



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 01:50 pm GMT

PDB ID : 6FF4
EMDB ID : EMD-4255
Title : human Bact spliceosome core structure
Authors : Haselbach, D.; Komarov, I.; Agafonov, D.; Hartmuth, K.; Graf, B.; Kastner, B.; Luehrmann, R.; Stark, H.
Deposited on : 2018-01-03
Resolution : 3.40 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:

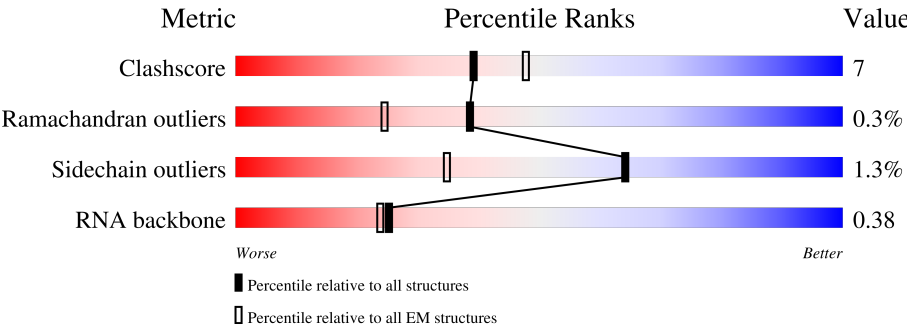
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	1	322	
2	2	188	
3	3	619	
4	5	116	
5	6	107	
6	7	464	
7	8	895	

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Mol	Chain	Length	Quality of chain
8	A	2335	
9	B	972	
10	C	536	
11	D	514	
12	E	579	
13	L	802	
14	O	848	
15	P	420	
16	Q	144	
17	R	229	
18	S	2752	
19	V	166	
20	Y	904	
21	Z	478	
22	s	472	
23	t	343	
24	u	1304	
25	v	1217	
26	x	86	
27	y	110	
28	z	125	

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
30	IHP	A	3001	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 72392 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 RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	122	Total	C	N	O	S	0	0
			981	623	168	187	3		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	60	Total	C	N	O	P	0	0
			1262	565	207	430	60		

- Molecule 3 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	118	Total	C	N	O	S	0	0
			981	609	185	182	5		

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	70	Total	C	N	O	P	0	0
			1470	659	243	498	70		

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	95	Total	C	N	O	P	0	0
			2035	910	377	653	95		

- Molecule 6 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	93	Total	C	N	O	S	0	0
			733	444	145	140	4		

- Molecule 7 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	144	Total	C	N	O	S	0	0
			1211	776	219	210	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2238	Total	C	N	O	S	0	0
			18569	11953	3245	3290	81		

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	902	Total	C	N	O	S	0	0
			7137	4566	1187	1349	35		

- Molecule 10 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	286	Total	C	N	O	S	0	0
			2287	1427	419	429	12		

- Molecule 11 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	320	Total	C	N	O	S	0	0
			2517	1588	457	464	8		

- Molecule 12 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	130	Total	C	N	O	S	0	0
			1054	664	175	211	4		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	103	Total	C	N	O	S	0	0
			858	548	157	149	4		

- Molecule 14 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	253	Total	C	N	O	S	0	0
			2235	1433	399	397	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	286	Total	C	N	O	S	0	0
			2305	1447	411	427	20		

- Molecule 16 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	138	Total	C	N	O	S	0	0
			1153	728	212	203	10		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	102	Total	C	N	O	S	0	0
			869	532	169	166	2		

- Molecule 18 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	34	Total	C	N	O	S	0	0
			261	158	56	46	1		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	95	Total	C	N	O	S	0	0
			762	494	121	142	5		

- Molecule 21 is a RNA chain called pre mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	48	Total	C	N	O	P	0	0
			1013	454	173	338	48		

- Molecule 22 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	175	Total	C	N	O	S	0	0
			1377	869	240	263	5		

- Molecule 23 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	172	Total	C	N	O	S	0	0
			1415	880	257	267	11		

- Molecule 24 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	881	Total	C	N	O	S	0	0
			7013	4496	1201	1274	42		

- Molecule 25 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	1189	Total	C	N	O	S	0	0
			9315	5908	1586	1776	45		

- Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	79	Total	C	N	O	S	0	0
			656	415	115	120	6		

- Molecule 27 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	100	Total	C	N	O	S	0	0
			766	473	135	145	13		

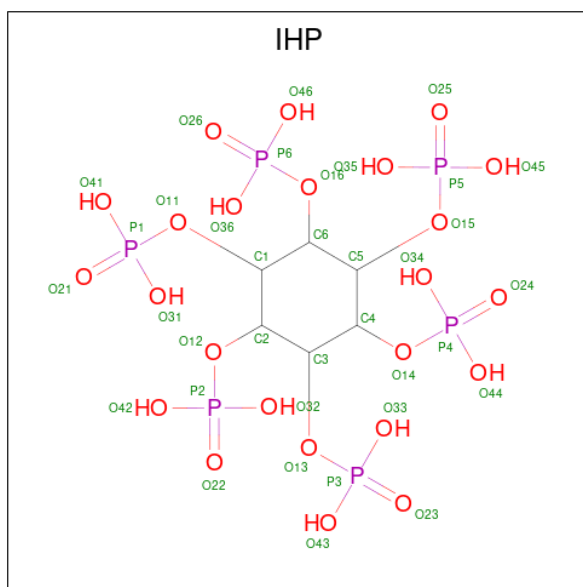
- Molecule 28 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	101	Total	C	N	O	S	0	0
			839	538	146	151	4		

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

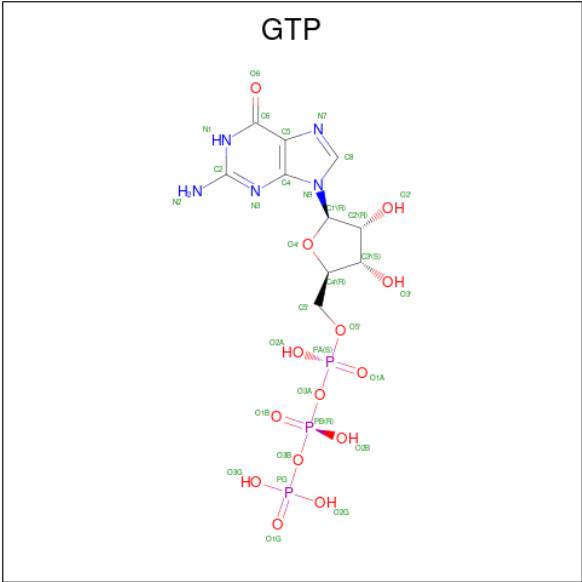
Mol	Chain	Residues	Atoms		AltConf
29	6	4	Total	Mg	0
			4	4	

- Molecule 30 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

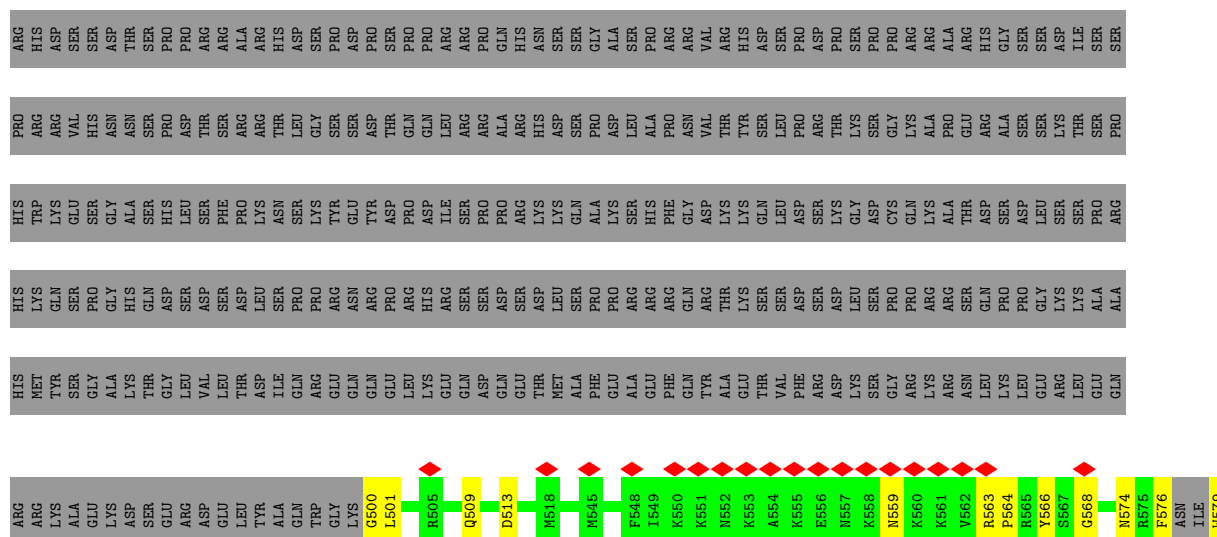
- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



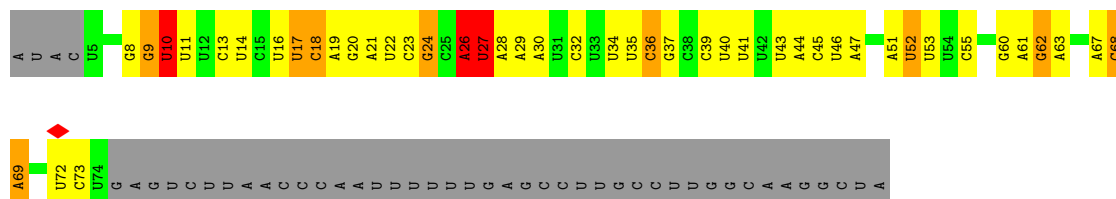
Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

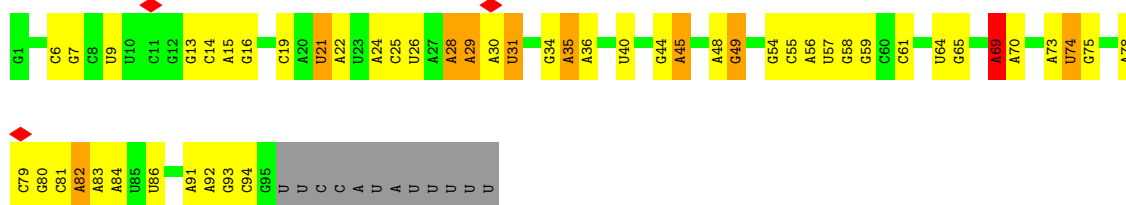
Mol	Chain	Residues	Atoms		AltConf
32	P	3	Total	Zn	0
			3	3	
32	Q	3	Total	Zn	0
			3	3	
32	t	1	Total	Zn	0
			1	1	
32	y	3	Total	Zn	0
			3	3	



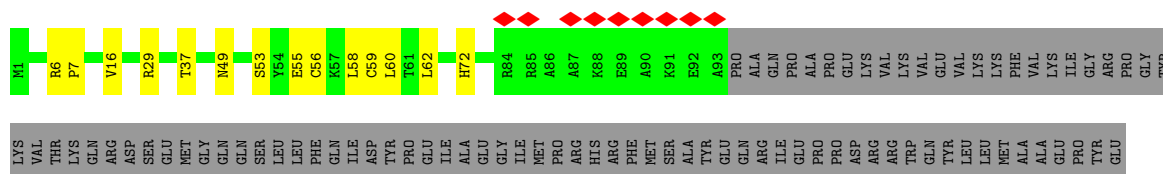
• Molecule 4: U5 snRNA



• Molecule 5: U6 snRNA



• Molecule 6: Splicing factor 3A subunit 2



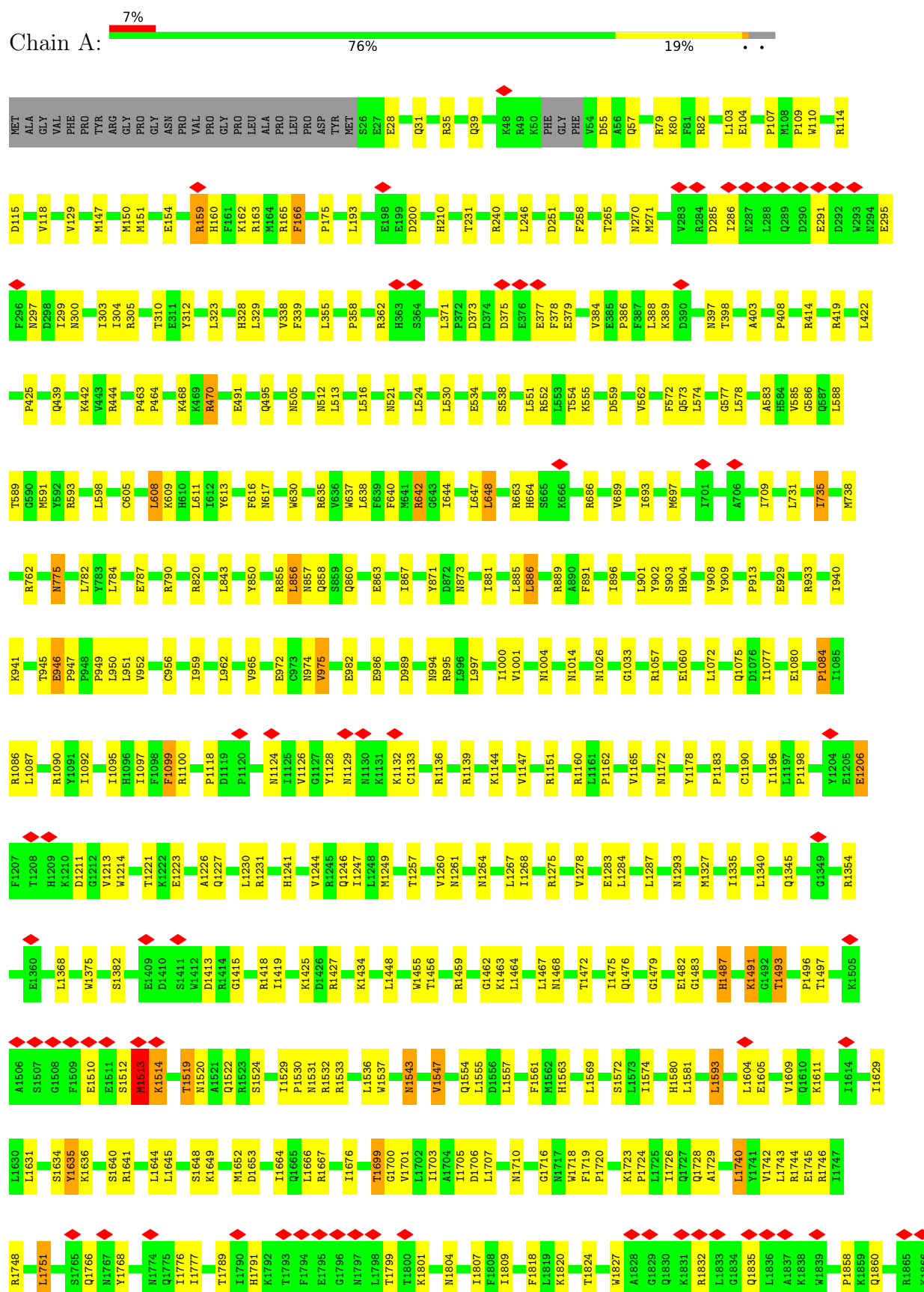
[illegible]

- Molecule 7: Splicing factor 3B subunit 2

Chain 8:  15% 84%

[illegible]

• Molecule 8: Pre-mRNA-processing-splicing factor 8



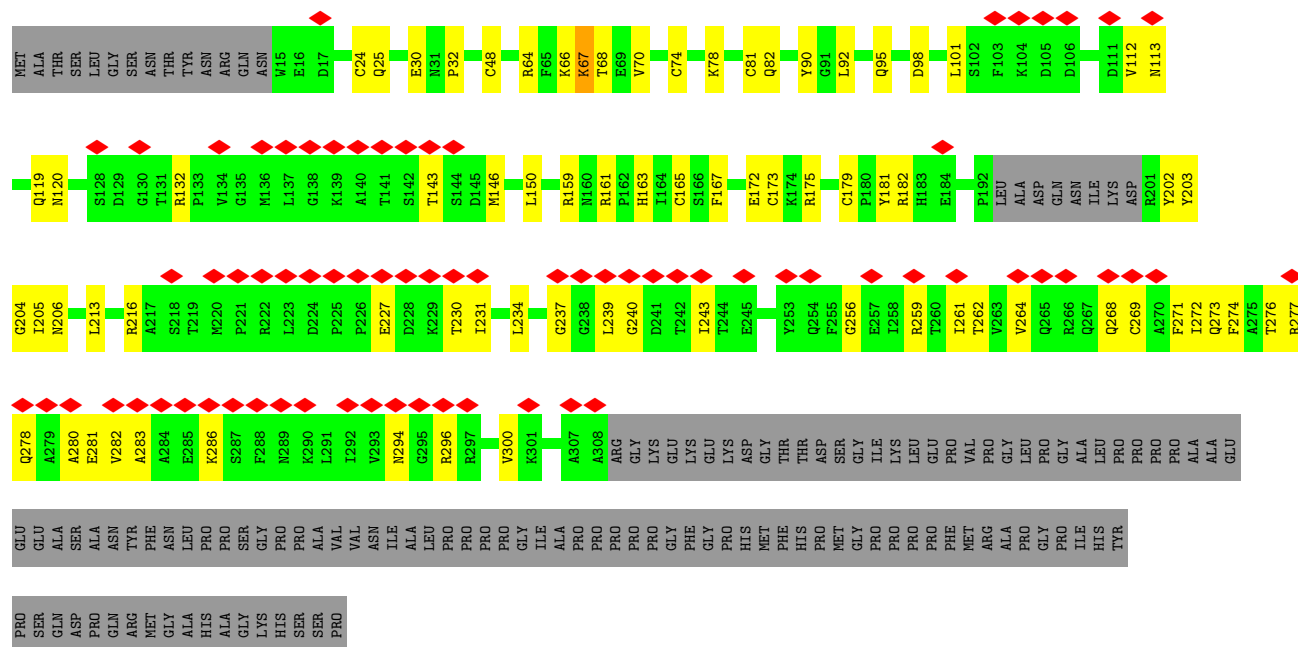


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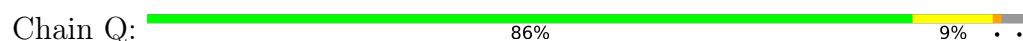
- Molecule 14: Crooked neck-like protein 1

[illegible]

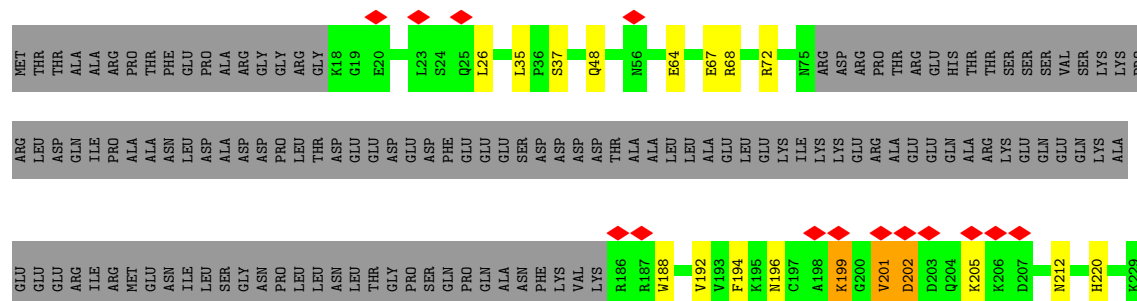
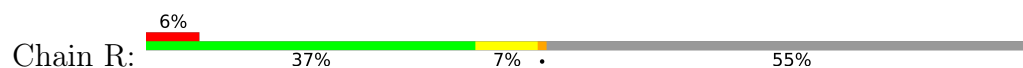
- Molecule 15: Pre-mRNA-splicing factor RBM22



- Molecule 16: Protein BUD31 homolog



- Molecule 17: Spliceosome-associated protein CWC15 homolog



- Molecule 18: Serine/arginine repetitive matrix protein 2

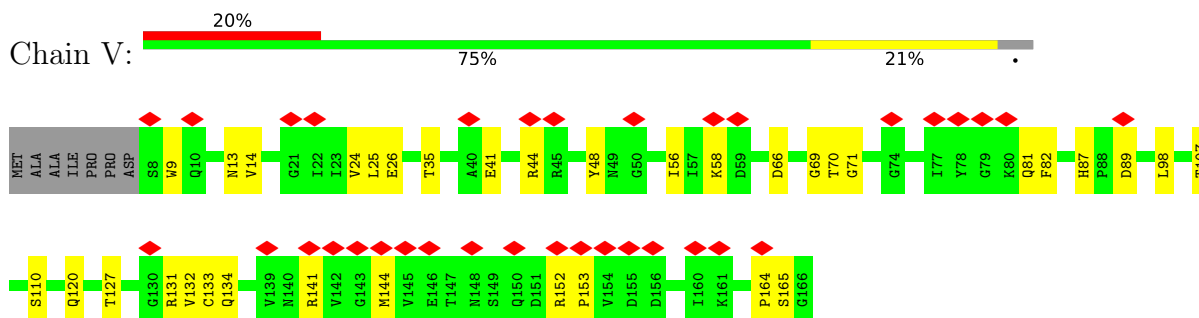
99%

[illegible]

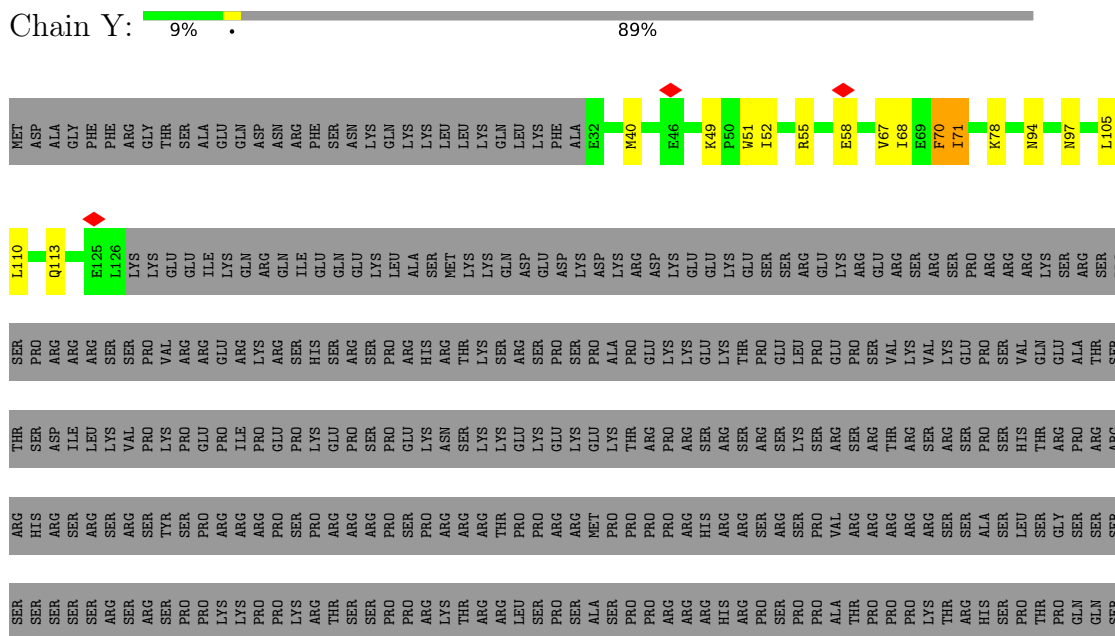


ARG	LYS	ALA	SER	ALA	SER	THR	GLU	LEU
GLN	PRO	LYS	SER	THR	SER	THR	GLU	ALA
ARG	SER	ARG	SER	ALA	SER	THR	ARG	ALA
GLY	PRO	ARG	SER	SER	SER	SER	PRO	SER
ASP	LYS	ARG	SER	SER	SER	SER	SER	LEU
ARG	LYS	SER	SER	SER	SER	ALA	PRO	THR
SER	PRO	SER	SER	SER	SER	GLY	SER	SER
SER	PRO	SER	SER	SER	SER	SER	SER	ALA
PRO	GLY	SER	SER	SER	SER	ASN	MET	WET
HIS	GLU	SER	SER	SER	SER	GLY	GLY	ALA
LYS	ARG	SER	SER	SER	SER	MET	GLN	PRO
ARG	ARG	SER	SER	SER	SER	LEU	ALA	ALA
ARG	ARG	SER	SER	SER	SER	SER	PRO	ALA
ARG	ARG	SER	SER	SER	SER	VAL	SER	SER
GLU	SER	SER	GLY	SER	GLY	PRO	GLN	GLY
THR	PRO	SER	SER	SER	SER	ALA	SER	ALA
PRO	ARG	SER	SER	SER	SER	PRO	LEU	ASN
SER	LYS	SER	SER	SER	SER	GLY	LEU	LEU
PRO	PRO	SER	SER	SER	SER	VAL	PRO	THR
ARG	ILE	SER	ASP	PRO	ASP	PRO	PRO	SER
PRO	ASP	SER	SER	SER	SER	HIS	ALA	PRO
MET	SER	SER	GLU	SER	GLY	SER	GLN	ARG
LEU	SER	SER	GLY	SER	GLY	ASP	ASP	VAL
HIS	ARG	SER	SER	SER	SER	VAL	GLN	PRO
ARG	ASP	SER	SER	SER	GLY	GLU	PRO	LEU
SER	ARG	SER	LEU	SER	LEU	ARG	SER	SER
SER	ARG	SER	PRO	SER	PRO	PRO	SER	ALA
ARG	SER	SER	VAL	SER	VAL	PRO	PRO	TYR
SER	LEU	SER	GLN	SER	GLN	ALA	VAL	GLU
SER	SER	SER	PRO	SER	PRO	SER	PRO	ARG
PRO	TYR	SER	GLU	GLU	GLU	THR	SER	VAL
		SER	VAL	VAL	VAL	GLY	ALA	SER
	PRO	SER	ALA	ALA	ALA	ALA	PHE	GLY
	VAL	SER	LEU	SER	LEU	GLN	SER	ARG
	GLU	SER	LYS	LYS	LYS	GLN	ASP	THR
	ARG	SER	ARG	ARG	ARG	PRO	GLN	SER
	ARG	SER	VAL	VAL	VAL	SER	SER	PRO
	PRO	SER	PRO	ARG	PRO	ALA	PRO	PRO
	ARG	SER	SER	SER	SER	LEU	CYS	LEU
	SER	SER	PRO	PRO	PRO	ALA	LEU	LEU
	PRO	SER	THR	THR	THR	ALA	ILE	ASP
	SER	SER	GLN	GLN	GLN	LEU	ALA	ARG
	PRO	SER	ALA	ALA	ALA	GLN	GLN	ALA
	PRO	SER	PRO	PRO	PRO	PRO	THR	ARG
	PRO	SER	LYS	LYS	GLY	ALA	THR	SER
	ARG	SER	GLU	GLU	GLU	LYS	PRO	ARG
	ASP	PRO	VAL	VAL	VAL	ALA	VAL	THR
	GLN	SER	SER	SER	SER	ARG	ALA	PRO
	GLN	PRO	GLY	GLY	GLY	ARG	GLY	PRO
	SER	ALA	GLU	GLU	GLU	SER	SER	ALA
	SER	LYS	GLY	GLY	GLY	SER	GLN	ALA
	SER	PRO	ARG	ARG	ARG	SER	SER	PRO
	SER	SER	PRO	PRO	PRO	SER	LEU	SER
	GLU	PRO	PRO	PRO	PRO	SER	GLN	SER
	ARG	GLN	GLU	GLU	GLU	SER	SER	GLY
	GLY	ALA	PRO	PRO	PRO	SER	GLY	ARG
	SER	LEU	THR	THR	THR	SER	WET	ALA
	ARG	PRO	PRO	PRO	PRO	SER	THR	THR

- Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

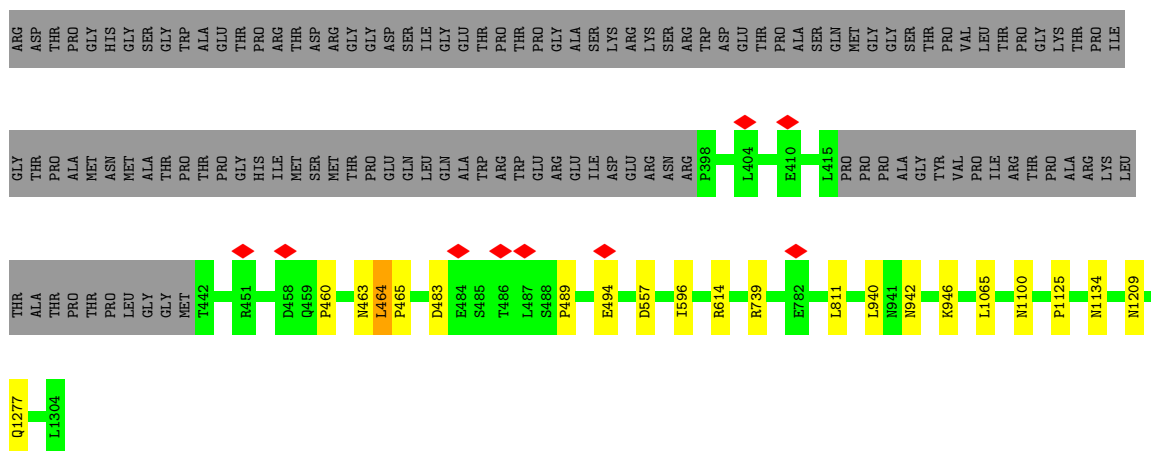


- Molecule 20: Serine/arginine repetitive matrix protein 1

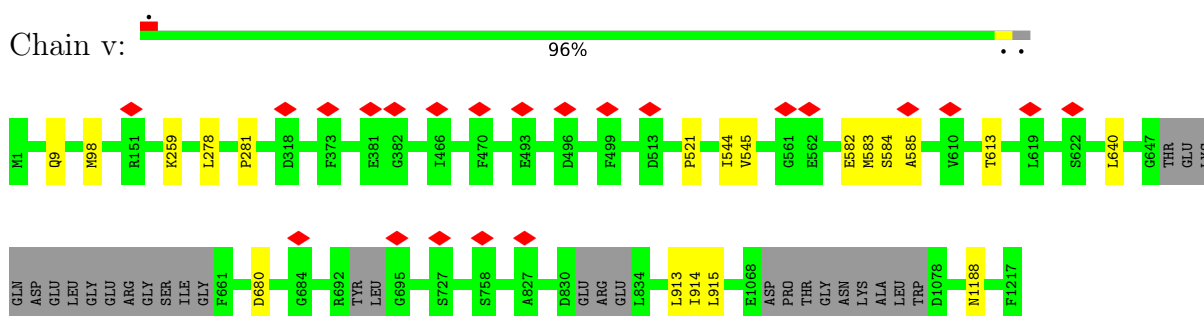




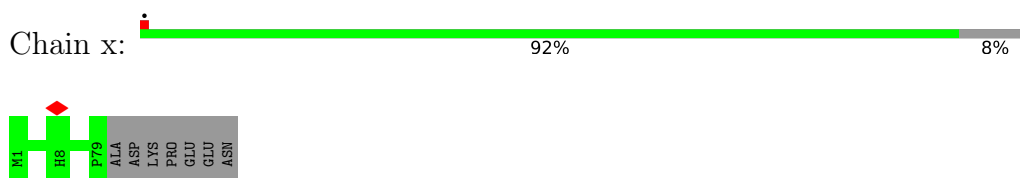




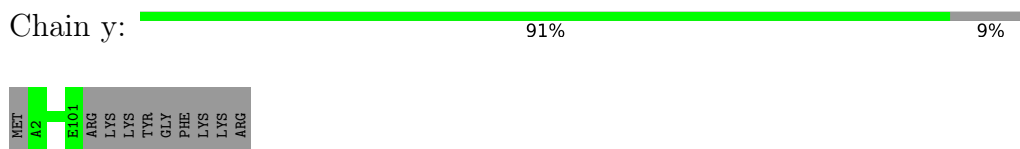
- Molecule 25: Splicing factor 3B subunit 3



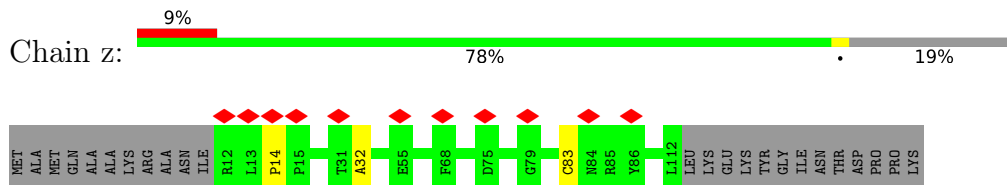
- Molecule 26: Splicing factor 3B subunit 5



- Molecule 27: PHD finger-like domain-containing protein 5A



- Molecule 28: Splicing factor 3B subunit 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.314	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	487.19998, 487.19998, 487.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.45	0/999	0.64	0/1347
2	2	0.78	0/1404	1.21	9/2177 (0.4%)
3	3	0.39	0/1002	0.68	1/1341 (0.1%)
4	5	0.97	1/1638 (0.1%)	1.41	32/2545 (1.3%)
5	6	0.91	0/2279	1.20	11/3551 (0.3%)
6	7	0.45	0/744	0.68	1/993 (0.1%)
7	8	0.48	0/1239	0.65	0/1660
8	A	0.59	2/19083 (0.0%)	0.73	14/25888 (0.1%)
9	B	0.44	1/7299 (0.0%)	0.75	7/9917 (0.1%)
10	C	0.47	0/2328	0.70	0/3128
11	D	0.63	0/2584	0.79	3/3522 (0.1%)
12	E	0.35	0/1079	0.65	0/1453
13	L	0.52	0/879	0.71	1/1184 (0.1%)
14	O	0.43	0/2295	0.66	0/3088
15	P	0.41	0/2354	0.70	1/3176 (0.0%)
16	Q	0.50	0/1178	0.73	0/1579
17	R	0.45	0/881	0.76	2/1169 (0.2%)
18	S	0.42	0/265	0.70	0/355
19	V	0.31	0/1268	0.56	0/1714
20	Y	0.37	0/775	0.60	0/1045
21	Z	0.85	0/1129	1.13	5/1752 (0.3%)
22	s	0.48	0/1411	0.68	2/1911 (0.1%)
23	t	0.45	0/1447	0.63	1/1945 (0.1%)
24	u	0.55	0/7147	0.72	3/9675 (0.0%)
25	v	0.49	0/9504	0.68	3/12894 (0.0%)
26	x	0.59	0/675	0.71	0/912
27	y	0.63	0/779	0.60	0/1047
28	z	0.42	1/857 (0.1%)	0.64	0/1157
All	All	0.56	5/74522 (0.0%)	0.78	96/102125 (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
3	3	0	1
8	A	0	19
9	B	0	8
10	C	0	3
11	D	0	5
13	L	0	1
14	O	0	2
15	P	0	3
22	s	0	1
23	t	0	1
24	u	0	6
25	v	0	5
28	z	0	2
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	z	14	PRO	C-N	6.42	1.46	1.34
4	5	26	A	N9-C4	-6.39	1.34	1.37
8	A	538	SER	CA-CB	-5.41	1.44	1.52
8	A	166	PHE	CB-CG	-5.07	1.42	1.51
9	B	566	THR	C-N	5.03	1.45	1.34

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	27	U	N1-C2-O2	13.25	132.08	122.80
4	5	27	U	N3-C2-O2	-12.05	113.77	122.20
4	5	27	U	C2-N1-C1'	11.36	131.33	117.70
2	2	23	A	C8-N9-C4	-8.76	102.30	105.80
4	5	36	C	C6-N1-C2	-8.40	116.94	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	568	GLY	Peptide
8	A	165	ARG	Peptide

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Mol	Chain	Res	Type	Group
8	A	175	PRO	Peptide
8	A	210	HIS	Peptide
8	A	521	ASN	Peptide

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	1	981	0	976	14	0
2	2	1262	0	640	10	0
3	3	981	0	961	13	0
4	5	1470	0	746	16	0
5	6	2035	0	1028	26	0
6	7	733	0	720	10	0
7	8	1211	0	1248	5	0
8	A	18569	0	18479	286	0
9	B	7137	0	7149	135	0
10	C	2287	0	2314	48	0
11	D	2517	0	2471	49	0
12	E	1054	0	988	10	0
13	L	858	0	868	21	0
14	O	2235	0	2153	29	0
15	P	2305	0	2282	45	0
16	Q	1153	0	1160	9	0
17	R	869	0	855	12	0
18	S	261	0	267	1	0
19	V	1236	0	1210	22	0
20	Y	762	0	779	8	0
21	Z	1013	0	515	16	0
22	s	1377	0	1314	0	0
23	t	1415	0	1337	0	0
24	u	7013	0	7199	0	0
25	v	9315	0	9235	0	0
26	x	656	0	622	0	0
27	y	766	0	738	0	0
28	z	839	0	841	0	0
29	6	4	0	0	0	0
30	A	36	0	6	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	B	32	0	12	1	0
32	P	3	0	0	0	0
32	Q	3	0	0	0	0
32	t	1	0	0	0	0
32	y	3	0	0	0	0
All	All	72392	0	69113	688	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 7.

The worst 5 of 688 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)
8:A:613:TYR:HE2	30:A:3001:IHP:O42	1.25	1.18
8:A:442:LYS:NZ	30:A:3001:IHP:O43	1.76	1.16
8:A:163:ARG:NH2	30:A:3001:IHP:O36	1.84	1.10
8:A:613:TYR:CE2	30:A:3001:IHP:O42	2.16	0.98
2:2:12:G:H1	5:6:86:U:H3	0.91	0.90

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	1	120/322 (37%)	105 (88%)	15 (12%)	0	100	100
3	3	116/619 (19%)	93 (80%)	23 (20%)	0	100	100
6	7	91/464 (20%)	85 (93%)	6 (7%)	0	100	100
7	8	142/895 (16%)	122 (86%)	18 (13%)	2 (1%)	9	31
8	A	2232/2335 (96%)	1953 (88%)	274 (12%)	5 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	B	900/972 (93%)	747 (83%)	149 (17%)	4 (0%)	30	60
10	C	282/536 (53%)	221 (78%)	61 (22%)	0	100	100
11	D	318/514 (62%)	269 (85%)	47 (15%)	2 (1%)	22	50
12	E	126/579 (22%)	112 (89%)	14 (11%)	0	100	100
13	L	101/802 (13%)	87 (86%)	13 (13%)	1 (1%)	13	39
14	O	251/848 (30%)	219 (87%)	31 (12%)	1 (0%)	30	60
15	P	282/420 (67%)	236 (84%)	45 (16%)	1 (0%)	30	60
16	Q	136/144 (94%)	115 (85%)	21 (15%)	0	100	100
17	R	98/229 (43%)	79 (81%)	19 (19%)	0	100	100
18	S	32/2752 (1%)	24 (75%)	8 (25%)	0	100	100
19	V	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
20	Y	93/904 (10%)	90 (97%)	3 (3%)	0	100	100
22	s	173/472 (37%)	152 (88%)	21 (12%)	0	100	100
23	t	166/343 (48%)	145 (87%)	20 (12%)	1 (1%)	22	50
24	u	877/1304 (67%)	803 (92%)	70 (8%)	4 (0%)	25	54
25	v	1179/1217 (97%)	1022 (87%)	153 (13%)	4 (0%)	37	66
26	x	77/86 (90%)	66 (86%)	11 (14%)	0	100	100
27	y	98/110 (89%)	90 (92%)	8 (8%)	0	100	100
28	z	99/125 (79%)	85 (86%)	14 (14%)	0	100	100
All	All	8146/17158 (48%)	7068 (87%)	1053 (13%)	25 (0%)	38	66

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	384	HIS
24	u	464	LEU
8	A	1519	THR
11	D	385	TYR
15	P	67	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	109/291 (38%)	109 (100%)	0	100	100
3	3	102/545 (19%)	101 (99%)	1 (1%)	73	83
6	7	77/382 (20%)	77 (100%)	0	100	100
7	8	132/776 (17%)	131 (99%)	1 (1%)	79	87
8	A	2026/2108 (96%)	1987 (98%)	39 (2%)	52	71
9	B	802/866 (93%)	793 (99%)	9 (1%)	70	81
10	C	242/459 (53%)	237 (98%)	5 (2%)	48	69
11	D	275/441 (62%)	269 (98%)	6 (2%)	47	68
12	E	111/502 (22%)	110 (99%)	1 (1%)	75	86
13	L	88/709 (12%)	87 (99%)	1 (1%)	70	81
14	O	229/751 (30%)	226 (99%)	3 (1%)	65	78
15	P	254/361 (70%)	251 (99%)	3 (1%)	67	80
16	Q	126/130 (97%)	124 (98%)	2 (2%)	58	75
17	R	94/203 (46%)	91 (97%)	3 (3%)	34	59
18	S	27/2432 (1%)	27 (100%)	0	100	100
19	V	129/134 (96%)	129 (100%)	0	100	100
20	Y	86/831 (10%)	84 (98%)	2 (2%)	45	67
22	s	149/416 (36%)	148 (99%)	1 (1%)	81	88
23	t	153/294 (52%)	152 (99%)	1 (1%)	81	88
24	u	763/1104 (69%)	754 (99%)	9 (1%)	67	80
25	v	1028/1051 (98%)	1020 (99%)	8 (1%)	79	87
26	x	71/77 (92%)	71 (100%)	0	100	100
27	y	86/95 (90%)	86 (100%)	0	100	100
28	z	90/109 (83%)	90 (100%)	0	100	100
All	All	7249/15067 (48%)	7154 (99%)	95 (1%)	64	78

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	D	385	TYR
17	R	72	ARG
11	D	427	LEU

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Mol	Chain	Res	Type
14	O	443	ILE
20	Y	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
11	D	394	ASN
22	s	127	HIS
11	D	408	ASN
16	Q	95	GLN
24	u	832	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	57/188 (30%)	16 (28%)	1 (1%)
21	Z	46/478 (9%)	19 (41%)	1 (2%)
4	5	69/116 (59%)	31 (44%)	1 (1%)
5	6	94/107 (87%)	30 (31%)	1 (1%)
All	All	266/889 (29%)	96 (36%)	4 (1%)

5 of 96 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	13	C
2	2	14	C
2	2	16	U
2	2	18	U
2	2	19	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	23	A
4	5	26	A
5	6	58	G
21	Z	261	A

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](#)

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	$\# Z > 2$
31	GTP	B	1500	-	26,34,34	1.35	2 (7%)	32,54,54	1.61	8 (25%)
30	IHP	A	3001	-	36,36,36	0.74	0	54,60,60	1.25	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
31	GTP	B	1500	-	-	5/18/38/38	0/3/3/3
30	IHP	A	3001	-	-	3/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	1500	GTP	C5-C6	-4.69	1.37	1.47
31	B	1500	GTP	C5-C4	-2.29	1.37	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	1500	GTP	PB-O3B-PG	-3.95	119.29	132.83
31	B	1500	GTP	C5-C6-N1	3.65	120.39	113.95
31	B	1500	GTP	C2-N1-C6	-3.07	119.45	125.10
30	A	3001	IHP	O12-C2-C1	2.96	115.66	108.69
31	B	1500	GTP	C8-N7-C5	2.91	108.54	102.99

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

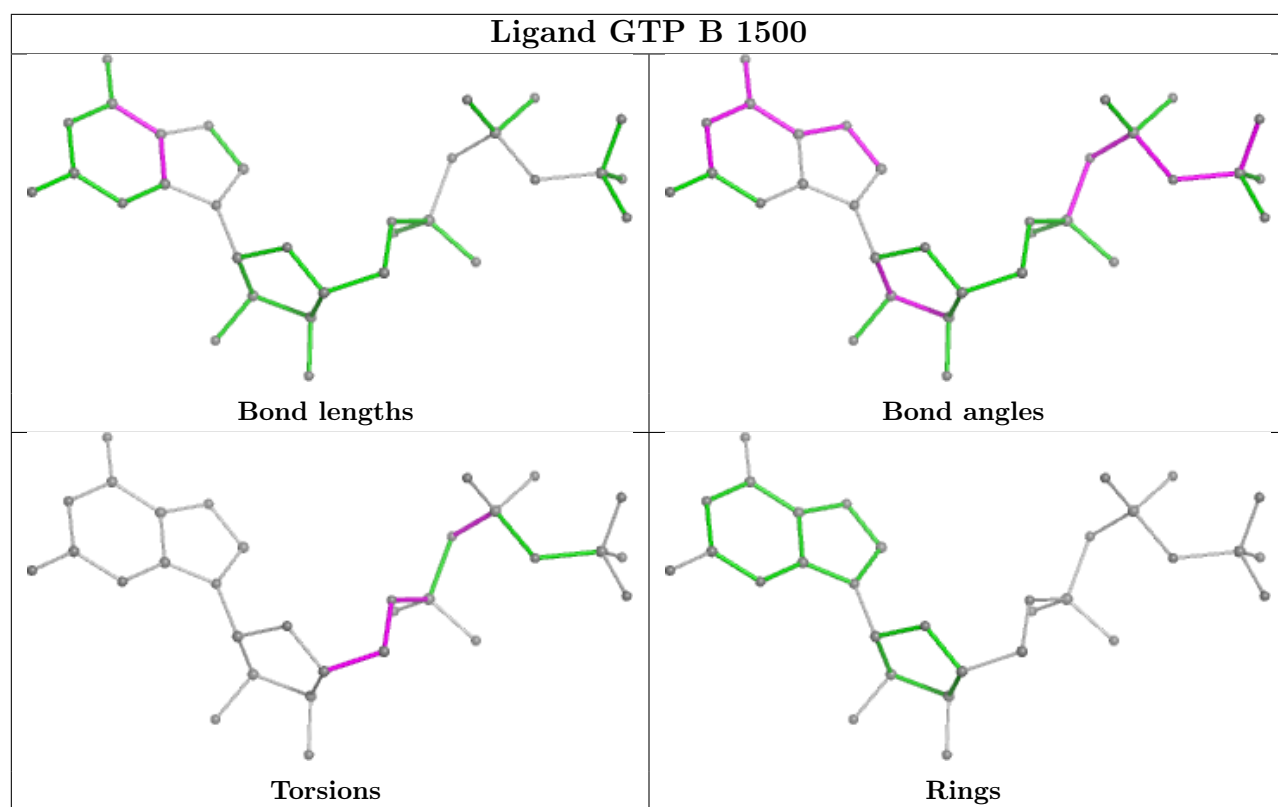
Mol	Chain	Res	Type	Atoms
30	A	3001	IHP	C1-C2-O12-P2
31	B	1500	GTP	C5'-O5'-PA-O3A
31	B	1500	GTP	C5'-O5'-PA-O1A
31	B	1500	GTP	PA-O3A-PB-O1B
31	B	1500	GTP	C4'-C5'-O5'-PA

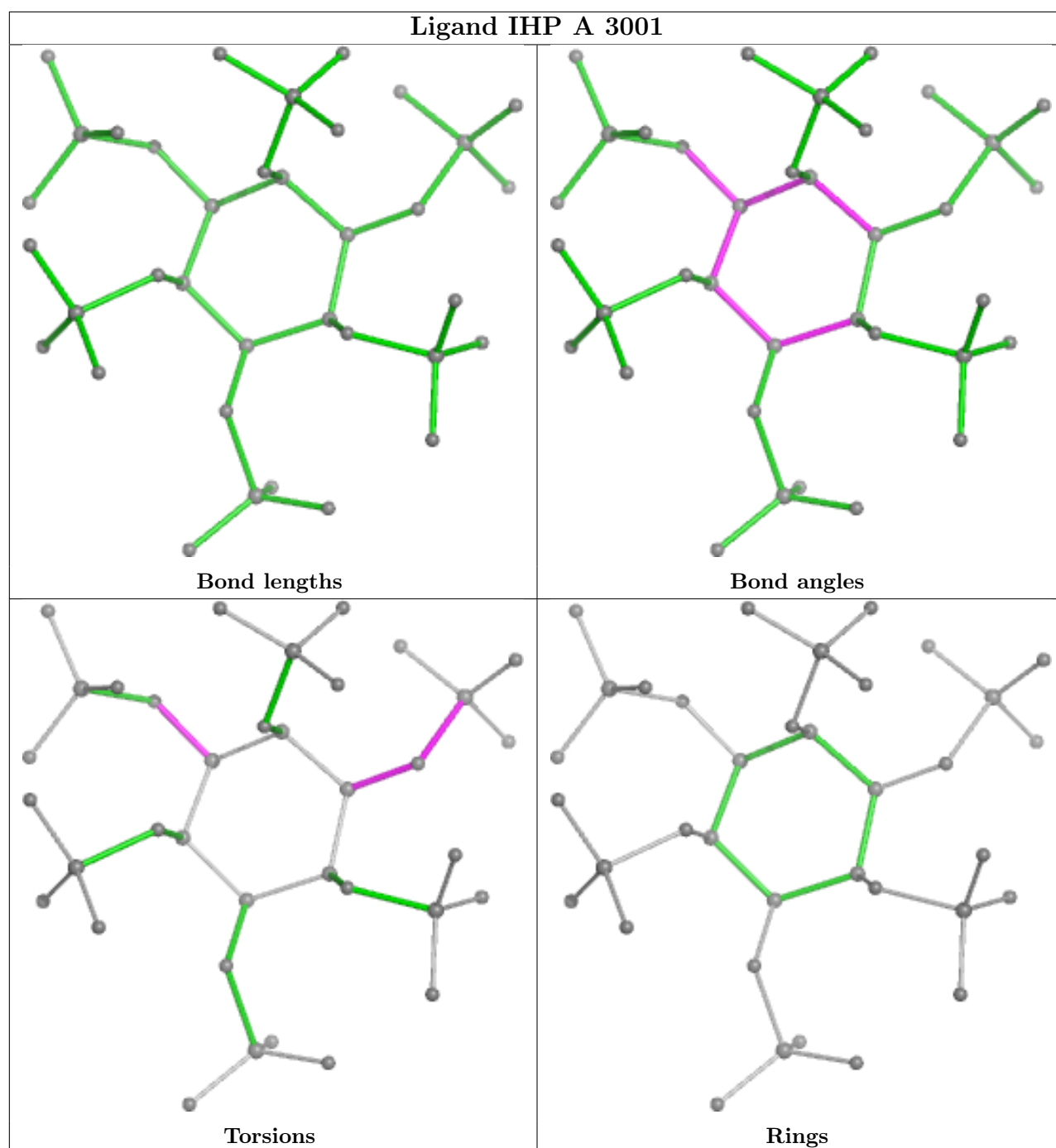
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	1500	GTP	1	0
30	A	3001	IHP	11	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	59:A	O3'	60:U	P	4.39

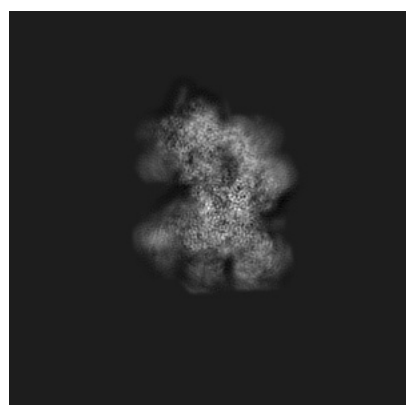
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4255. These allow visual inspection of the internal detail of the map and identification of artifacts.

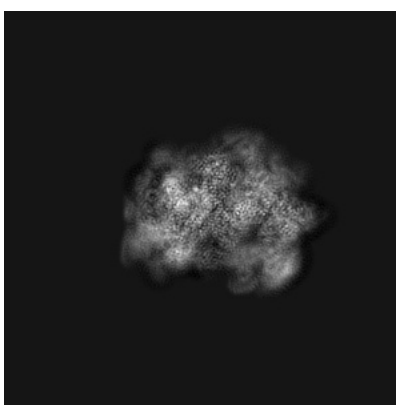
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

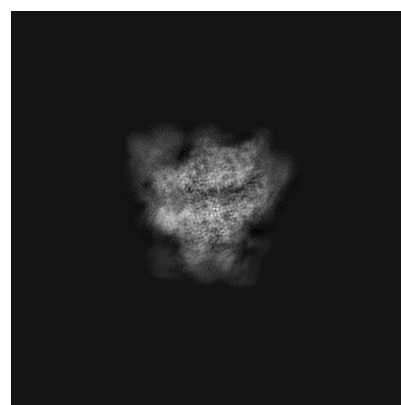
6.1.1 Primary map



X



Y

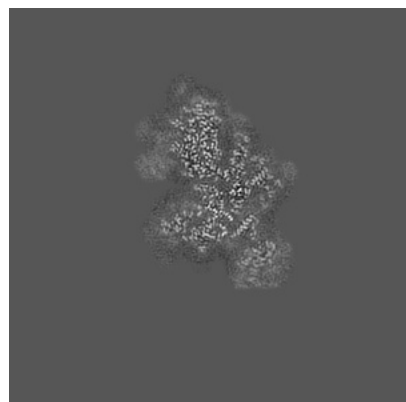


Z

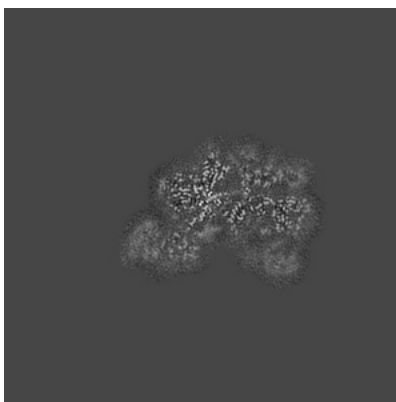
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210

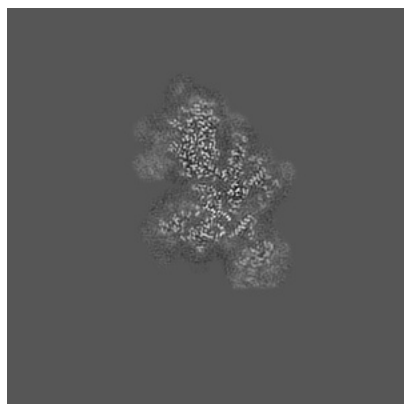


Z Index: 210

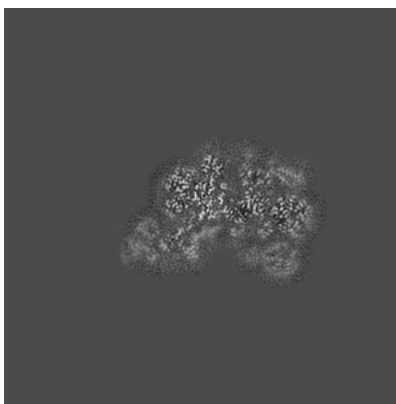
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

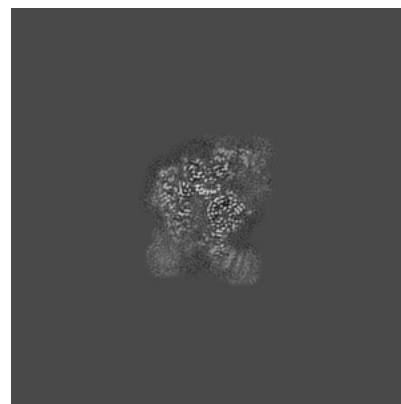
6.3.1 Primary map



X Index: 210



Y Index: 207

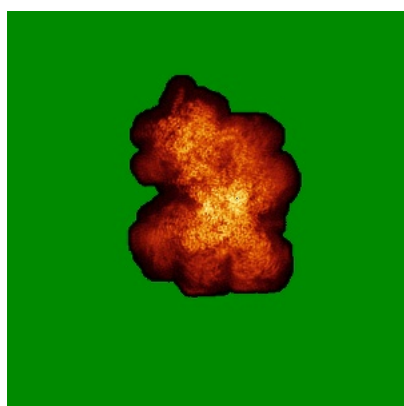


Z Index: 184

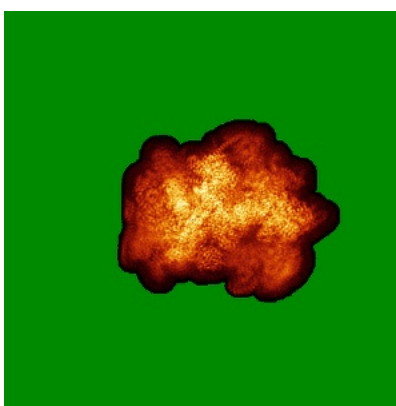
The images above show the largest variance slices of the map in three orthogonal directions.

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

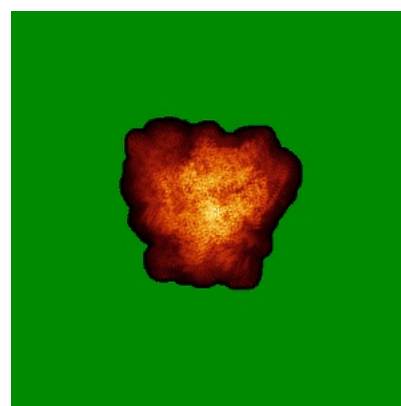
6.4.1 Primary map



X



Y

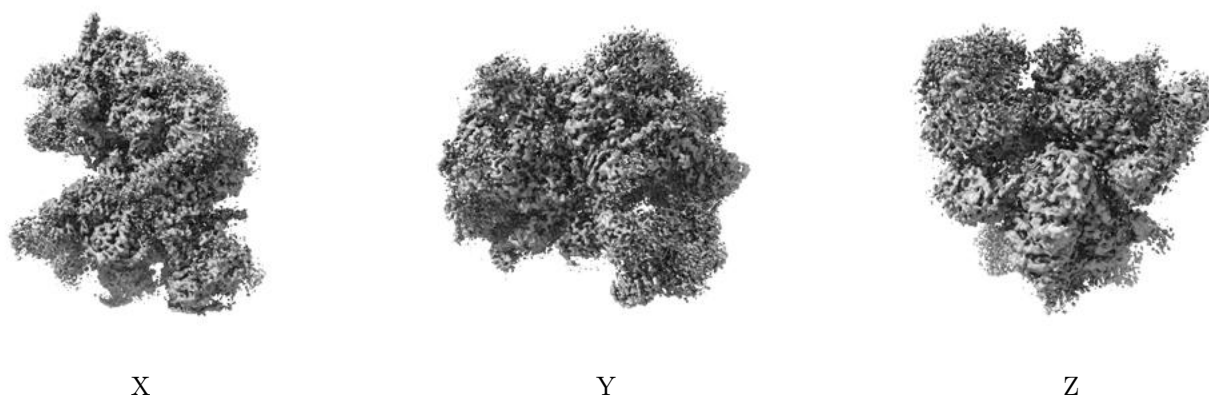


Z

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

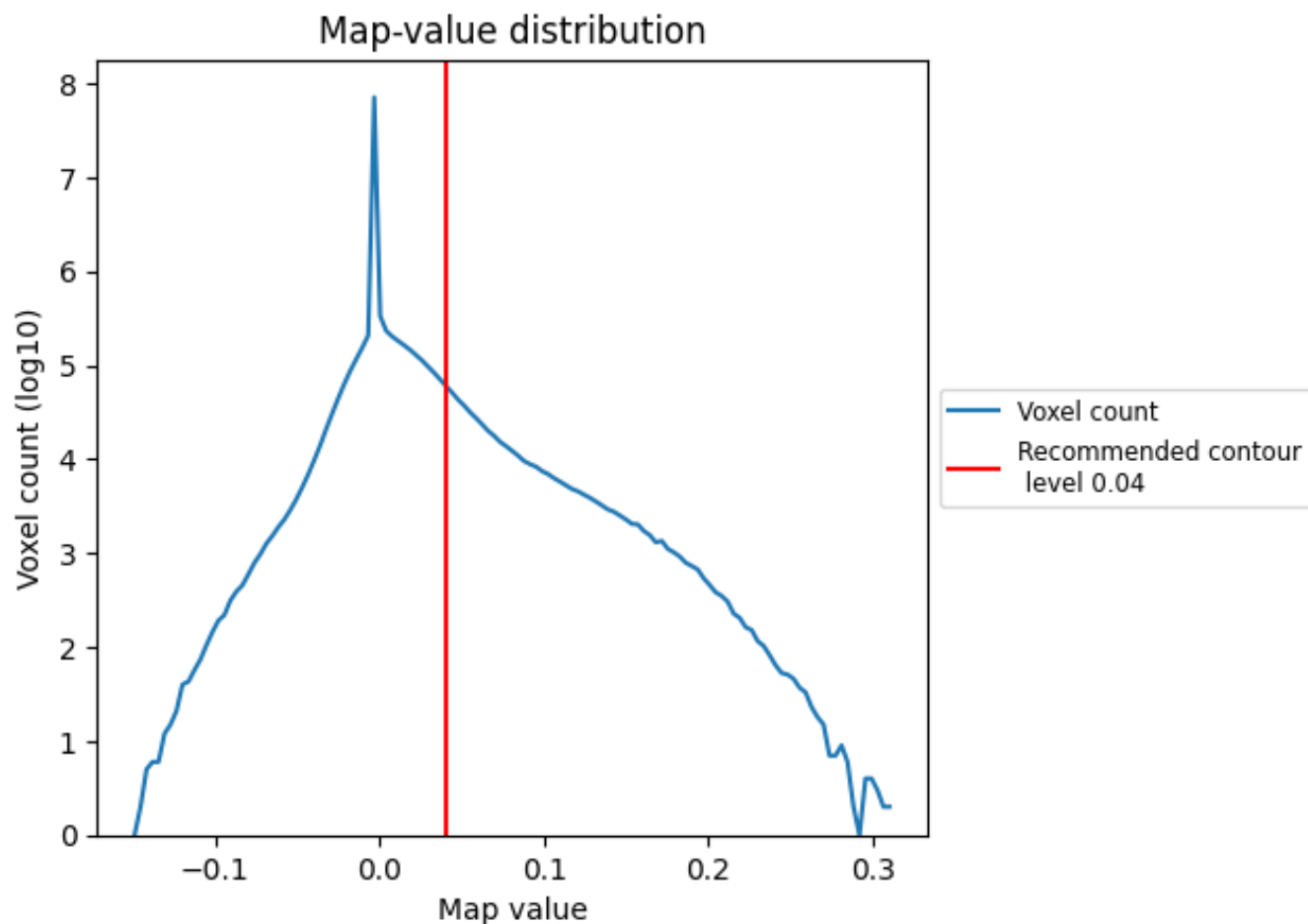
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

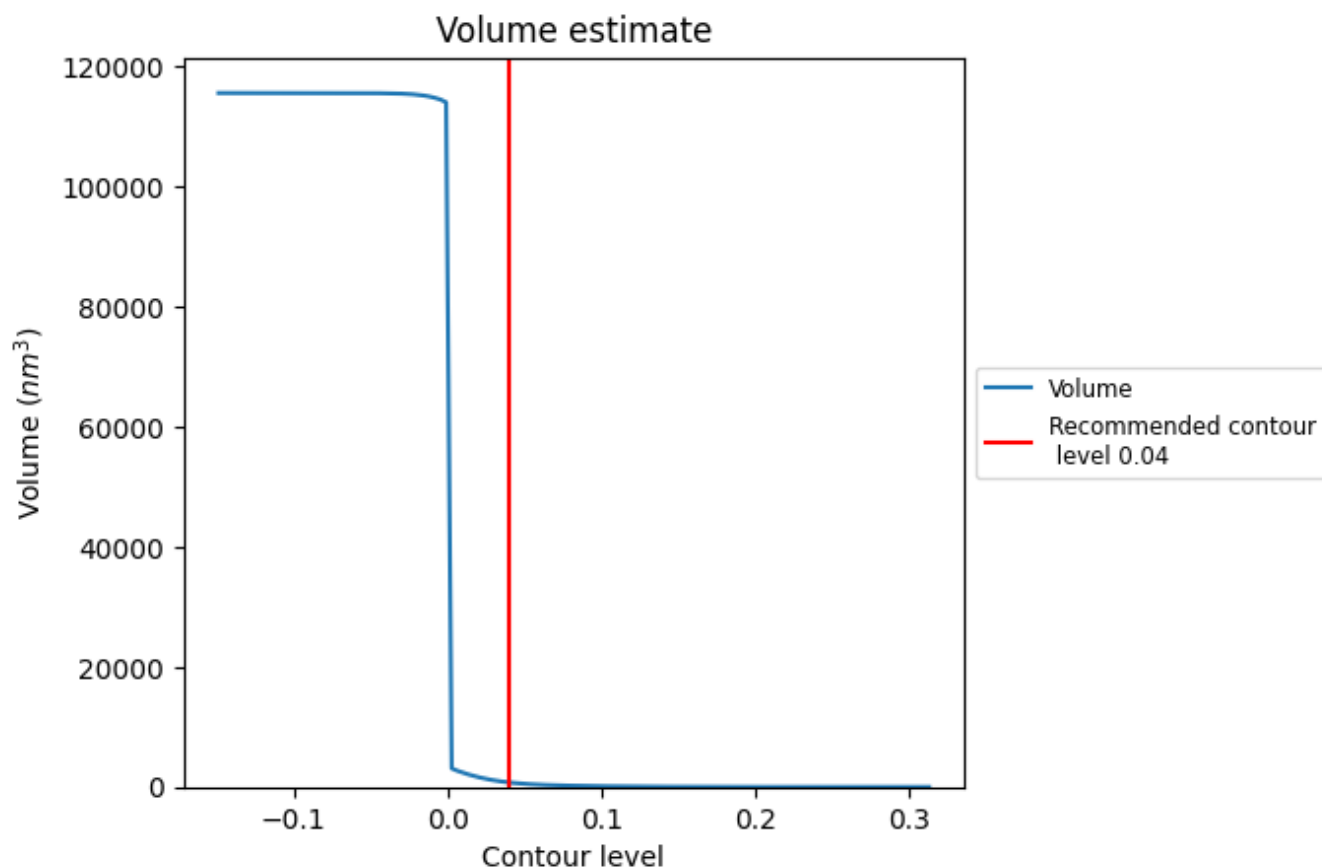
This section contains the results of statistical analysis of the map.

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.

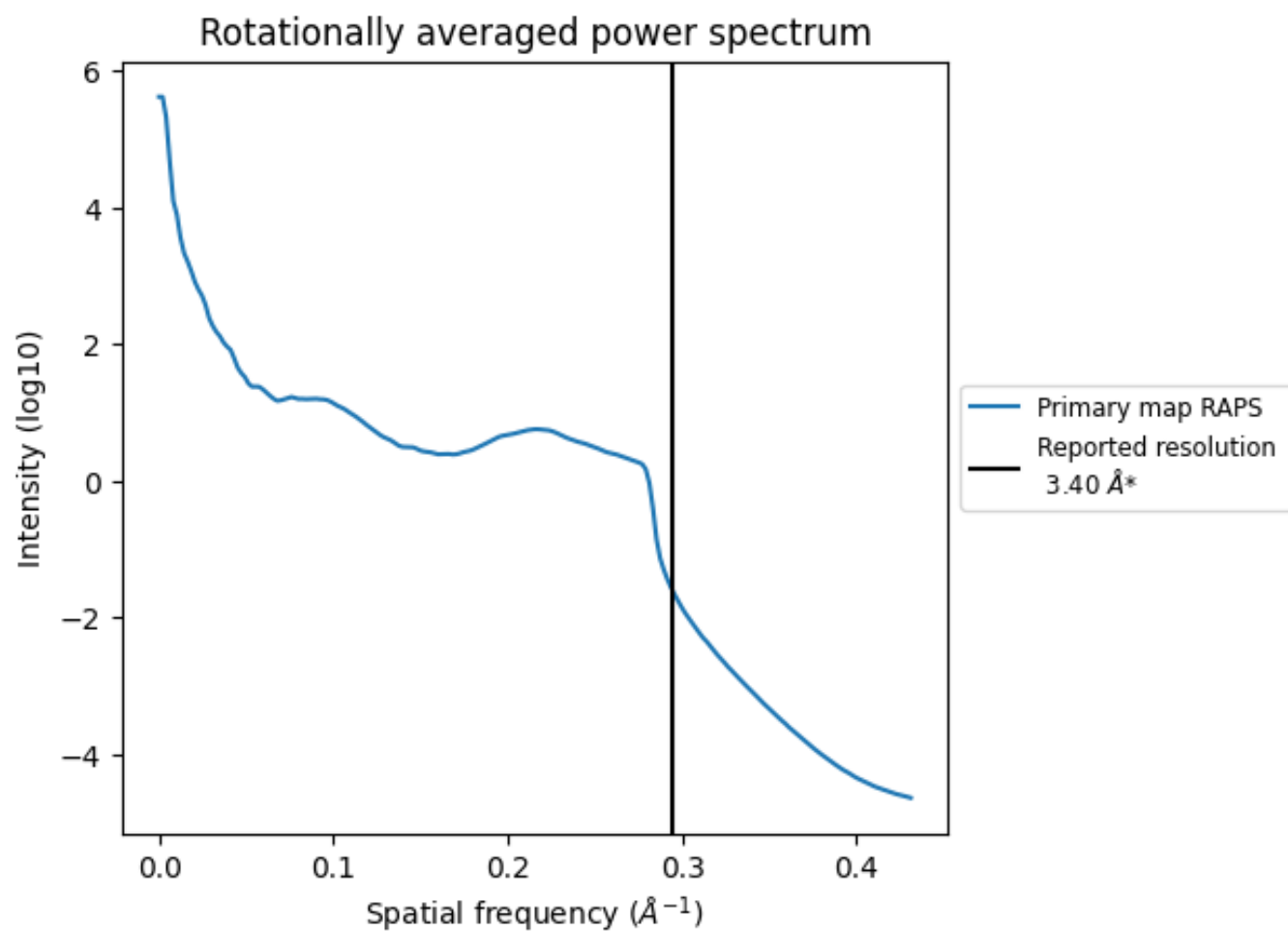
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 759 nm³; this corresponds to an approximate mass of 686 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 0.294 Å⁻¹

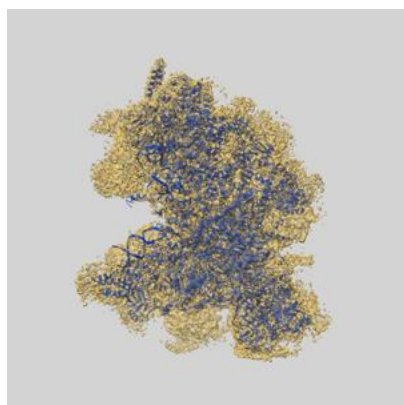
8 Fourier-Shell correlation ⓘ

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

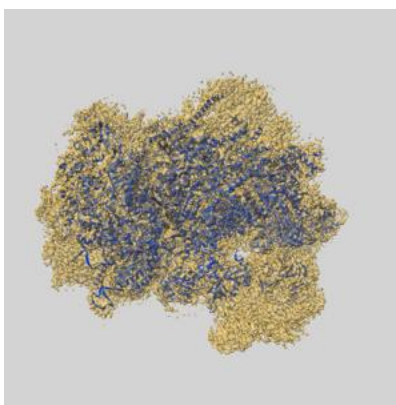
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4255 and PDB model 6FF4. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

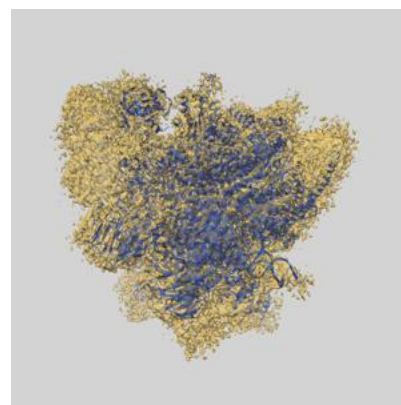
9.1 Map-model overlay [i](#)



X



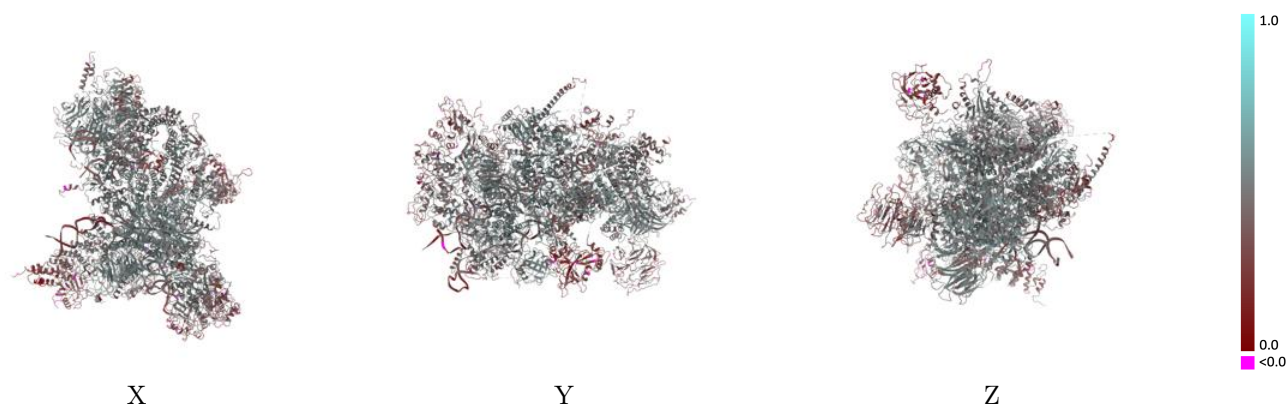
Y



Z

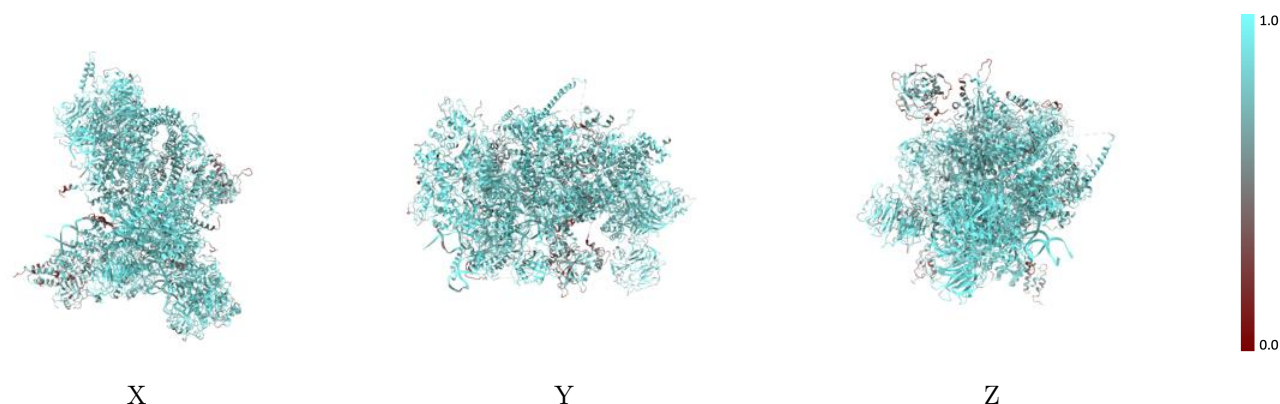
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



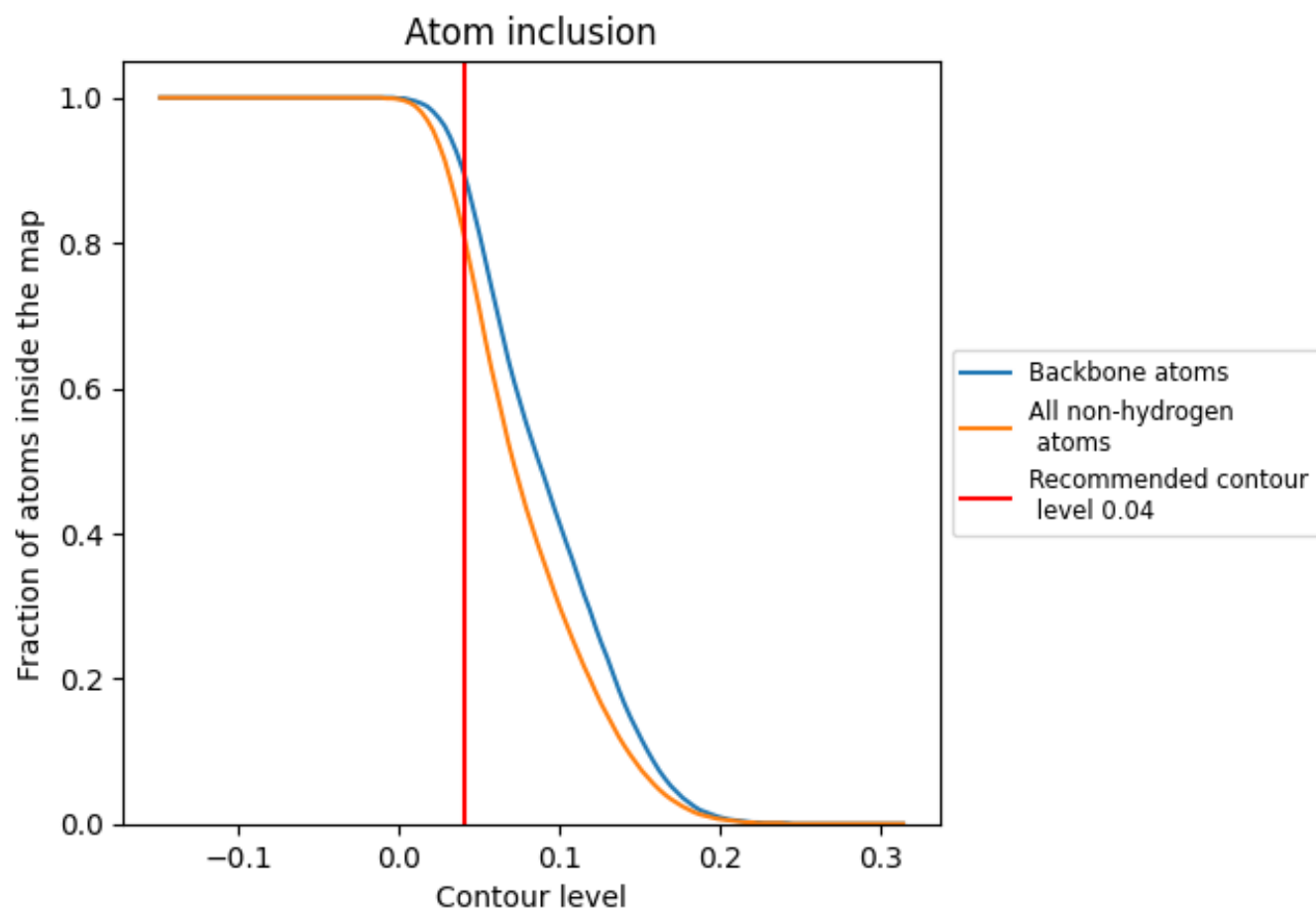
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.4430
1	 0.7840	 0.4600
2	 0.8790	 0.3980
3	 0.6360	 0.3860
5	 0.9210	 0.4110
6	 0.8970	 0.3970
7	 0.7870	 0.4660
8	 0.8410	 0.4890
A	 0.8170	 0.4700
B	 0.7990	 0.4050
C	 0.7260	 0.4190
D	 0.9220	 0.5210
E	 0.6100	 0.3610
L	 0.8220	 0.4690
O	 0.7280	 0.3770
P	 0.6410	 0.3540
Q	 0.8840	 0.4650
R	 0.6960	 0.4550
S	 0.6760	 0.4570
V	 0.6450	 0.2470
Y	 0.7920	 0.3720
Z	 0.9230	 0.4510
s	 0.8790	 0.4940
t	 0.6740	 0.4330
u	 0.8420	 0.4910
v	 0.8660	 0.4530
x	 0.8810	 0.4890
y	 0.8740	 0.5160
z	 0.7090	 0.3410

