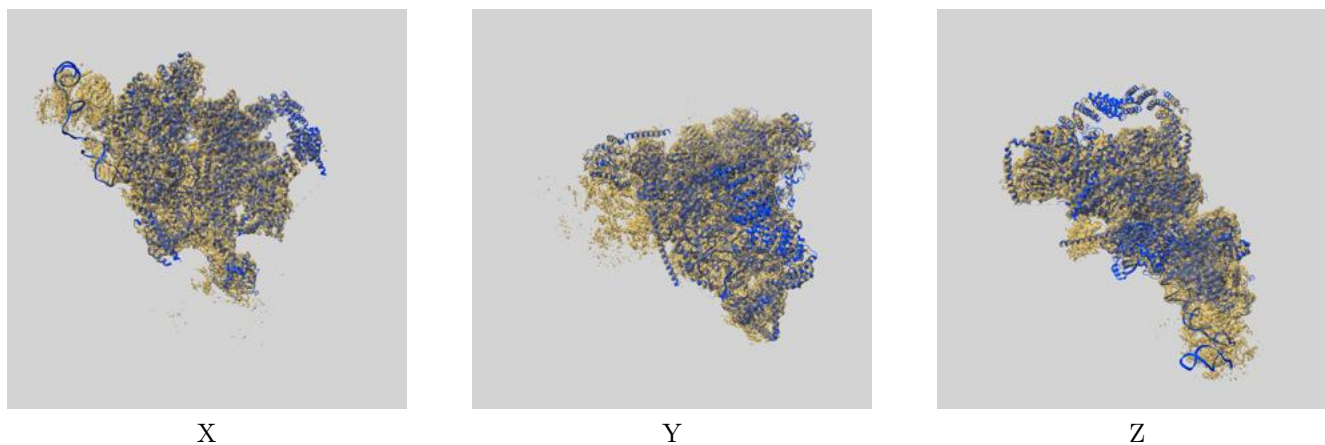
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.51	3.13
Unmasked-calculated*	3.81	7.44	3.90

*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 3.81 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

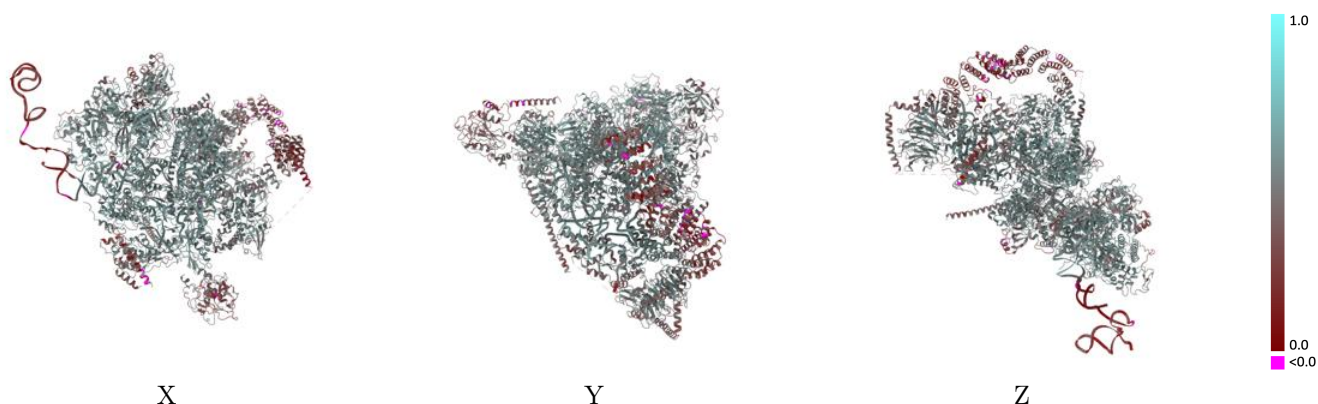
This section contains information regarding the fit between EMDB map EMD-18548 and PDB model 8QPE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



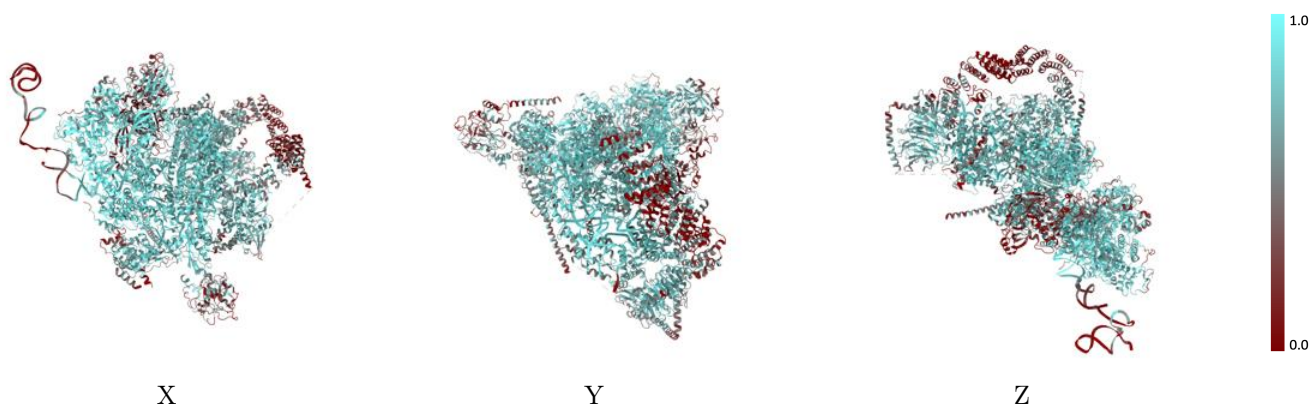
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



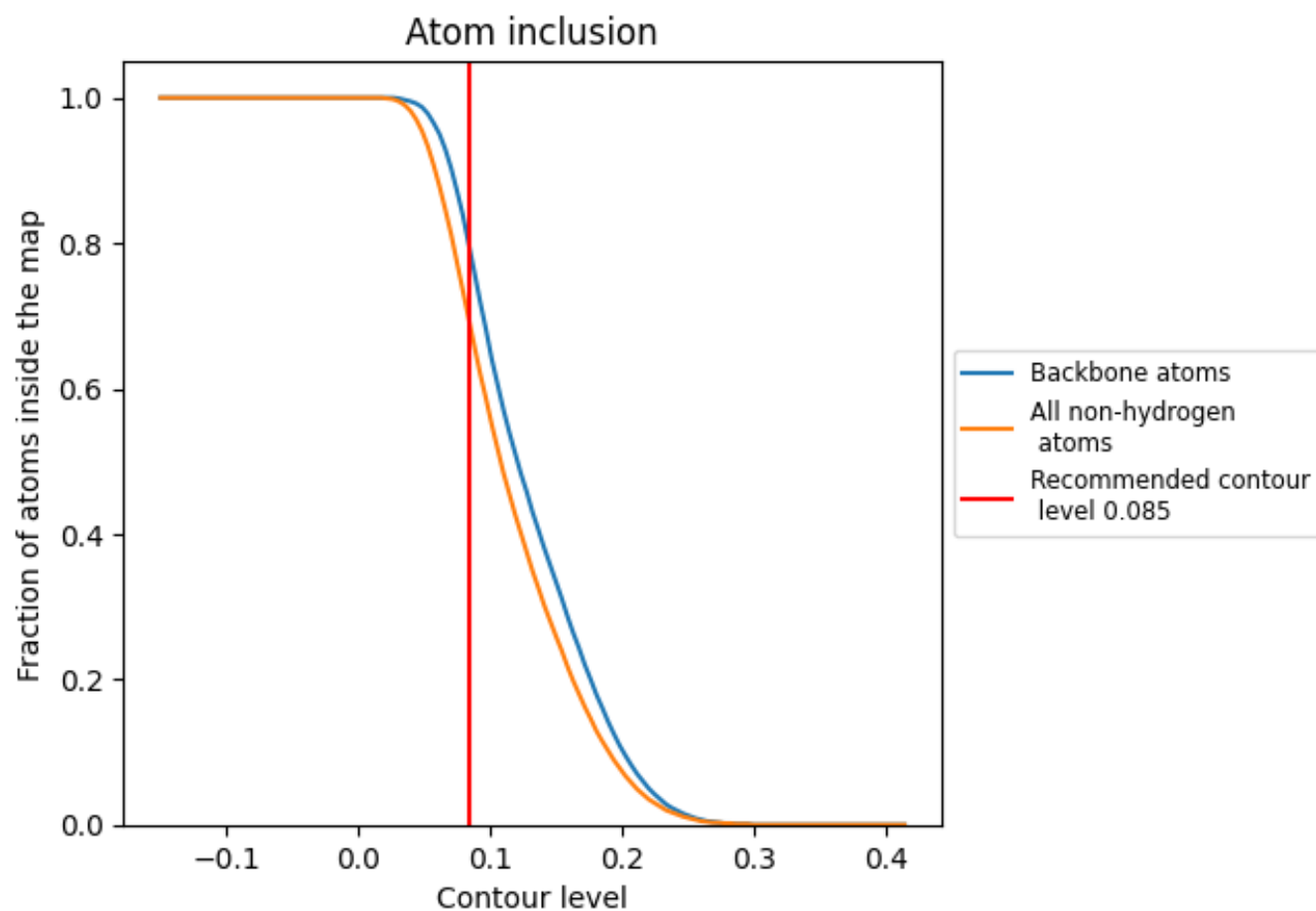
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.4950
4	 0.9140	 0.5610
5	 0.5940	 0.3690
6	 0.8790	 0.5290
7	 0.6710	 0.5000
A	 0.8010	 0.5370
C	 0.7790	 0.5290
D	 0.9300	 0.5950
F	 0.6700	 0.4770
I	 0.6840	 0.4810
J	 0.6300	 0.4570
K	 0.4090	 0.2530
L	 0.7200	 0.5040
M	 0.8320	 0.5570
N	 0.4990	 0.4000
S	 0.4900	 0.4290
U	 0.1980	 0.4540
X	 0.6320	 0.4670
r	 0.5890	 0.4630
z1	 0.9830	 0.6020
z2	 0.9330	 0.5430

