



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 10:38 AM JST

PDB ID : 6ID1
EMDB ID : EMD-9647
Title : Cryo-EM structure of a human intron lariat spliceosome after Prp43 loaded (ILS2 complex) at 2.9 angstrom resolution
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on : 2018-09-07
Resolution : 2.86 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:

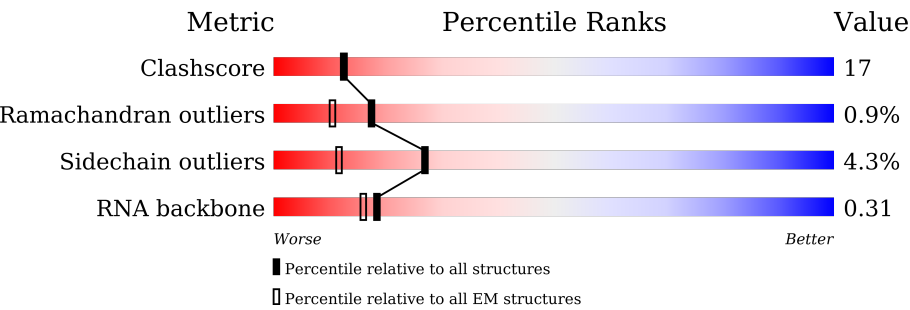
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.86 Å.

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



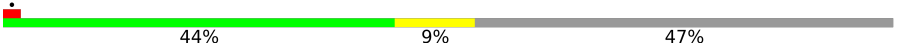

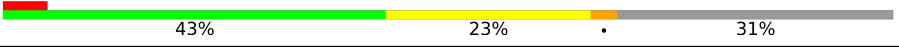
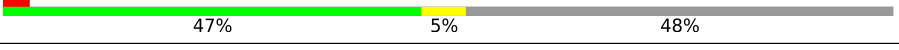


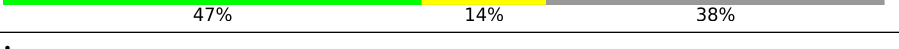
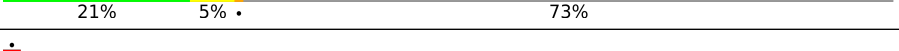

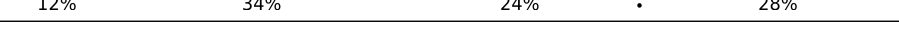
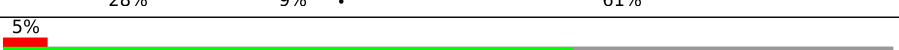



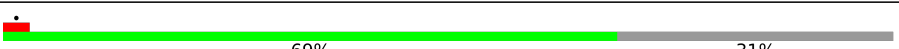





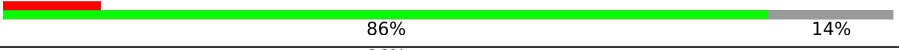

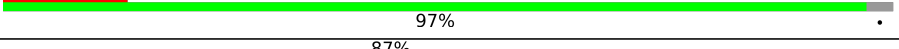


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	2335	<div><div>70%14%•15%</div></div>
2	B	117	<div><div>24%28%32%16%</div></div>
3	C	972	<div><div>70%20%•9%</div></div>
4	E	357	<div><div>34%36%14%•15%</div></div>
5	F	107	<div><div>36%31%15%8%9%</div></div>
6	J	848	<div><div>30%60%7%33%</div></div>
7	L	802	<div><div>23%48%9%•41%</div></div>

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Mol	Chain	Length	Quality of chain
8	M	243	
9	N	144	
10	O	420	
11	P	229	
12	R	536	
13	S	166	
14	T	514	
15	W	579	
16	G	272	
17	H	188	
18	U	894	
19	a	126	
19	h	126	
20	b	231	
20	i	231	
21	c	119	
21	j	119	
22	d	118	
22	k	118	
23	f	86	
23	m	86	
24	e	92	
24	l	92	
25	g	76	
25	n	76	

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Mol	Chain	Length	Quality of chain
26	q	504	
26	r	504	
26	s	504	
26	t	504	
27	K	225	
28	I	855	
29	Q	1485	
30	y	301	
31	o	255	
32	p	225	
33	V	795	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GTP	C	1500	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 79882 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1981	Total	C	N	O	S	0	0
			16477	10621	2883	2902	71		

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2060	923	341	698	98		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	888	Total	C	N	O	S	0	0
			7022	4494	1172	1322	34		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 5 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	568	Total	C	N	O	S	0	0
			3817	2379	717	715	6		

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	475	Total	C	N	O	S	0	0
			3369	2094	634	635	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	290	Total	C	N	O	S	0	0
			2340	1469	415	436	20		

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			985	601	194	188	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	272	Total	C	N	O	P	S	0	0
			2165	1357	393	401	2	12		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	317	Total	C	N	O	S	0	0
			2496	1574	453	461	8		

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	158	Total	C	N	O	S	0	0
			1276	803	217	252	4		

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	68	Total	C	N	O	P	0	0
			1201	529	148	456	68		

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	136	Total	C	N	O	P	0	0
			2884	1289	496	963	136		

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	347	Total	C	N	O	S	0	0
			2864	1817	496	529	22		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	81	Total	C	N	O	0	0
			399	237	81	81		
19	h	80	Total	C	N	O	0	0
			393	233	80	80		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	86	Total	C	N	O	0	0
			424	252	86	86		
20	i	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	82	Total	C	N	O	0	0
			406	242	82	82		
21	j	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	d	97	Total	C	N	O	0	0
			480	286	97	97		
22	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	f	74	Total	C	N	O	0	0
			361	213	74	74		
23	m	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	79	Total	C	N	O	0	0
			391	233	79	79		
24	l	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	g	74	Total	C	N	O	0	0
			363	215	74	74		
25	n	67	Total	C	N	O	0	0
			329	195	67	67		

- Molecule 26 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	q	132	Total	C	N	O	0	0
			659	395	132	132		
26	r	131	Total	C	N	O	0	0
			654	392	131	131		
26	s	67	Total	C	N	O	0	0
			335	201	67	67		
26	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 27 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	152	Total	C	N	O	S	0	0
			980	612	177	189	2		

- Molecule 28 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	576	Total	C	N	O	S	0	0
			2875	1716	579	579	1		

- Molecule 29 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Q	1322	Total	C	N	O	0	0
			6554	3910	1322	1322		

- Molecule 30 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	162	Total	C	N	O	0	0
			804	480	162	162		

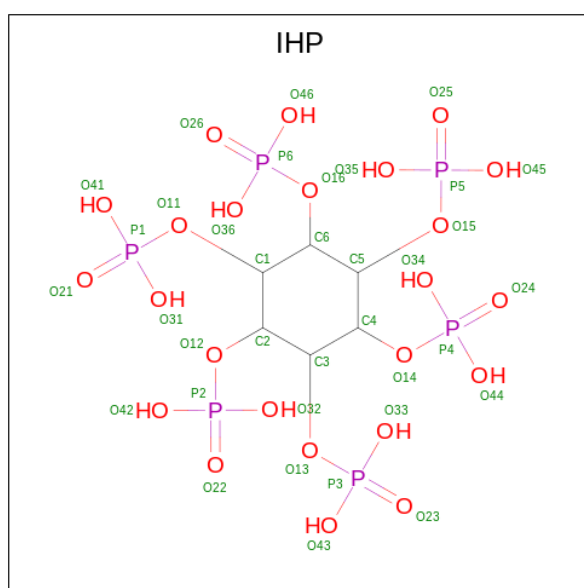
- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	94	Total	C	N	O	0	0
			464	276	94	94		

- Molecule 33 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15.

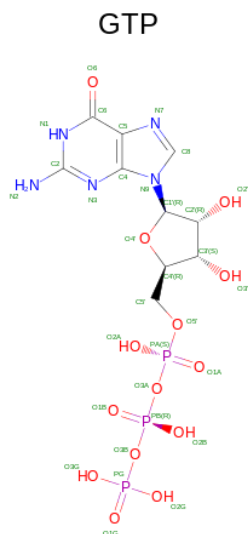
Mol	Chain	Residues	Atoms				AltConf	Trace
33	V	663	Total	C	N	O	0	0
			3285	1959	663	663		

- Molecule 34 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



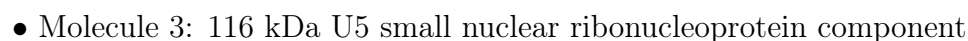
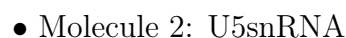
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

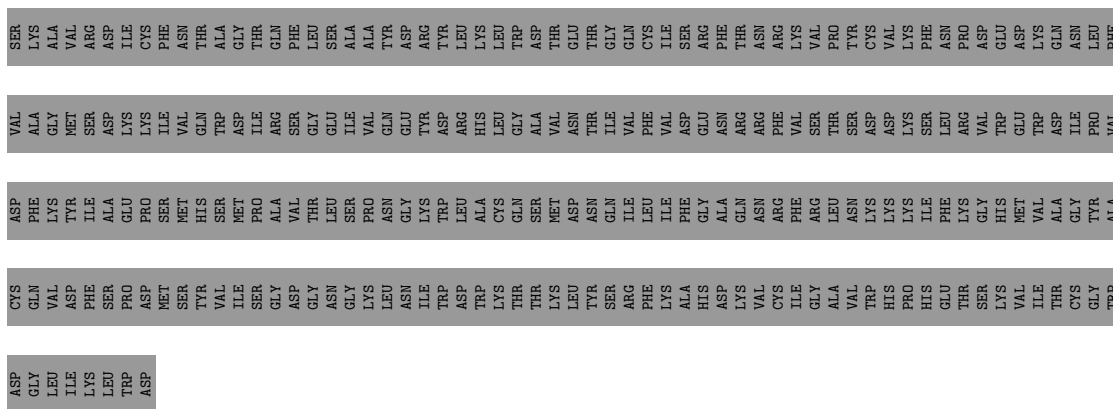
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	C	1	Total Mg 1 1	0
36	F	6	Total Mg 6 6	0

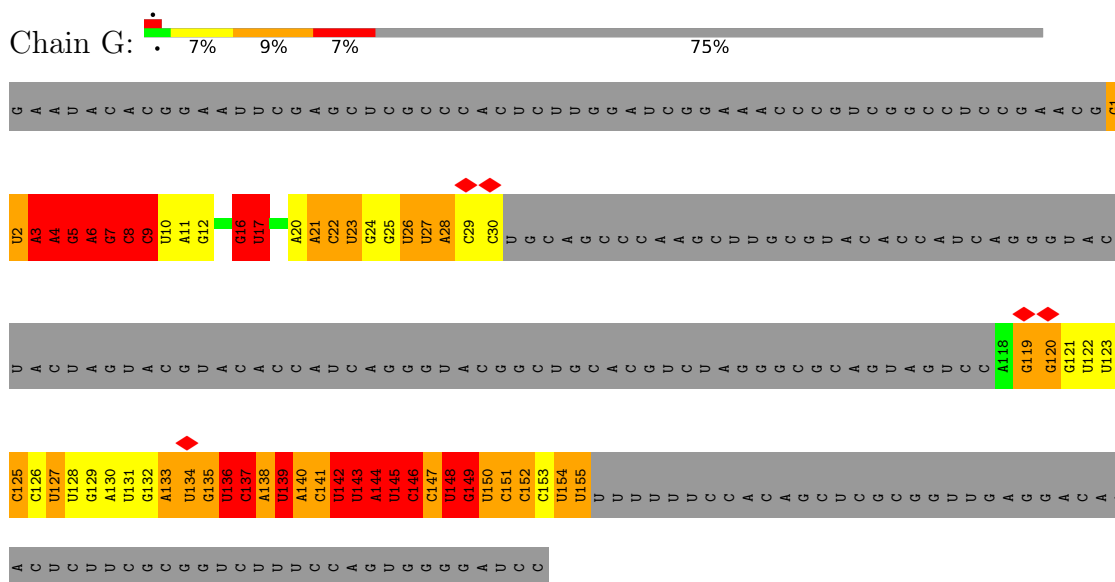
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
37	N	3	Total Zn 3 3	0
37	O	3	Total Zn 3 3	0
37	U	1	Total Zn 1 1	0

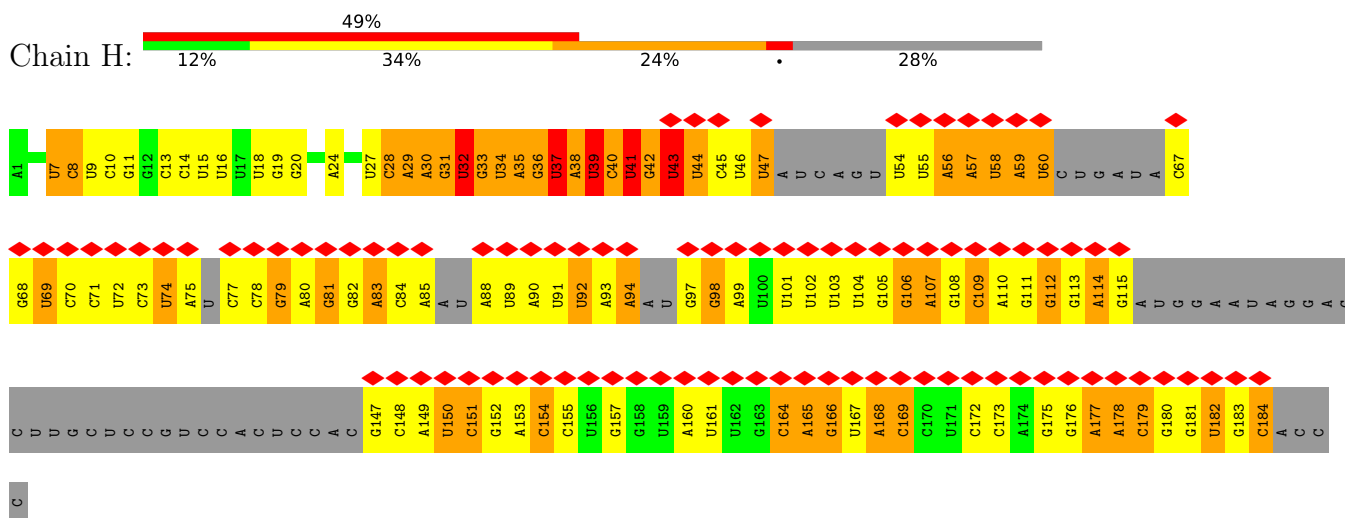




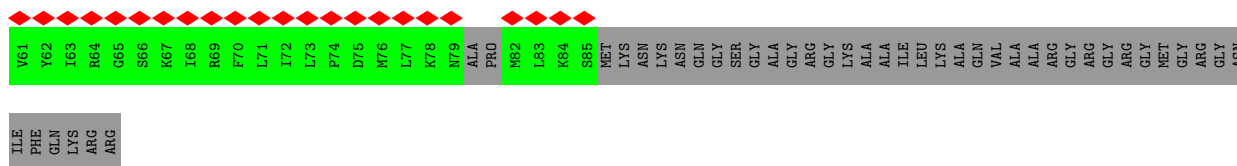
- Molecule 16: pre-mRNA



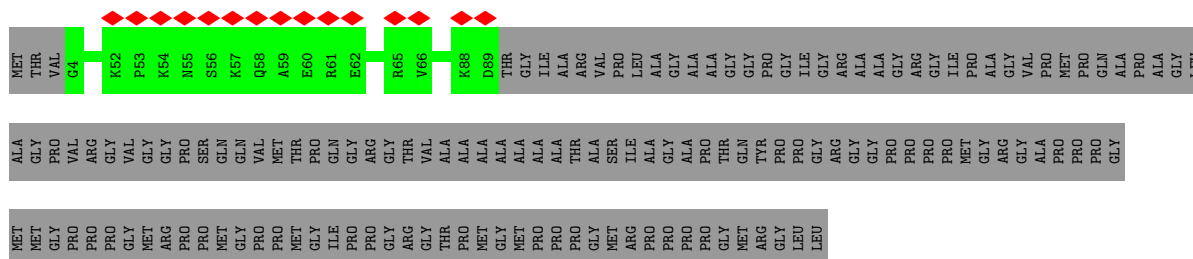
- Molecule 17: U2snRNA



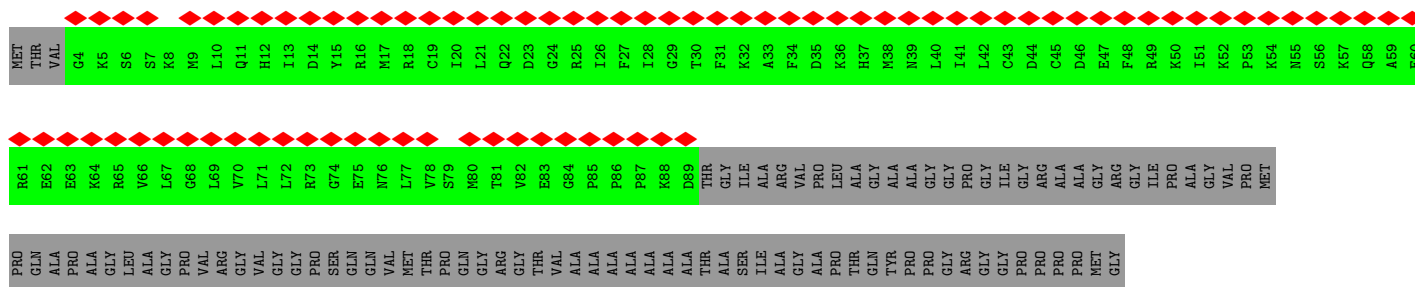
- Molecule 18: CWF19-like protein 2



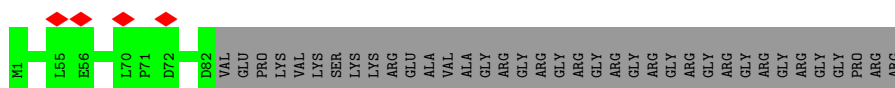
- Molecule 20: Small nuclear ribonucleoprotein-associated protein



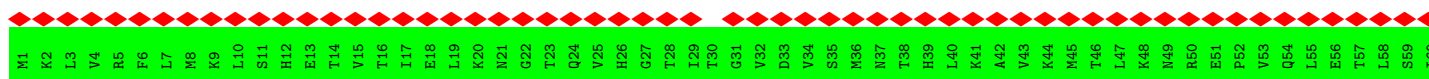
- Molecule 20: Small nuclear ribonucleoprotein-associated protein



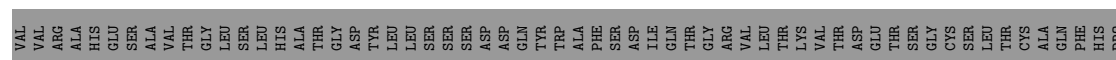
- Molecule 21: Small nuclear ribonucleoprotein Sm D1



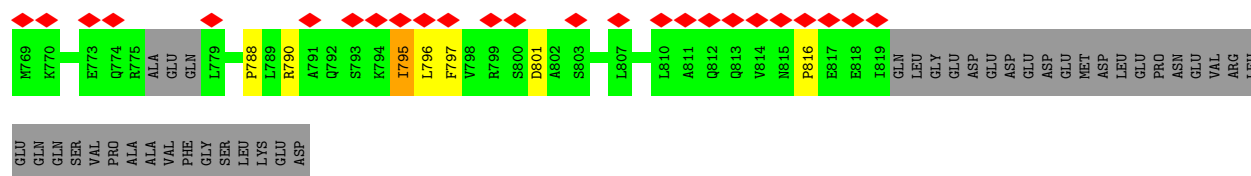
- Molecule 21: Small nuclear ribonucleoprotein Sm D1



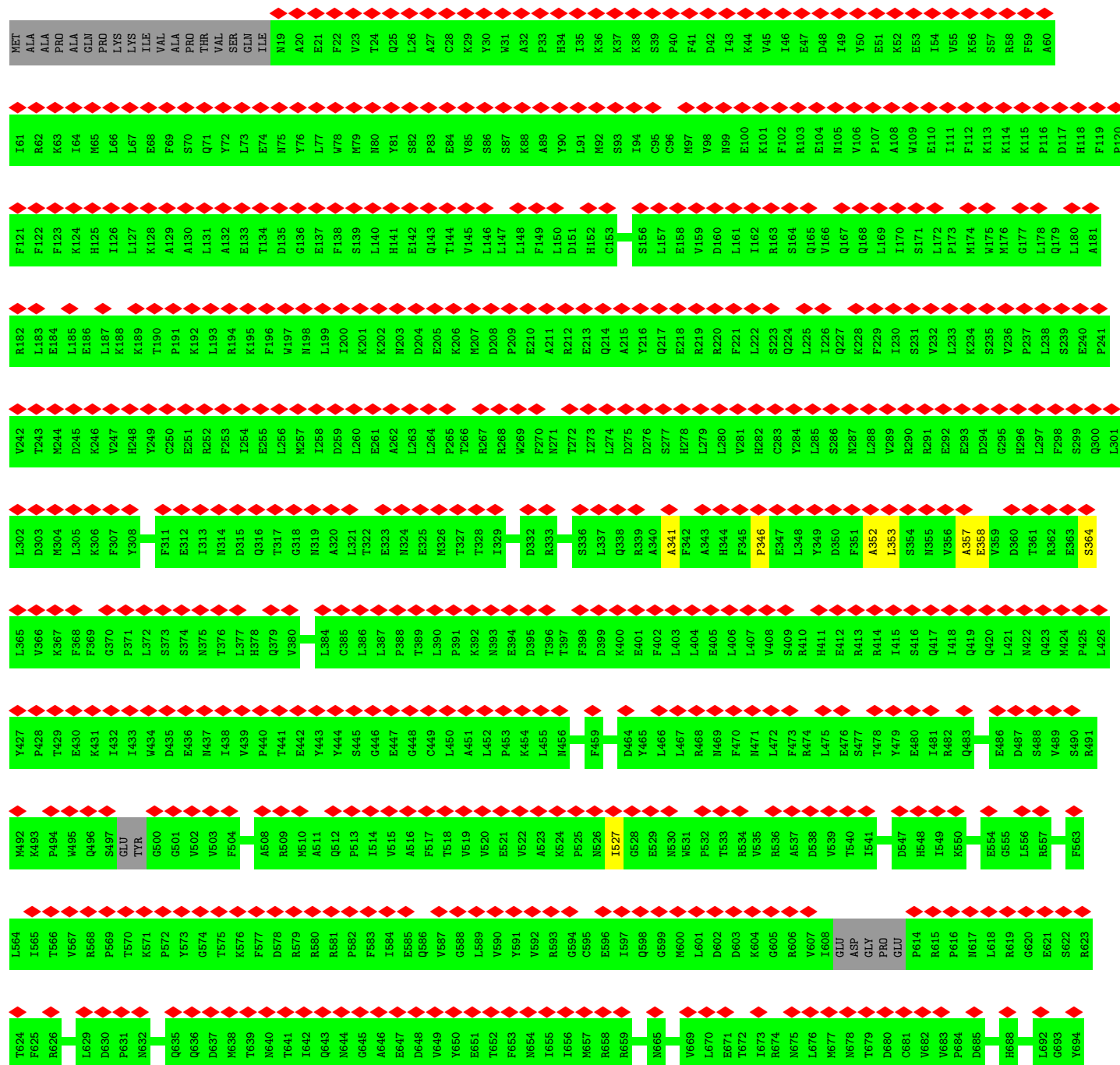
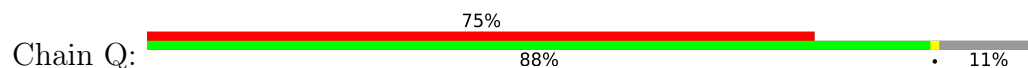








• Molecule 29: RNA helicase aquarius





Government	Percentage
Current government	76%
Previous government	81%
Next government	17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	499840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.577	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, IHP, ZN, MG, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/16926	0.61	7/22947 (0.0%)
2	B	0.43	1/2296 (0.0%)	0.88	0/3569
3	C	0.30	0/7181	0.62	3/9758 (0.0%)
4	E	0.42	0/2420	0.69	0/3281
5	F	0.56	4/2323 (0.2%)	1.11	13/3619 (0.4%)
6	J	0.33	0/3863	0.55	6/5250 (0.1%)
7	L	0.39	2/3401 (0.1%)	0.59	10/4570 (0.2%)
8	M	0.27	0/1119	0.55	1/1497 (0.1%)
9	N	1.19	7/1210 (0.6%)	0.76	0/1622
10	O	0.38	0/2390	0.62	1/3227 (0.0%)
11	P	0.30	0/1000	0.54	0/1330
12	R	0.32	0/2186	0.69	3/2937 (0.1%)
13	S	0.29	0/1268	0.57	1/1714 (0.1%)
14	T	0.42	1/2562 (0.0%)	0.69	0/3492
15	W	0.30	0/1306	0.60	1/1760 (0.1%)
16	G	0.89	10/1327 (0.8%)	1.60	40/2053 (1.9%)
17	H	0.58	9/3214 (0.3%)	0.99	9/4989 (0.2%)
18	U	0.33	0/2928	0.68	3/3928 (0.1%)
19	a	0.47	0/397	0.61	0/549
19	h	0.47	0/391	0.61	0/540
20	b	0.51	0/423	0.72	0/587
20	i	0.50	0/423	0.73	0/587
21	c	0.58	0/405	0.73	0/563
21	j	0.57	0/405	0.73	0/563
22	d	0.69	0/479	0.85	0/666
22	k	0.70	0/420	0.85	0/583
23	f	0.75	0/360	0.82	0/497
23	m	0.75	0/360	0.81	0/497
24	e	0.66	0/390	0.80	0/542
24	l	0.64	0/390	0.80	0/542
25	g	0.54	0/362	0.71	0/501
25	n	0.53	0/327	0.72	0/451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	q	0.35	0/658	0.58	3/919 (0.3%)
26	r	0.33	0/653	0.59	3/912 (0.3%)
26	s	0.27	0/334	0.37	0/466
26	t	0.31	0/334	0.38	0/466
27	K	1.05	9/982 (0.9%)	0.69	5/1318 (0.4%)
28	I	0.35	0/2858	0.61	11/3948 (0.3%)
29	Q	0.22	0/6545	0.43	0/9115
30	y	0.29	0/389	0.73	0/540
31	o	0.64	0/803	1.49	4/1119 (0.4%)
32	p	0.62	0/463	1.26	0/643
33	V	0.66	0/3284	0.75	0/4578
All	All	0.45	43/81755 (0.1%)	0.72	124/113235 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
3	C	0	3
5	F	0	1
6	J	0	1
7	L	0	2
11	P	0	1
12	R	0	1
14	T	0	2
15	W	0	2
16	G	0	8
18	U	0	2
22	d	0	1
22	k	0	1
29	Q	0	1
33	V	0	1
All	All	0	37

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	106	CYS	CB-SG	-23.11	1.43	1.82
9	N	101	CYS	CB-SG	-16.04	1.54	1.82
9	N	137	CYS	CB-SG	-12.01	1.61	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	119	CYS	CB-SG	-10.98	1.63	1.82
9	N	142	CYS	CB-SG	-9.64	1.65	1.82

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	4	A	O4'-C1'-N9	18.63	123.10	108.20
16	G	3	A	N9-C1'-C2'	13.62	131.71	114.00
16	G	8	C	N1-C1'-C2'	10.36	127.47	114.00
5	F	35	A	C4'-C3'-O3'	10.21	133.43	113.00
16	G	143	U	N1-C1'-C2'	9.61	126.49	114.00

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PRO	Peptide
1	A	1305	SER	Peptide
1	A	135	VAL	Peptide
1	A	1555	LEU	Peptide
1	A	166	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16477	0	16462	280	0
2	B	2060	0	1044	98	0
3	C	7022	0	7046	168	0
4	E	2366	0	2303	421	0
5	F	2075	0	1048	127	0
6	J	3817	0	2912	46	0
7	L	3369	0	2929	157	0
8	M	1098	0	1082	19	0
9	N	1184	0	1189	15	0
10	O	2340	0	2316	193	0
11	P	985	0	965	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	R	2165	0	2214	74	0
13	S	1236	0	1210	31	0
14	T	2496	0	2446	47	0
15	W	1276	0	1221	66	0
16	G	1201	0	609	232	0
17	H	2884	0	1461	279	0
18	U	2864	0	2814	146	0
19	a	399	0	173	0	0
19	h	393	0	170	0	0
20	b	424	0	179	0	0
20	i	424	0	179	0	0
21	c	406	0	170	0	0
21	j	406	0	170	0	0
22	d	480	0	200	0	0
22	k	422	0	175	0	0
23	f	361	0	158	0	0
23	m	361	0	158	0	0
24	e	391	0	163	0	0
24	l	391	0	163	0	0
25	g	363	0	160	0	0
25	n	329	0	138	0	0
26	q	659	0	296	0	0
26	r	654	0	294	0	0
26	s	335	0	168	0	0
26	t	335	0	168	0	0
27	K	980	0	741	158	0
28	I	2875	0	1374	82	0
29	Q	6554	0	2828	23	0
30	y	390	0	190	0	0
31	o	804	0	350	0	0
32	p	464	0	205	0	0
33	V	3285	0	1442	5	0
34	A	36	0	6	2	0
35	C	32	0	12	9	0
36	C	1	0	0	0	0
36	F	6	0	0	0	0
37	N	3	0	0	0	0
37	O	3	0	0	0	0
37	U	1	0	0	0	0
All	All	79882	0	61701	2254	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 17.

The worst 5 of 2254 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)
10:O:155:PRO:HG3	12:R:188:PHE:CD1	1.21	1.62
16:G:120:G:H2'	29:Q:1019:SER:CB	1.24	1.60
6:J:658:ARG:HA	6:J:667:ILE:CB	1.39	1.53
6:J:496:ASP:CB	6:J:536:LEU:H	1.23	1.51
10:O:260:THR:HG23	10:O:273:GLN:CB	1.32	1.50

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1977/2335 (85%)	1799 (91%)	160 (8%)	18 (1%)	14	29
3	C	886/972 (91%)	799 (90%)	84 (10%)	3 (0%)	37	55
4	E	301/357 (84%)	268 (89%)	22 (7%)	11 (4%)	2	5
6	J	536/848 (63%)	495 (92%)	37 (7%)	4 (1%)	19	36
7	L	459/802 (57%)	421 (92%)	33 (7%)	5 (1%)	12	25
8	M	128/243 (53%)	115 (90%)	13 (10%)	0	100	100
9	N	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
10	O	288/420 (69%)	262 (91%)	24 (8%)	2 (1%)	19	36
11	P	114/229 (50%)	96 (84%)	17 (15%)	1 (1%)	14	29
12	R	268/536 (50%)	234 (87%)	30 (11%)	4 (2%)	8	19
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	297 (94%)	16 (5%)	2 (1%)	22	40
15	W	156/579 (27%)	134 (86%)	18 (12%)	4 (3%)	4	10
18	U	343/894 (38%)	289 (84%)	49 (14%)	5 (2%)	8	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
19	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
20	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
20	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
21	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
21	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
22	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
22	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
23	f	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
23	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
24	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
24	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
25	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
25	n	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
26	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	8
26	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	8	18
26	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	19
26	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	19
27	K	144/225 (64%)	130 (90%)	7 (5%)	7 (5%)	2	3
28	I	538/855 (63%)	501 (93%)	25 (5%)	12 (2%)	5	12
29	Q	1304/1485 (88%)	1278 (98%)	25 (2%)	1 (0%)	48	69
30	y	77/301 (26%)	74 (96%)	3 (4%)	0	100	100
31	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	22
32	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
33	V	661/795 (83%)	614 (93%)	40 (6%)	7 (1%)	12	25
All	All	10524/16892 (62%)	9733 (92%)	695 (7%)	96 (1%)	17	29

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1519	THR
1	A	1639	VAL

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Mol	Chain	Res	Type
1	A	1653	ASP
1	A	1948	ASP

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	A	1792/2108 (85%)	1754 (98%)	38 (2%)	48	72
3	C	787/866 (91%)	762 (97%)	25 (3%)	34	60
4	E	259/300 (86%)	203 (78%)	56 (22%)	1	0
6	J	242/751 (32%)	241 (100%)	1 (0%)	89	95
7	L	248/709 (35%)	233 (94%)	15 (6%)	16	32
8	M	117/209 (56%)	114 (97%)	3 (3%)	41	67
9	N	130/130 (100%)	130 (100%)	0	100	100
10	O	259/361 (72%)	237 (92%)	22 (8%)	8	18
11	P	104/203 (51%)	102 (98%)	2 (2%)	52	74
12	R	227/457 (50%)	217 (96%)	10 (4%)	24	46
13	S	129/134 (96%)	127 (98%)	2 (2%)	58	79
14	T	273/441 (62%)	272 (100%)	1 (0%)	89	95
15	W	135/502 (27%)	131 (97%)	4 (3%)	36	62
18	U	313/806 (39%)	292 (93%)	21 (7%)	13	27
27	K	54/196 (28%)	44 (82%)	10 (18%)	1	1
28	I	12/749 (2%)	6 (50%)	6 (50%)	0	0
All	All	5081/8922 (57%)	4865 (96%)	216 (4%)	27	47

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	318	ARG
10	O	220	MET
18	U	810	ILE

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Mol	Chain	Res	Type
6	J	591	LEU
7	L	731	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
10	O	254	GLN
15	W	184	ASN
11	P	75	ASN
12	R	281	ASN
1	A	1784	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	67/272 (24%)	55 (82%)	14 (20%)
17	H	129/188 (68%)	53 (41%)	2 (1%)
2	B	97/117 (82%)	57 (58%)	4 (4%)
5	F	96/107 (89%)	42 (43%)	7 (7%)
All	All	389/684 (56%)	207 (53%)	27 (6%)

5 of 207 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	12	U

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	G	7	G
16	G	21	A
16	G	150	U
16	G	16	G
16	G	22	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
12	SEP	R	224	12	8,9,10	0.83	0	8,12,14	1.08	0
12	SEP	R	232	12	8,9,10	0.98	0	8,12,14	2.08	2 (25%)

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
12	SEP	R	224	12	-	0/5/8/10	-
12	SEP	R	232	12	-	1/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	232	SEP	OG-CB-CA	4.44	112.47	108.14
12	R	232	SEP	P-OG-CB	-2.36	111.81	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	232	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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
35	GTP	C	1500	36	26,34,34	0.98	1 (3%)	32,54,54	1.49	5 (15%)
34	IHP	A	3000	-	36,36,36	0.71	0	54,60,60	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GTP	C	1500	36	-	4/18/38/38	0/3/3/3
34	IHP	A	3000	-	-	5/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	1500	GTP	C6-N1	-2.98	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	1500	GTP	PA-O3A-PB	-3.99	119.15	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	1500	GTP	PB-O3B-PG	-3.76	119.91	132.83
35	C	1500	GTP	C5-C6-N1	2.66	118.65	113.95
35	C	1500	GTP	O6-C6-C5	-2.35	119.78	124.37
35	C	1500	GTP	C8-N7-C5	2.27	107.32	102.99

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

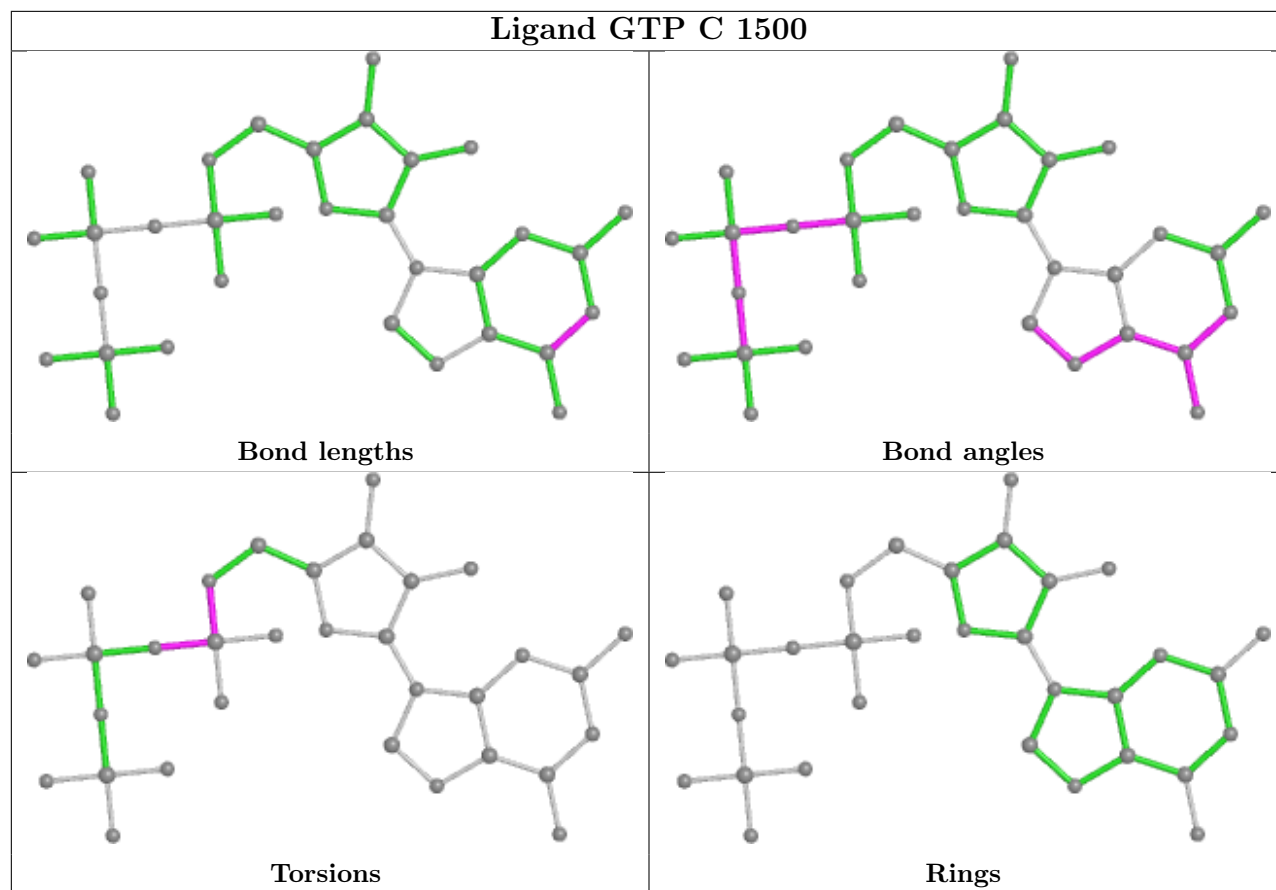
Mol	Chain	Res	Type	Atoms
35	C	1500	GTP	C5'-O5'-PA-O3A
35	C	1500	GTP	C5'-O5'-PA-O1A
35	C	1500	GTP	C5'-O5'-PA-O2A
34	A	3000	IHP	C1-O11-P1-O21
34	A	3000	IHP	C3-O13-P3-O23

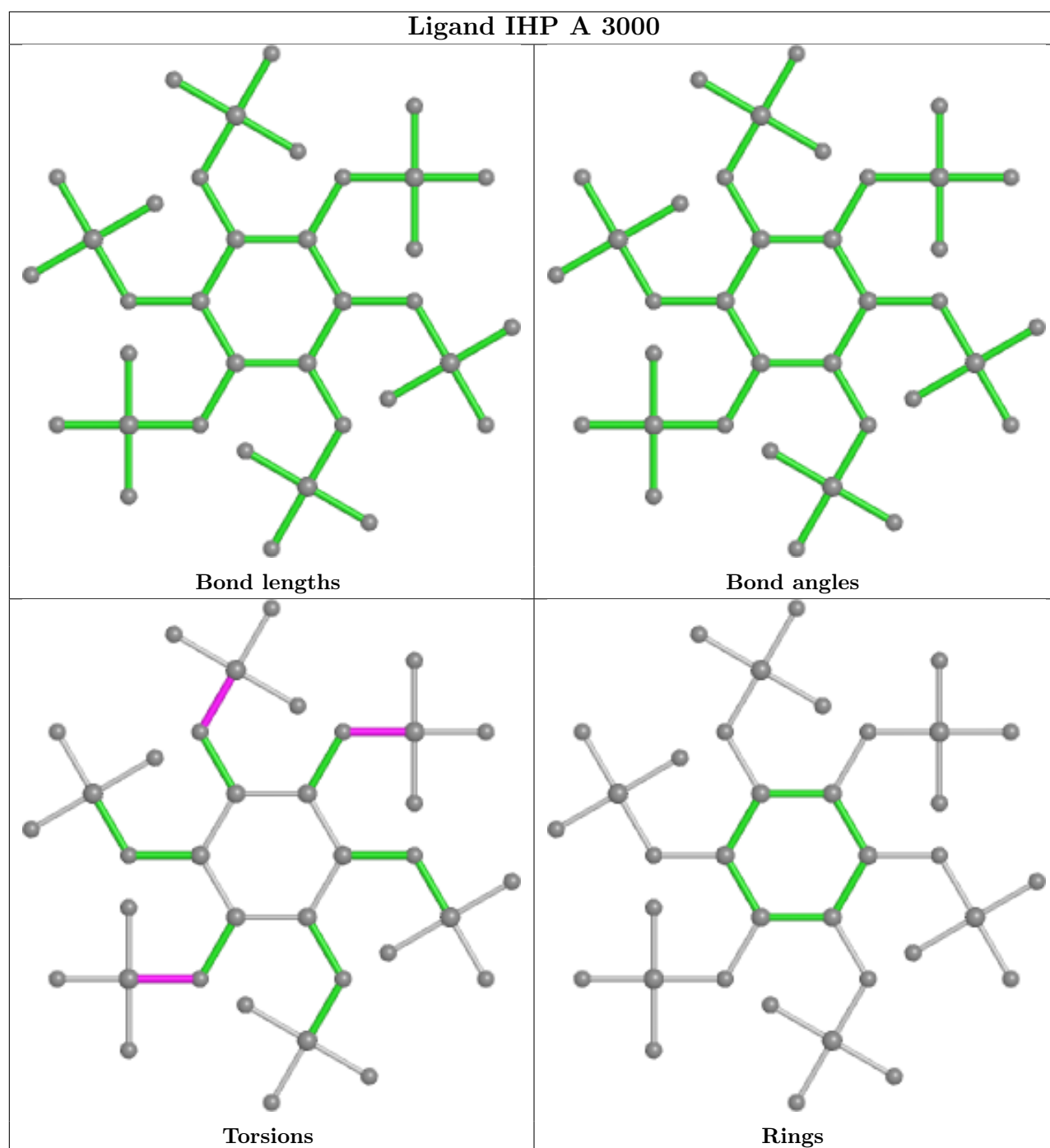
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	1500	GTP	9	0
34	A	3000	IHP	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

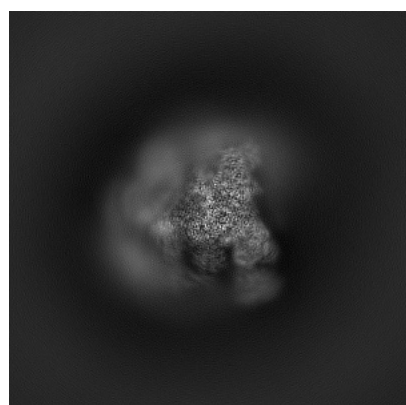
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9647. These allow visual inspection of the internal detail of the map and identification of artifacts.

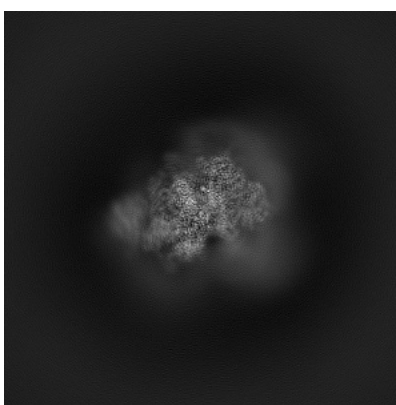
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

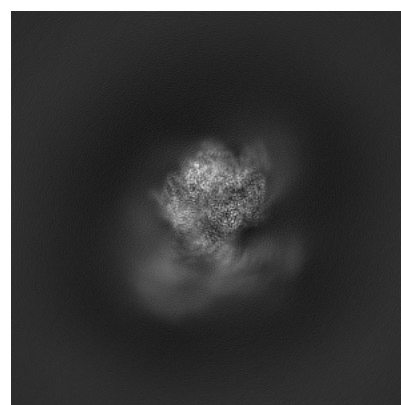
6.1.1 Primary map



X



Y

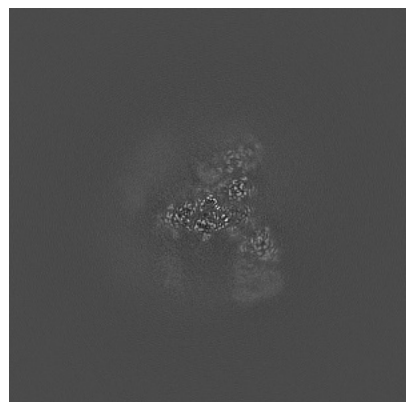


Z

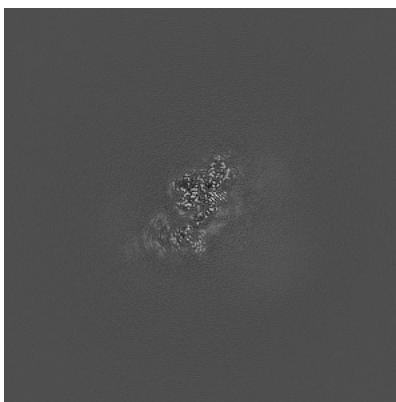
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

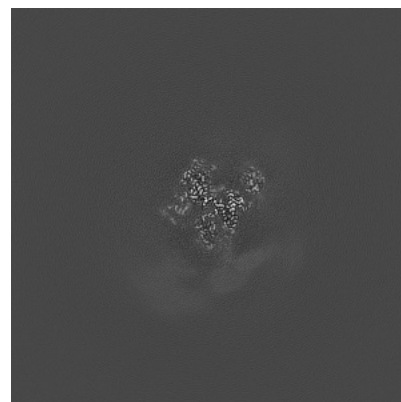
6.2.1 Primary map



X Index: 200



Y Index: 200

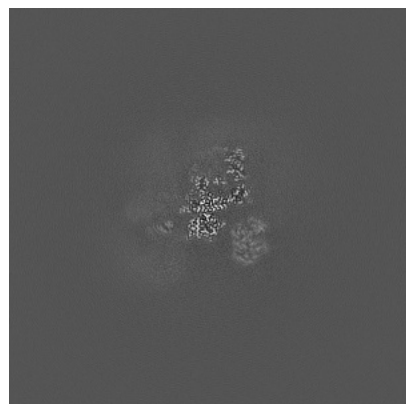


Z Index: 200

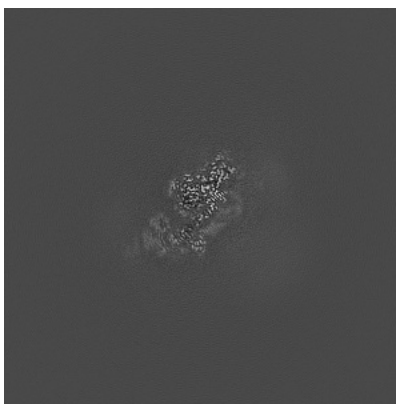
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

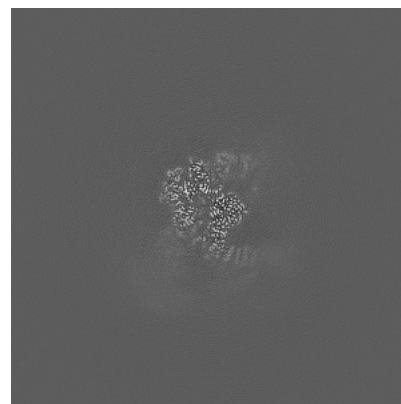
6.3.1 Primary map



X Index: 221



Y Index: 201

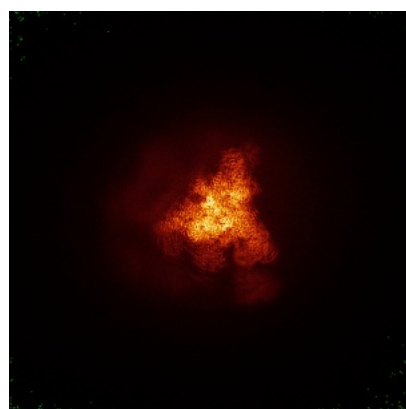


Z Index: 185

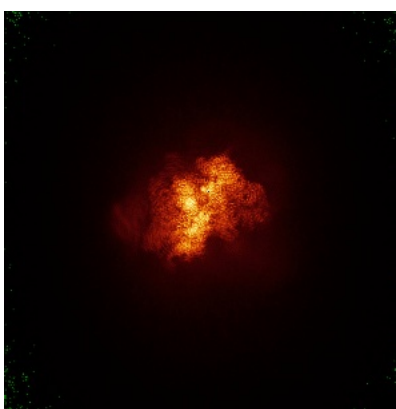
The images above show the largest variance slices of the map in three orthogonal directions.

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

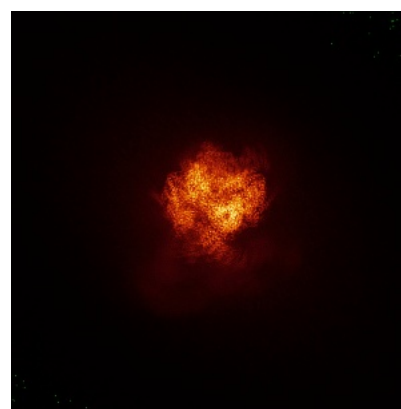
6.4.1 Primary map



X



Y

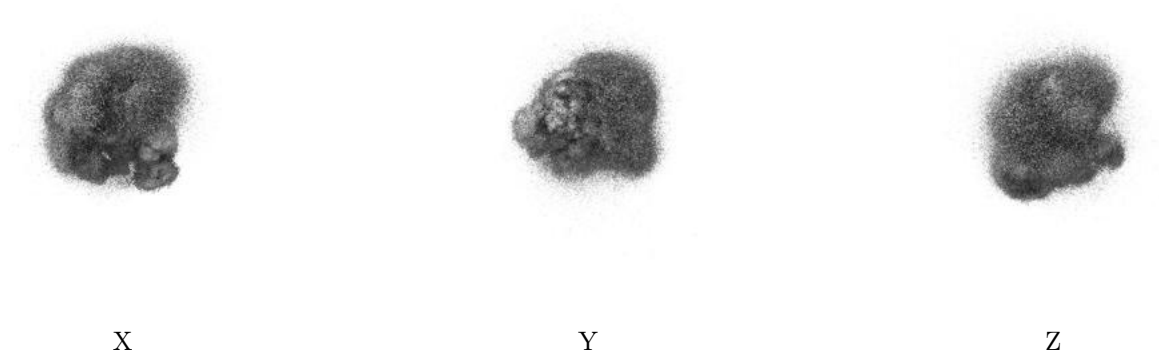


Z

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

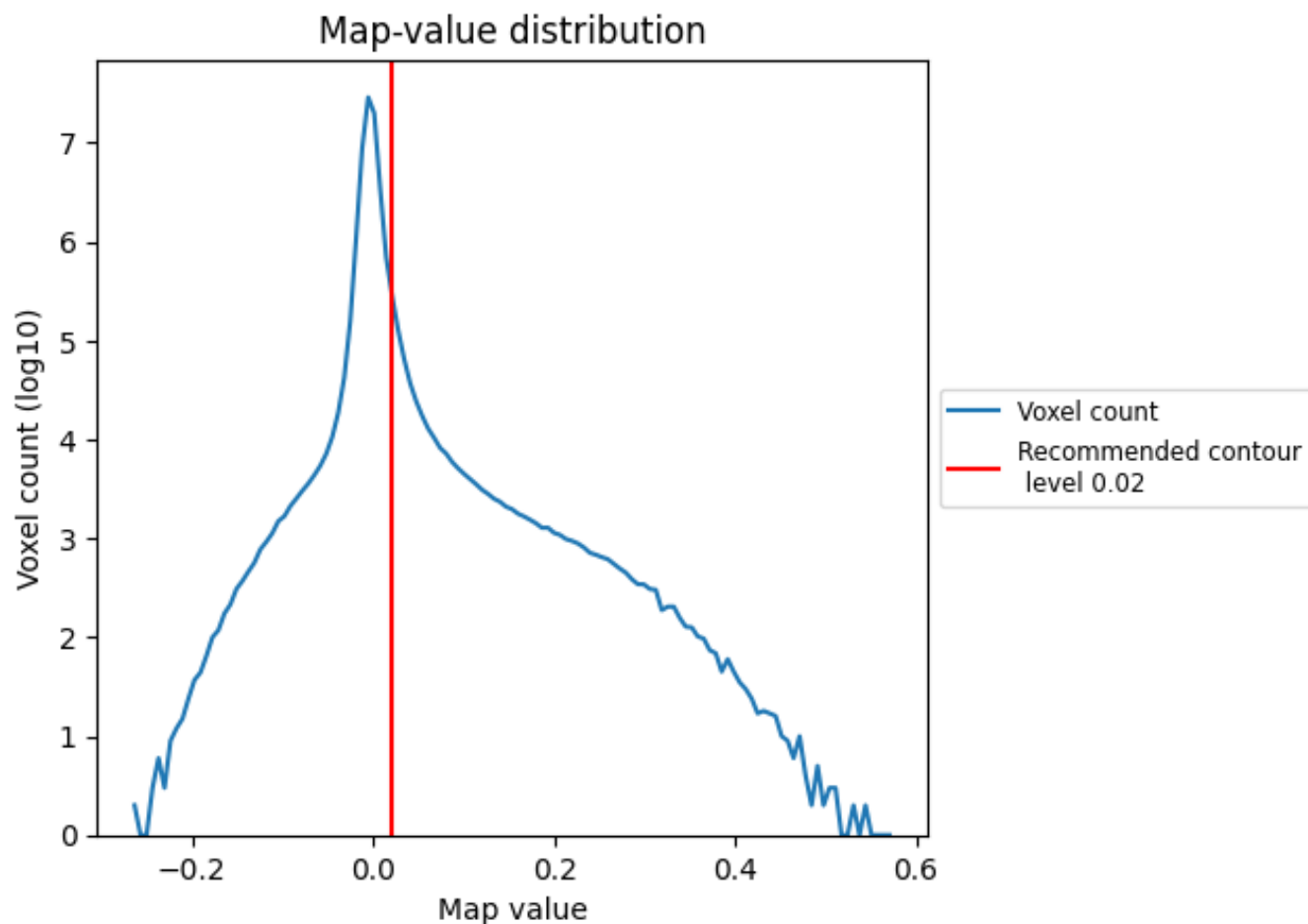
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

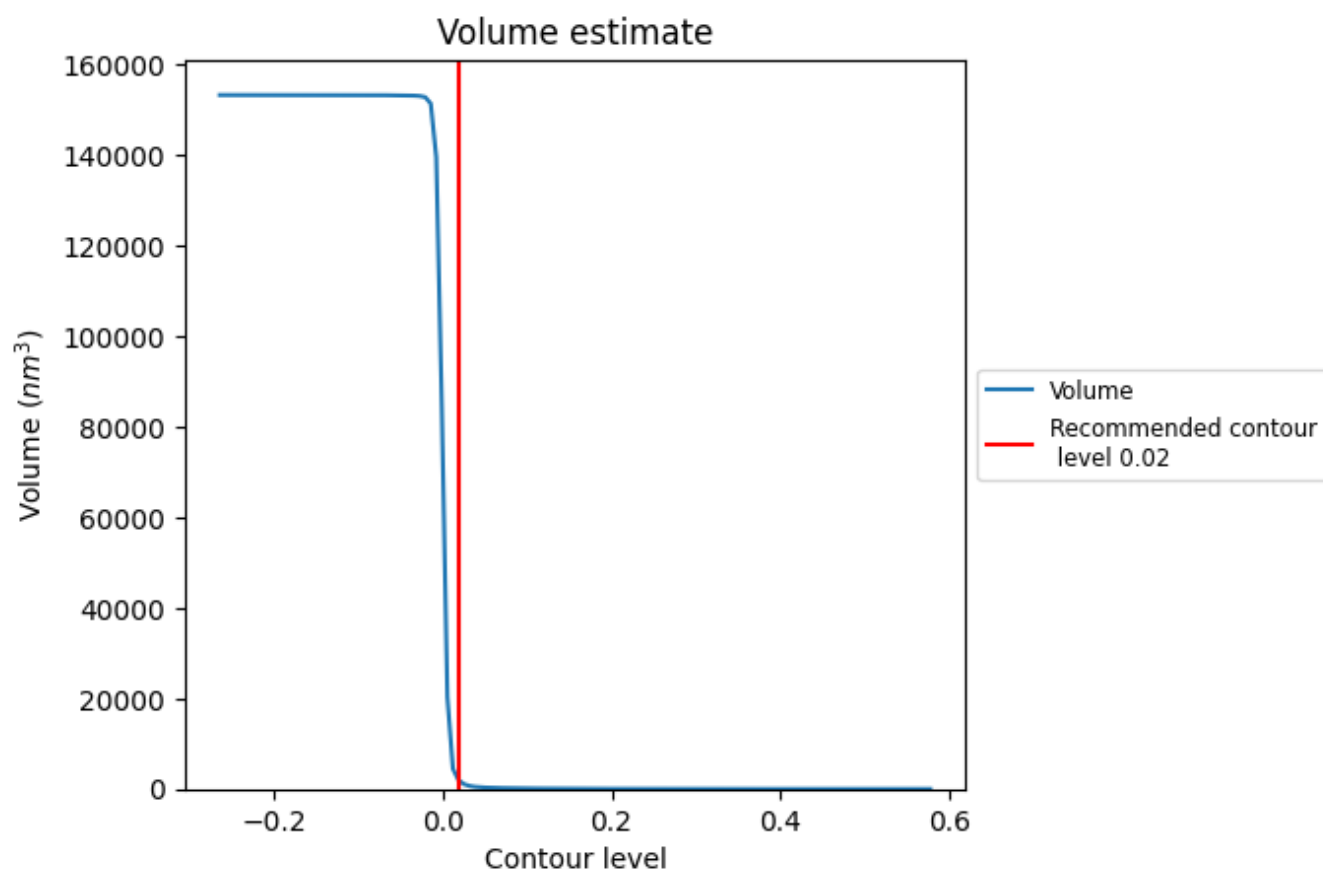
This section contains the results of statistical analysis of the map.

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.

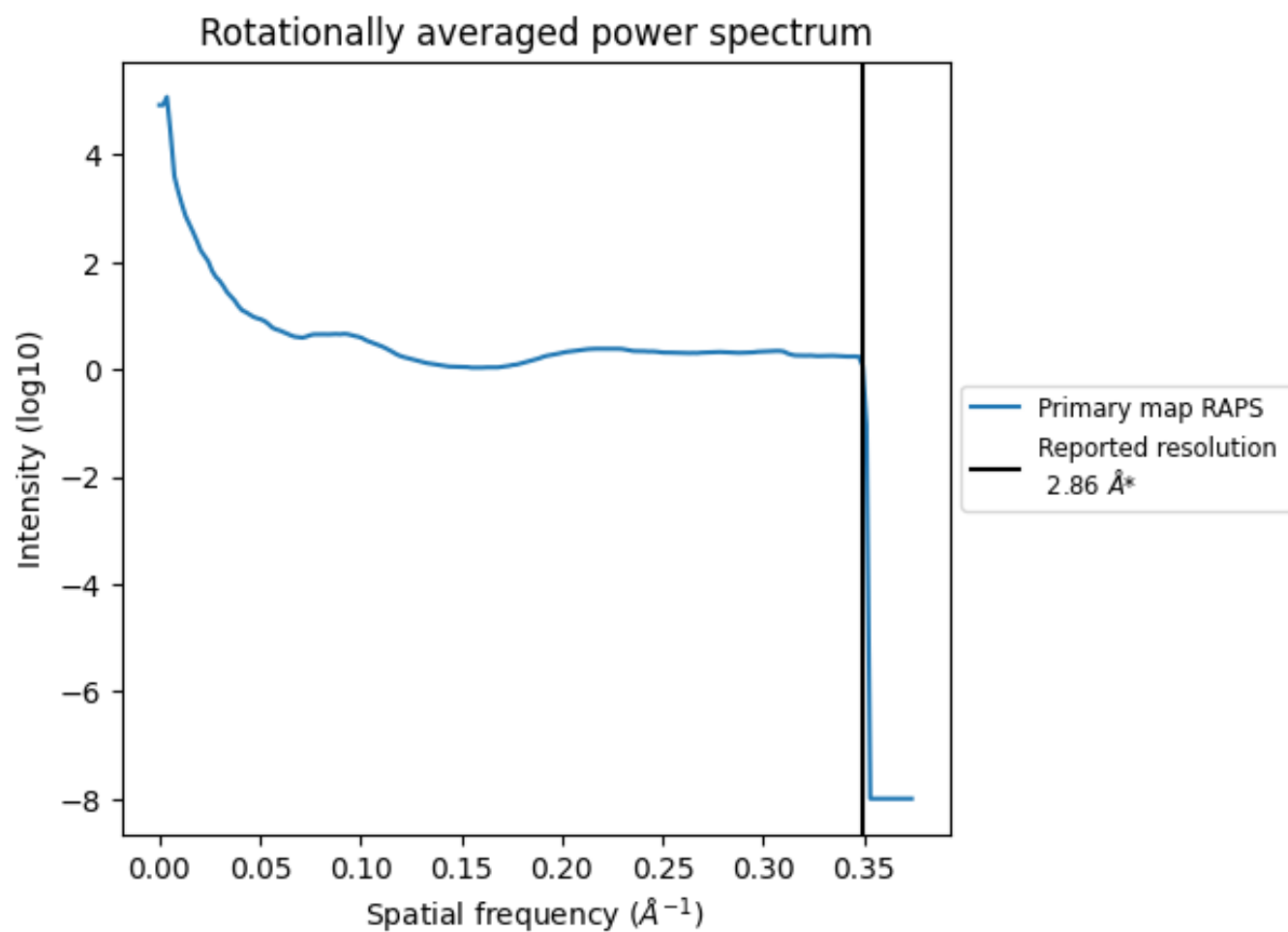
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1797 nm^3 ; this corresponds to an approximate mass of 1623 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 0.350 Å⁻¹

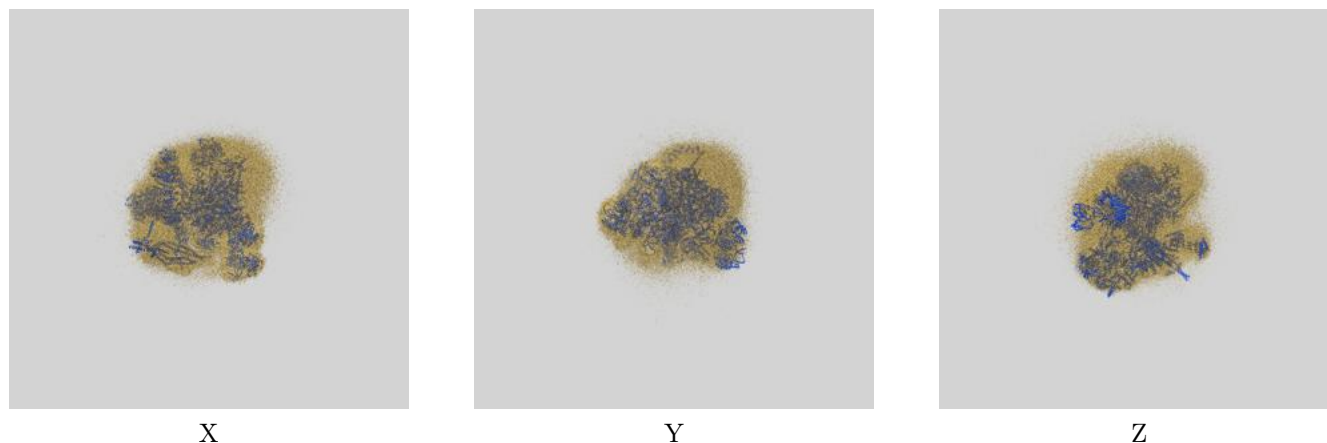
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

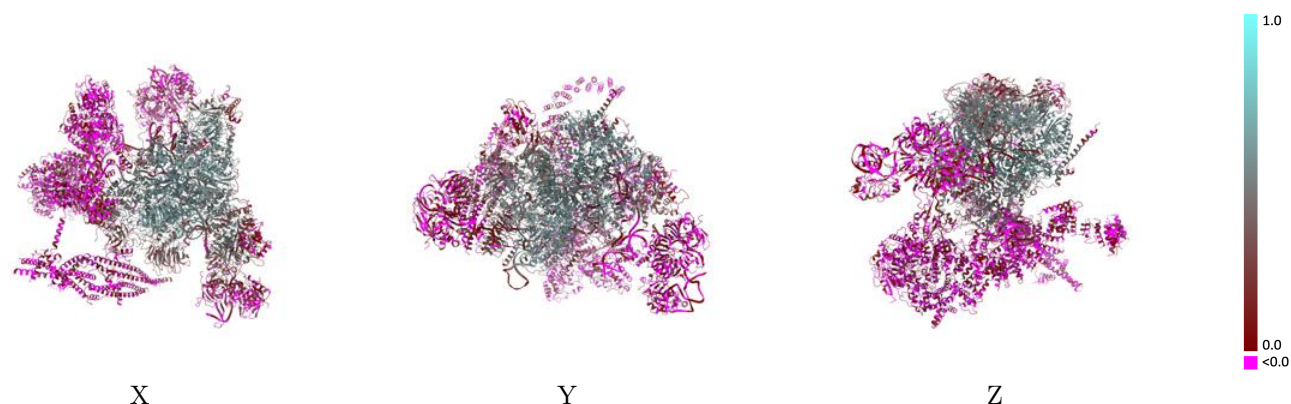
This section contains information regarding the fit between EMDB map EMD-9647 and PDB model 6ID1. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



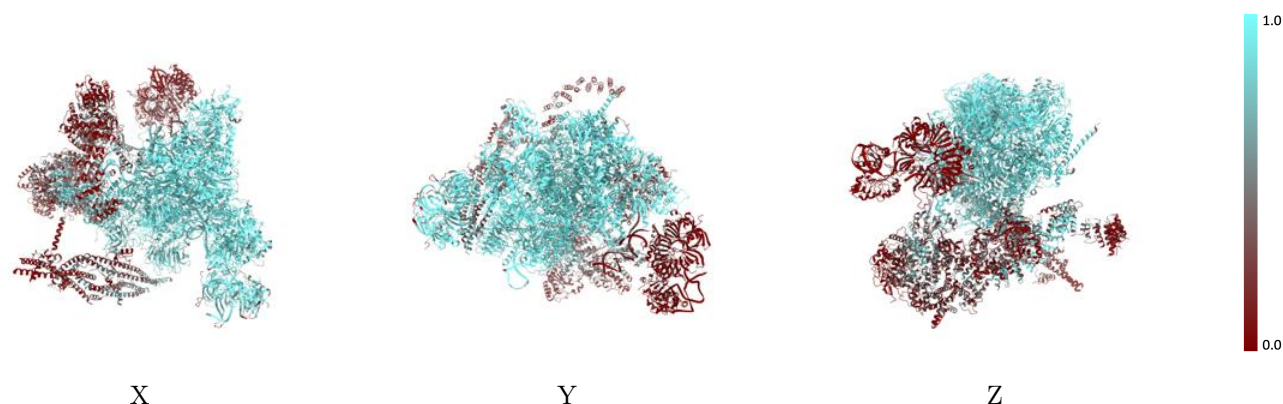
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



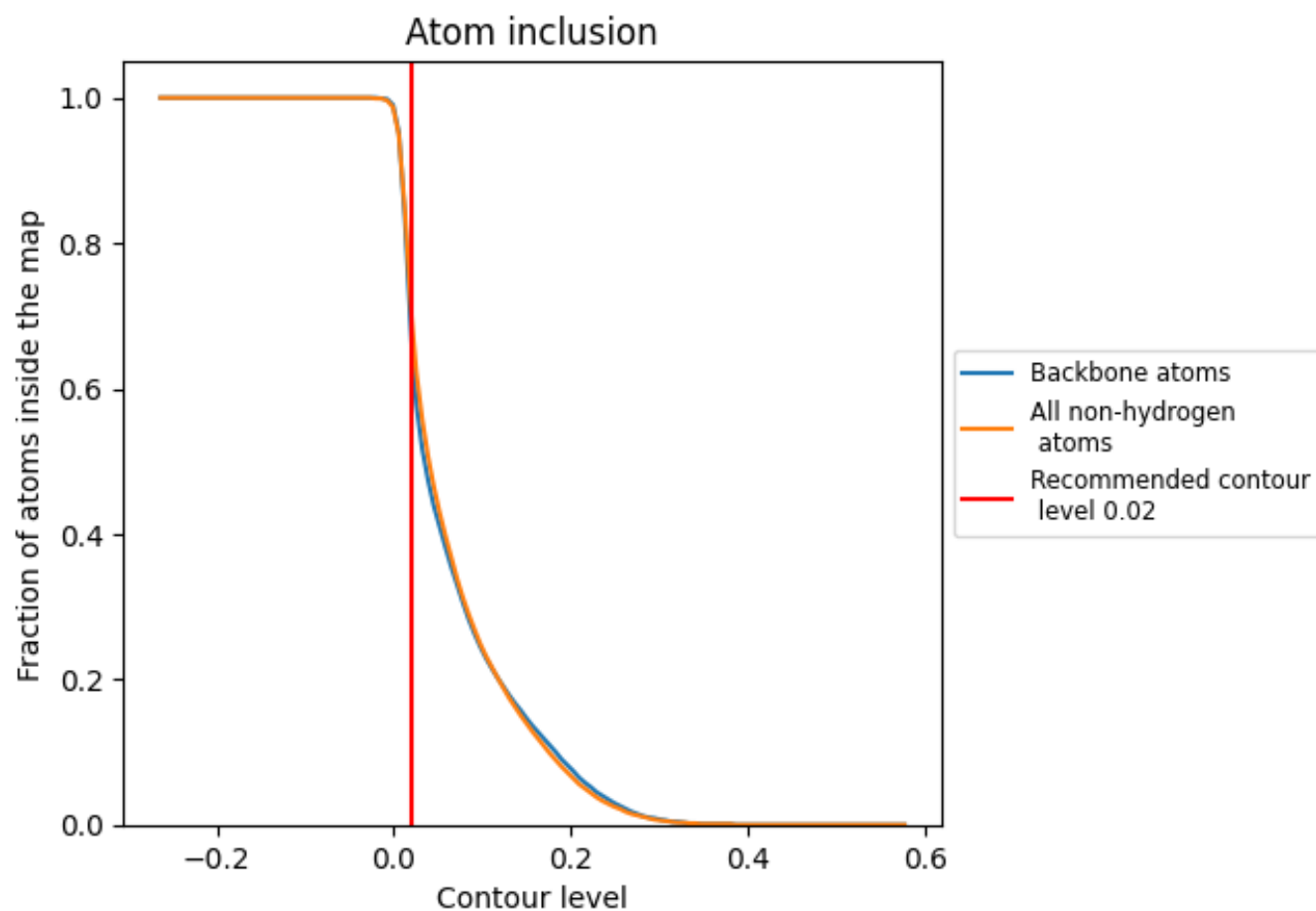
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7010	 0.2910
A	 0.9460	 0.5070
B	 0.9160	 0.3290
C	 0.9180	 0.3560
E	 0.9000	 0.2990
F	 0.9430	 0.4390
G	 0.7810	 0.1720
H	 0.3200	 0.0900
I	 0.6000	 0.0420
J	 0.6430	 0.2780
K	 0.3970	 0.0550
L	 0.6340	 0.2560
M	 0.8280	 0.4070
N	 0.9670	 0.5630
O	 0.8550	 0.3890
P	 0.8590	 0.4360
Q	 0.2360	 0.0140
R	 0.8910	 0.4260
S	 0.8480	 0.2520
T	 0.9800	 0.5940
U	 0.9240	 0.4780
V	 0.1900	 0.0130
W	 0.8400	 0.3760
a	 0.8900	 0.2050
b	 0.7920	 0.1000
c	 0.9060	 0.1090
d	 0.8460	 0.0450
e	 0.7800	 0.0620
f	 0.7950	 -0.0090
g	 0.7580	 0.0680
h	 0.1090	 0.0110
i	 0.1180	 0.0280
j	 0.0890	 0.0510
k	 0.0170	 -0.0070
l	 0.0280	 0.0100



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Chain	Atom inclusion	Q-score
m	 0.0170	 -0.0010
n	 0.0940	 0.0070
o	 0.0590	 0.0290
p	 0.0600	 0.0360
q	 0.1210	 -0.0070
r	 0.3720	 0.0170
s	 0.4000	 -0.0250
t	 0.1640	 0.0090
y	 0.4690	 0.0440