



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:59 pm GMT

PDB ID : 6FF7
EMDB ID : EMD-4240
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 : 4.50 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:

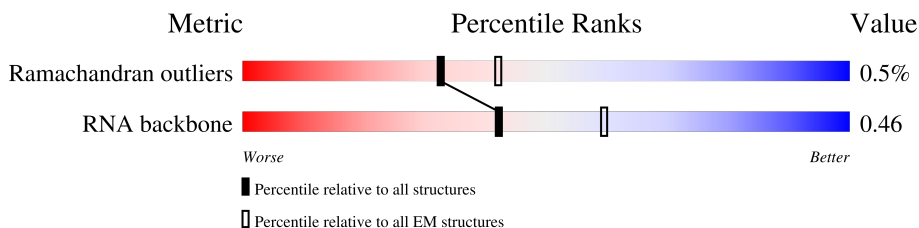
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.50 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)
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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	
8	A	2335	
9	B	972	

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Mol	Chain	Length	Quality of chain
10	C	536	53% 47%
11	D	514	62% 38%
12	E	579	22% 78%
13	L	802	13% 87%
14	O	848	30% 70%
15	P	420	68% 32%
16	Q	144	96%
17	R	229	44% 55%
18	S	2752	99%
19	V	166	95%
20	Y	904	11% 89%
21	Z	369	8% 5% 87%
22	s	472	37% 63%
23	t	343	50% 50%
24	u	1304	67% 32%
25	v	1217	97%
26	x	86	92% 8%
27	y	110	91% 9%
28	N	125	79% 19%
28	z	125	78% 19%
29	0	396	37% 61%
30	9	501	71% 84% 14%
31	F	357	82% 16%
32	G	504	7% 26% 74%
32	H	504	6% 27% 73%



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Mol	Chain	Length	Quality of chain
32	I	504	27% 73%
32	J	504	8% 26% 73%
33	K	225	30% 92% 5%
34	M	855	37% 85% 14%
35	T	908	7% 50% 49%
36	U	1485	28% 89% 11%
37	W	255	59% 61% 36%
38	X	225	48% 75% 24%
39	a	118	6% 75% 25%
39	h	118	58% 82% 17%
40	b	86	84% 15%
40	i	86	26% 86% 14%
41	c	92	7% 84% 15%
41	j	92	30% 86% 14%
42	d	76	9% 95%
42	k	76	32% 97%
43	e	126	8% 69% 30%
43	l	126	34% 66% 34%
44	f	240	7% 37% 63%
44	m	240	25% 30% 70%
45	g	119	78% 22%
45	n	119	51% 69% 31%
46	o	301	60% 75% 24%
47	p	793	16% 22% 78%
48	q	1041	5% 60% 40%

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Mol	Chain	Length	Quality of chain
49	r	2136	 80% 19%
50	w	285	 20% 19% 80%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 88879 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
			Total	C	N	O		
1	1	122	601	357	122	122	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

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

- Molecule 3 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	118	584	348	118	118	0	0

- Molecule 4 is a RNA chain called U5 snRNA.

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

- Molecule 5 is a RNA chain called U6 snRNA.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	7	93	457	271	93	93	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	8	144	Total	C	N	O	0	0
			714	426	144	144		

- 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	0	0
			11093	6617	2238	2238		

- 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	0	0
			4456	2652	902	902		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	C	286	Total	C	N	O	0	0
			1418	846	286	286		

- Molecule 11 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	D	320	Total	C	N	O	0	0
			1578	938	320	320		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	E	130	Total	C	N	O	0	0
			642	382	130	130		

- 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	0	0
			511	305	103	103		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	253	Total	C	N	O	0	0
			1260	754	253	253		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	286	Total	C	N	O	0	0
			1413	841	286	286		

- Molecule 16 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	138	Total	C	N	O	0	0
			683	407	138	138		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	102	Total	C	N	O	0	0
			507	303	102	102		

- 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	0	0
			163	95	34	34		

- 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	0	0
			775	457	159	159		

- 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	0	0
			470	280	95	95		

- Molecule 21 is a RNA chain called pre-mRNA.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	s	175	859	509	175	175	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	t	172	849	505	172	172	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	u	881	4357	2595	881	881	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	v	1189	5862	3484	1189	1189	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	x	79	391	233	79	79	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	y	100	490	290	100	100	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	z	101	Total	C	N	O	0	0
			500	298	101	101		
28	N	101	Total	C	N	O	0	0
			500	298	101	101		

- Molecule 29 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	0	155	Total	C	N	O	0	0
			766	456	155	155		

- Molecule 30 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	9	432	Total	C	N	O	0	0
			2139	1275	432	432		

- Molecule 31 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	F	299	Total	C	N	O	0	0
			1471	873	299	299		

- Molecule 32 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	G	132	Total	C	N	O	0	0
			659	395	132	132		
32	H	135	Total	C	N	O	0	0
			674	404	135	135		
32	I	134	Total	C	N	O	0	0
			669	401	134	134		
32	J	135	Total	C	N	O	0	0
			674	404	135	135		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	K	213	Total	C	N	O	0	0
			1059	633	213	213		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	M	738	3665	2189	738	738	0	0

- Molecule 35 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	T	462	2292	1368	462	462	0	0

- Molecule 36 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	U	1329	6588	3930	1329	1329	0	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	W	162	804	480	162	162	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	89	ASP	CYS	conflict	UNP P09661
W	119	CYS	SER	conflict	UNP P09661

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	X	171	844	502	171	171	0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	a	89	440	262	89	89	0	0
39	h	98	485	289	98	98	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	73	Total	C	N	O	0	0
			356	210	73	73		
40	i	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	c	78	Total	C	N	O	0	0
			386	230	78	78		
41	j	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	d	73	Total	C	N	O	0	0
			358	212	73	73		
42	k	74	Total	C	N	O	0	0
			363	215	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	e	88	Total	C	N	O	0	0
			434	258	88	88		
43	l	83	Total	C	N	O	0	0
			409	243	83	83		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	f	89	Total	C	N	O	0	0
			439	261	89	89		
44	m	71	Total	C	N	O	0	0
			349	207	71	71		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	g	93	Total	C	N	O	0	0
			461	275	93	93		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	n	82	406	242	82	82	0	0

- Molecule 46 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	o	229	1119	661	229	229	0	0

- Molecule 47 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	p	175	870	520	175	175	0	0

- Molecule 48 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	q	625	3091	1841	625	625	0	0

- Molecule 49 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	r	1722	8530	5086	1722	1722	0	0

- Molecule 50 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	56	276	164	56	56	0	0

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	2	1	Total	Zn	0
			1	1	
51	P	3	Total	Zn	0
			3	3	

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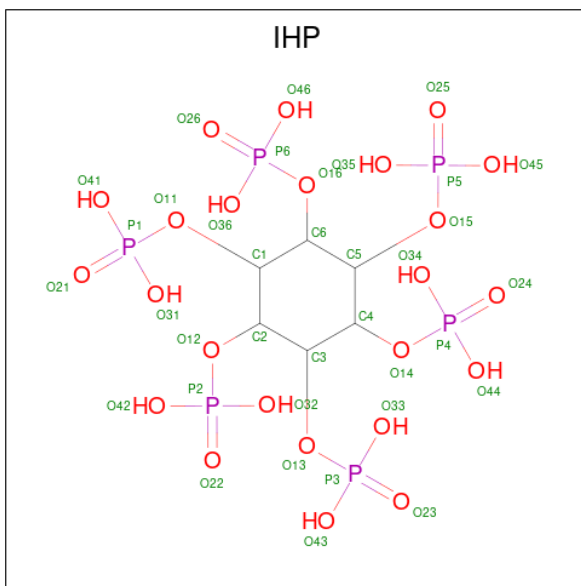
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Mol	Chain	Residues	Atoms		AltConf
51	Q	3	Total	Zn	0
			3	3	
51	Z	1	Total	Zn	0
			1	1	
51	y	3	Total	Zn	0
			3	3	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	6	4	Total	Mg	0
			4	4	
52	r	1	Total	Mg	0
			1	1	

- Molecule 53 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



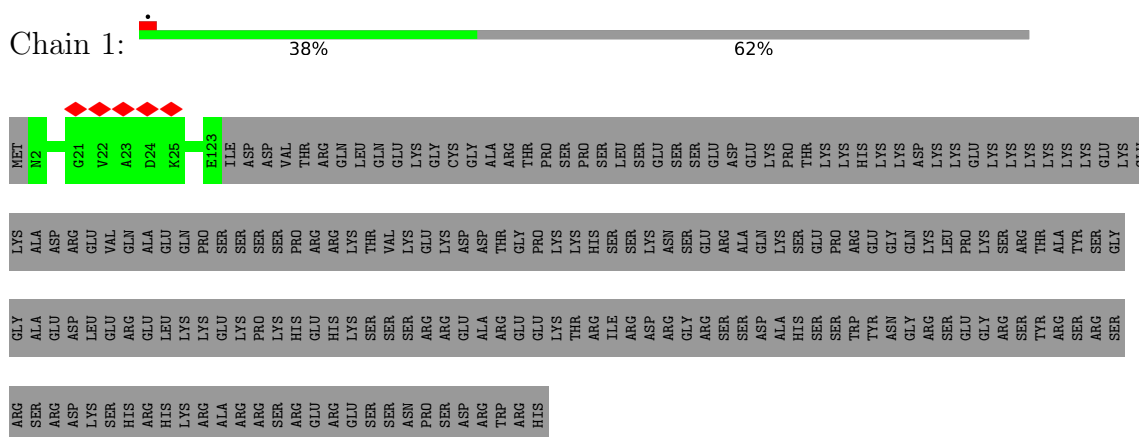
Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

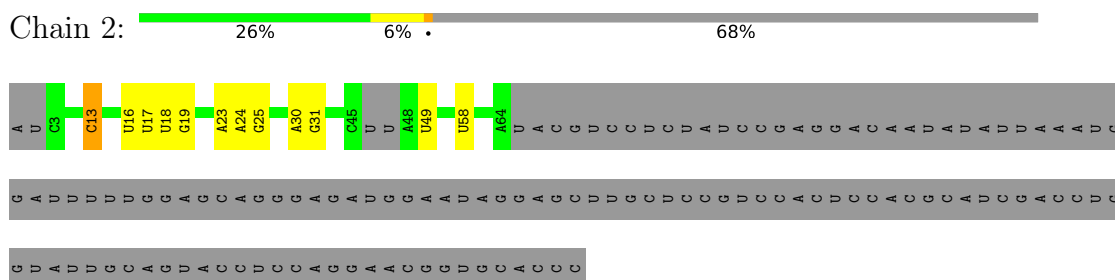
3 Residue-property plots [i](#)

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.

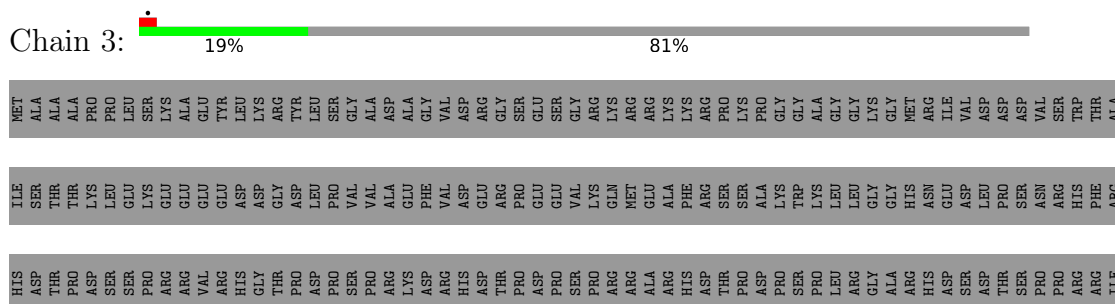
- Molecule 1: RNA-binding motif protein, X-linked 2

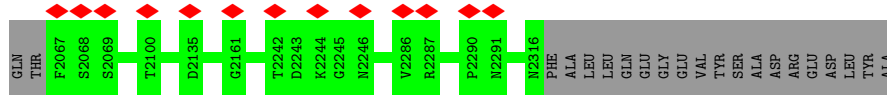
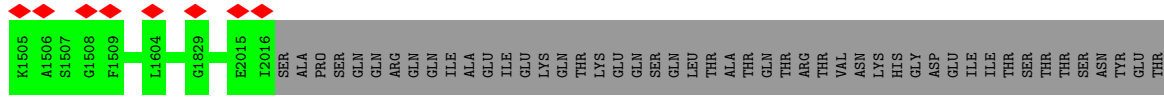


- Molecule 2: U2 snRNA

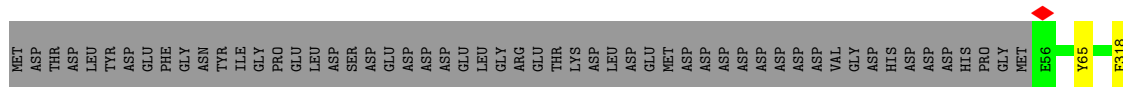
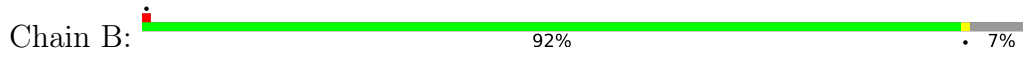


- Molecule 3: BUD13 homolog

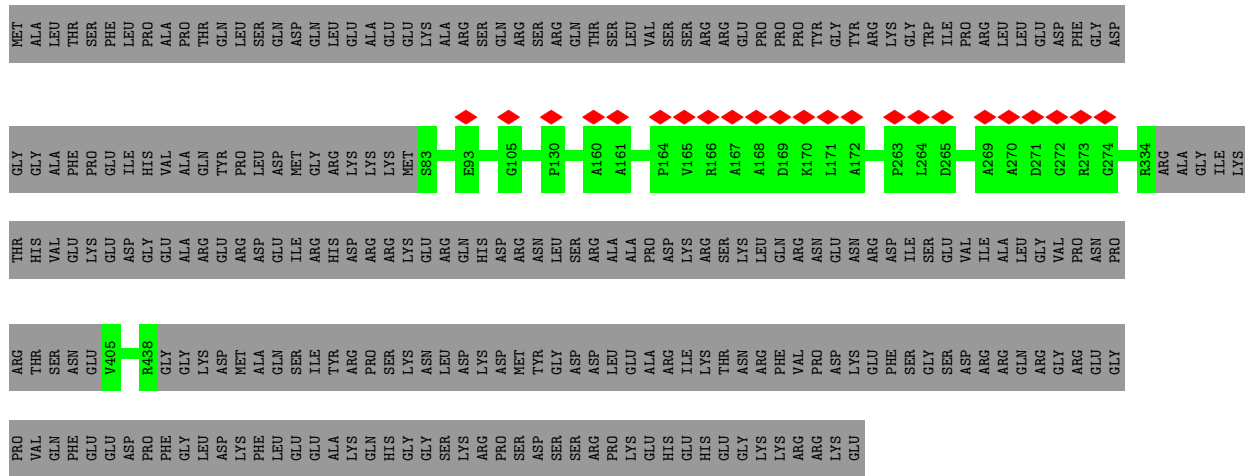




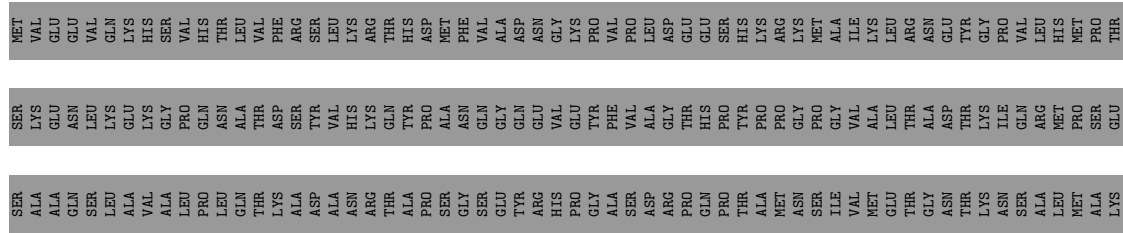
- Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component

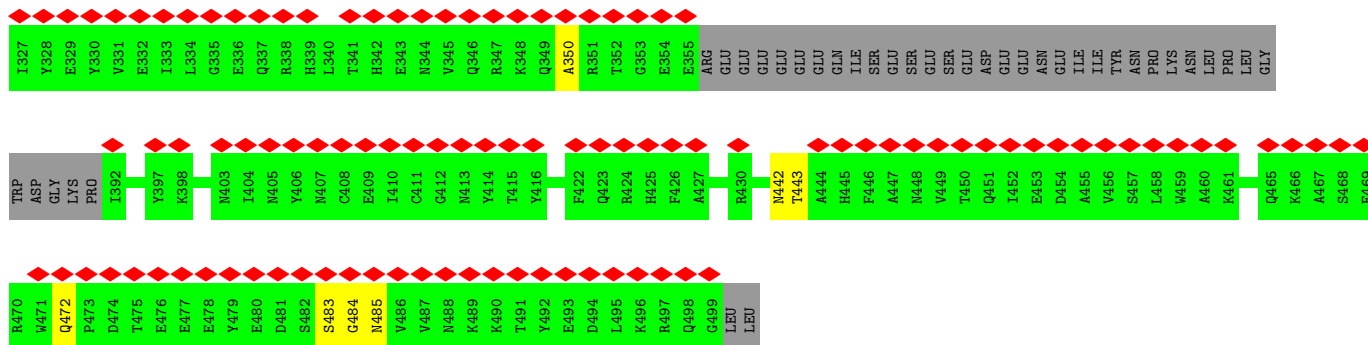


- Molecule 10: SNW domain-containing protein 1

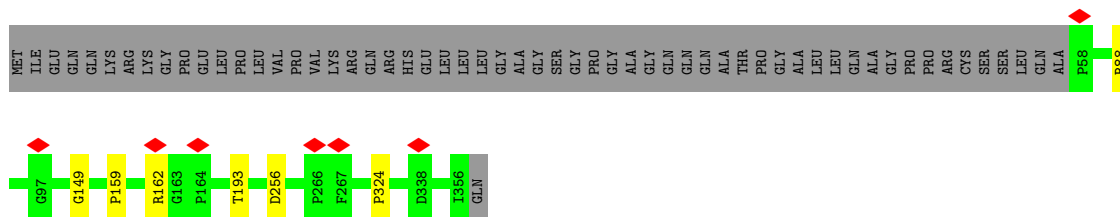
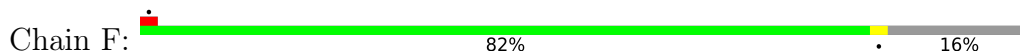


- Molecule 11: Pleiotropic regulator 1

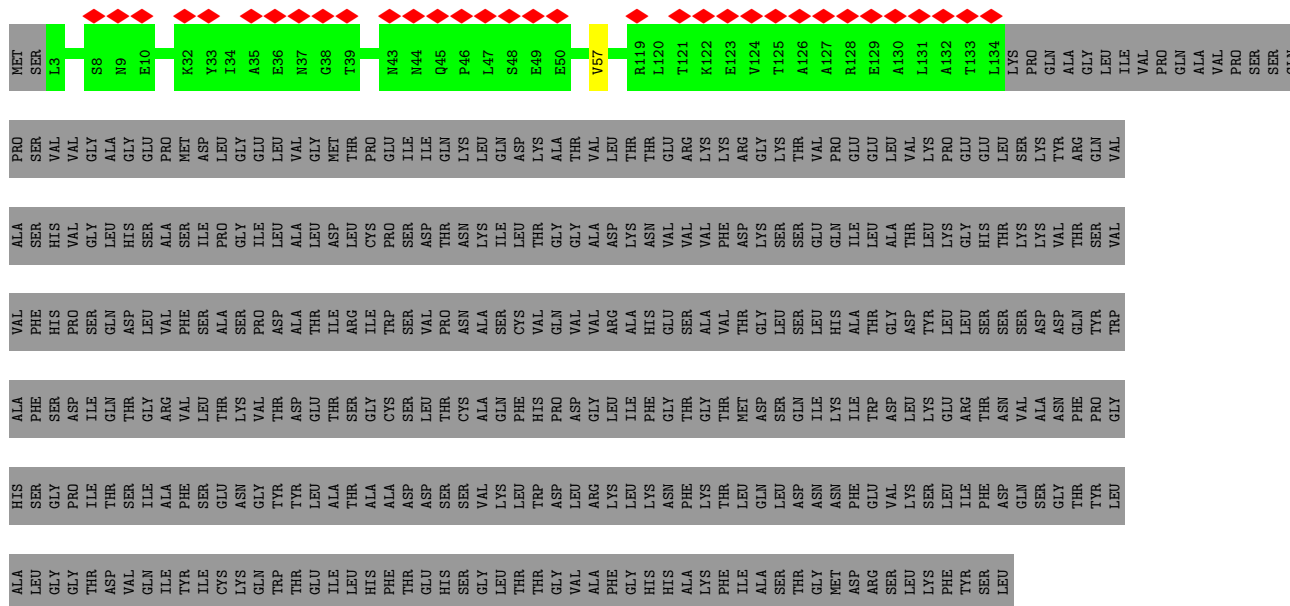




• Molecule 31: U5 small nuclear ribonucleoprotein 40 kDa protein

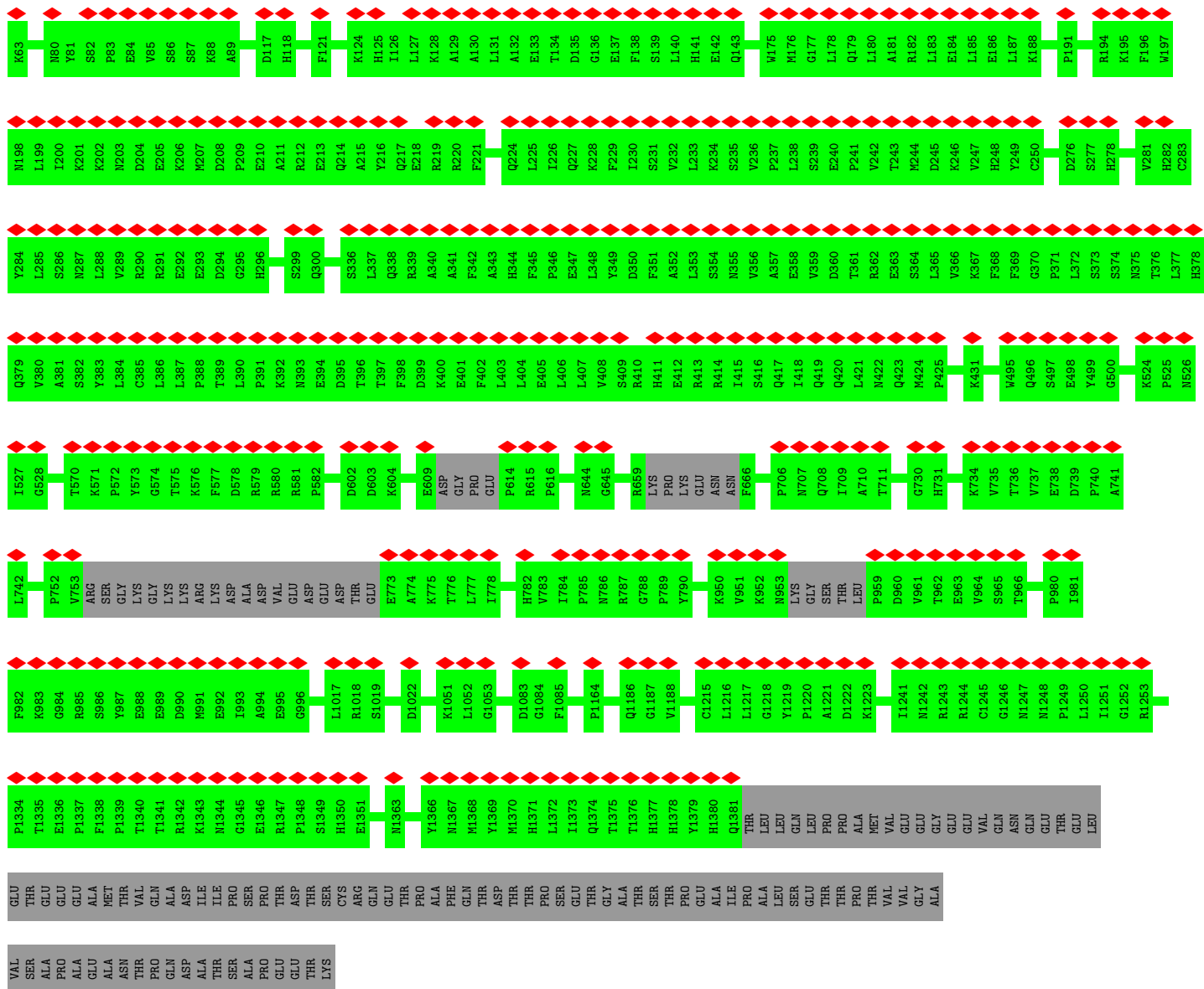


• Molecule 32: Pre-mRNA-processing factor 19

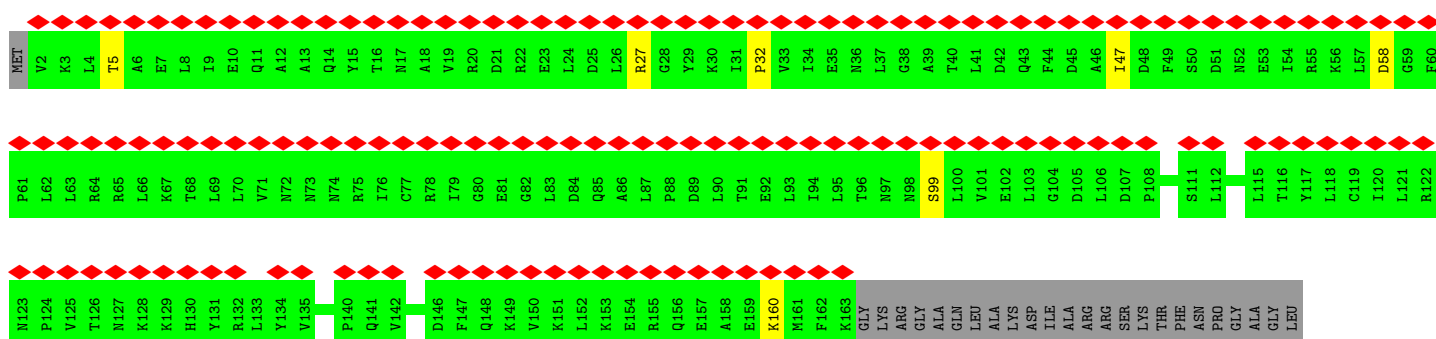


• Molecule 32: Pre-mRNA-processing factor 19





• Molecule 37: U2 small nuclear ribonucleoprotein A'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	165853	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, GTP, ZN, MG, 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	1	0.25	0/600	0.51	0/833
2	2	0.21	0/1404	0.88	1/2177 (0.0%)
3	3	0.27	0/583	0.53	0/811
4	5	0.26	0/1638	0.99	6/2545 (0.2%)
5	6	0.25	0/2279	0.89	1/3551 (0.0%)
6	7	0.26	0/456	0.52	0/632
7	8	0.24	0/713	0.50	0/993
8	A	0.26	0/11090	0.55	0/15463
9	B	0.29	0/4455	0.59	0/6203
10	C	0.27	0/1416	0.58	0/1972
11	D	0.27	0/1577	0.63	0/2193
12	E	0.25	0/640	0.56	0/888
13	L	0.28	0/510	0.59	0/710
14	O	0.25	0/1259	0.54	0/1758
15	P	0.26	0/1411	0.57	0/1962
16	Q	0.26	0/682	0.53	0/949
17	R	0.27	0/505	0.65	1/702 (0.1%)
18	S	0.26	0/162	0.57	0/221
19	V	0.24	0/774	0.52	0/1070
20	Y	0.25	0/469	0.45	0/652
21	Z	0.24	0/1129	0.89	1/1752 (0.1%)
22	s	0.27	0/858	0.61	1/1190 (0.1%)
23	t	0.25	0/846	0.52	0/1173
24	u	0.27	0/4355	0.53	0/6065
25	v	0.26	0/5857	0.57	0/8142
26	x	0.26	0/390	0.49	0/542
27	y	0.24	0/489	0.48	0/677
28	N	0.33	0/499	0.64	0/694
28	z	0.37	1/499 (0.2%)	0.58	0/694
29	0	0.60	0/765	1.13	2/1064 (0.2%)
30	9	0.34	0/2131	0.55	0/2958
31	F	0.48	0/1470	0.67	0/2042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.24	0/658	0.42	0/919
32	H	0.25	0/673	0.44	0/940
32	I	0.23	0/668	0.41	0/933
32	J	0.25	0/673	0.50	1/940 (0.1%)
33	K	0.35	0/1058	0.59	0/1476
34	M	0.34	1/3662 (0.0%)	0.49	2/5107 (0.0%)
35	T	0.40	1/2290 (0.0%)	0.57	0/3192
36	U	0.21	0/6582	0.42	0/9171
37	W	0.64	0/803	1.49	5/1119 (0.4%)
38	X	0.77	0/841	1.20	1/1166 (0.1%)
39	a	0.54	0/439	0.73	0/610
39	h	0.66	0/484	0.81	0/673
40	b	0.58	0/355	0.72	0/490
40	i	0.68	0/360	0.79	0/497
41	c	0.60	0/385	0.72	0/535
41	j	0.64	0/390	0.81	0/542
42	d	0.58	0/357	0.74	0/494
42	k	0.51	0/362	0.70	0/501
43	e	0.54	0/433	0.68	0/601
43	l	0.45	0/408	0.60	0/566
44	f	0.55	0/438	0.68	0/608
44	m	0.47	0/347	0.64	0/479
45	g	0.60	0/459	0.74	0/637
45	n	0.56	0/405	0.71	0/563
46	o	0.45	0/1115	0.61	0/1539
47	p	0.35	0/867	3.21	4/1206 (0.3%)
48	q	0.41	0/3090	0.99	0/4304
49	r	0.33	0/8529	0.59	0/11891
50	w	0.87	0/275	0.92	0/381
All	All	0.34	3/89317 (0.0%)	0.72	26/125358 (0.0%)

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	2
9	B	0	6
11	D	0	1
14	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	1
19	V	0	1
24	u	0	1
25	v	0	5
28	z	0	2
29	0	0	1
30	9	0	2
32	J	1	0
33	K	0	3
34	M	0	2
39	h	0	1
47	p	0	4
49	r	0	1
All	All	1	36

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	208	ARG	C-N	14.63	1.67	1.34
35	T	616	LEU	C-N	7.88	1.49	1.34
28	z	14	PRO	C-N	6.17	1.46	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	p	232	GLU	O-C-N	-65.44	18.00	122.70
47	p	222	PRO	O-C-N	-61.17	24.82	122.70
47	p	236	PRO	O-C-N	-61.09	24.95	122.70
34	M	208	ARG	O-C-N	-13.69	100.80	122.70
32	J	100	ARG	N-CA-CB	-8.48	95.33	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	J	100	ARG	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	568	GLY	Peptide
8	A	1213	VAL	Peptide

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Mol	Chain	Res	Type	Group
8	A	1457	HIS	Peptide
9	B	318	PHE	Peptide
9	B	65	TYR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	109 (91%)	11 (9%)	0	100	100
3	3	116/619 (19%)	96 (83%)	20 (17%)	0	100	100
6	7	91/464 (20%)	84 (92%)	7 (8%)	0	100	100
7	8	142/895 (16%)	127 (89%)	15 (11%)	0	100	100
8	A	2232/2335 (96%)	1989 (89%)	243 (11%)	0	100	100
9	B	900/972 (93%)	769 (85%)	131 (15%)	0	100	100
10	C	282/536 (53%)	232 (82%)	50 (18%)	0	100	100
11	D	318/514 (62%)	283 (89%)	33 (10%)	2 (1%)	25	65
12	E	126/579 (22%)	115 (91%)	11 (9%)	0	100	100
13	L	101/802 (13%)	88 (87%)	13 (13%)	0	100	100
14	O	251/848 (30%)	227 (90%)	24 (10%)	0	100	100
15	P	282/420 (67%)	247 (88%)	35 (12%)	0	100	100
16	Q	136/144 (94%)	121 (89%)	15 (11%)	0	100	100
17	R	98/229 (43%)	78 (80%)	20 (20%)	0	100	100
18	S	32/2752 (1%)	27 (84%)	5 (16%)	0	100	100
19	V	157/166 (95%)	151 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	93/904 (10%)	92 (99%)	1 (1%)	0	100	100
22	s	173/472 (37%)	155 (90%)	18 (10%)	0	100	100
23	t	166/343 (48%)	140 (84%)	26 (16%)	0	100	100
24	u	877/1304 (67%)	812 (93%)	64 (7%)	1 (0%)	51	85
25	v	1179/1217 (97%)	1055 (90%)	122 (10%)	2 (0%)	47	81
26	x	77/86 (90%)	70 (91%)	7 (9%)	0	100	100
27	y	98/110 (89%)	92 (94%)	6 (6%)	0	100	100
28	N	99/125 (79%)	76 (77%)	21 (21%)	2 (2%)	7	40
28	z	99/125 (79%)	88 (89%)	11 (11%)	0	100	100
29	0	153/396 (39%)	133 (87%)	14 (9%)	6 (4%)	3	26
30	9	416/501 (83%)	375 (90%)	31 (8%)	10 (2%)	6	36
31	F	297/357 (83%)	273 (92%)	17 (6%)	7 (2%)	6	36
32	G	130/504 (26%)	120 (92%)	9 (7%)	1 (1%)	19	60
32	H	133/504 (26%)	119 (90%)	13 (10%)	1 (1%)	19	60
32	I	132/504 (26%)	123 (93%)	9 (7%)	0	100	100
32	J	133/504 (26%)	116 (87%)	14 (10%)	3 (2%)	6	37
33	K	211/225 (94%)	178 (84%)	30 (14%)	3 (1%)	11	47
34	M	732/855 (86%)	623 (85%)	103 (14%)	6 (1%)	19	60
35	T	458/908 (50%)	417 (91%)	34 (7%)	7 (2%)	10	46
36	U	1317/1485 (89%)	1292 (98%)	25 (2%)	0	100	100
37	W	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	48
38	X	165/225 (73%)	158 (96%)	4 (2%)	3 (2%)	8	42
39	a	87/118 (74%)	76 (87%)	10 (12%)	1 (1%)	14	52
39	h	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
40	b	71/86 (83%)	66 (93%)	4 (6%)	1 (1%)	11	47
40	i	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
41	c	76/92 (83%)	67 (88%)	8 (10%)	1 (1%)	12	48
41	j	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
42	d	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	11	47
42	k	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
43	e	86/126 (68%)	83 (96%)	2 (2%)	1 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	l	81/126 (64%)	80 (99%)	1 (1%)	0	100	100
44	f	87/240 (36%)	81 (93%)	6 (7%)	0	100	100
44	m	67/240 (28%)	66 (98%)	1 (2%)	0	100	100
45	g	89/119 (75%)	81 (91%)	8 (9%)	0	100	100
45	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
46	o	221/301 (73%)	203 (92%)	15 (7%)	3 (1%)	11	47
47	p	169/793 (21%)	164 (97%)	3 (2%)	2 (1%)	13	50
48	q	623/1041 (60%)	598 (96%)	21 (3%)	4 (1%)	25	65
49	r	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	47	81
50	w	54/285 (19%)	52 (96%)	0	2 (4%)	3	28
All	All	16581/30776 (54%)	15092 (91%)	1414 (8%)	75 (0%)	32	68

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	384	HIS
29	0	246	TYR
29	0	267	ASP
29	0	270	LEU
29	0	362	PHE

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	57/188 (30%)	12 (21%)	1 (1%)
21	Z	46/369 (12%)	18 (39%)	1 (2%)
4	5	69/116 (59%)	27 (39%)	1 (1%)
5	6	94/107 (87%)	25 (26%)	1 (1%)
All	All	266/780 (34%)	82 (30%)	4 (1%)

5 of 82 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	13	C
2	2	16	U
2	2	17	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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
53	IHP	A	3001	-	36,36,36	1.52	6 (16%)	54,60,60	0.71	1 (1%)
55	ADP	r	2202	52	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
55	ADP	r	2201	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
54	GTP	B	1500	-	26,34,34	1.13	2 (7%)	32,54,54	1.50	7 (21%)

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
53	IHP	A	3001	-	-	7/30/54/54	0/1/1/1
55	ADP	r	2202	52	-	2/12/32/32	0/3/3/3
55	ADP	r	2201	-	-	8/12/32/32	0/3/3/3
54	GTP	B	1500	-	-	6/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B	1500	GTP	C5-C6	-4.01	1.39	1.47
53	A	3001	IHP	P2-O12	3.55	1.66	1.59
53	A	3001	IHP	P1-O11	3.23	1.65	1.59
53	A	3001	IHP	P3-O13	3.19	1.65	1.59
53	A	3001	IHP	P4-O14	3.15	1.65	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	r	2202	ADP	PA-O3A-PB	-4.00	119.09	132.83
54	B	1500	GTP	C5-C6-N1	3.25	119.69	113.95
55	r	2201	ADP	N3-C2-N1	-3.23	123.64	128.68
54	B	1500	GTP	PB-O3B-PG	-3.19	121.88	132.83
55	r	2202	ADP	C3'-C2'-C1'	3.15	105.72	100.98

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

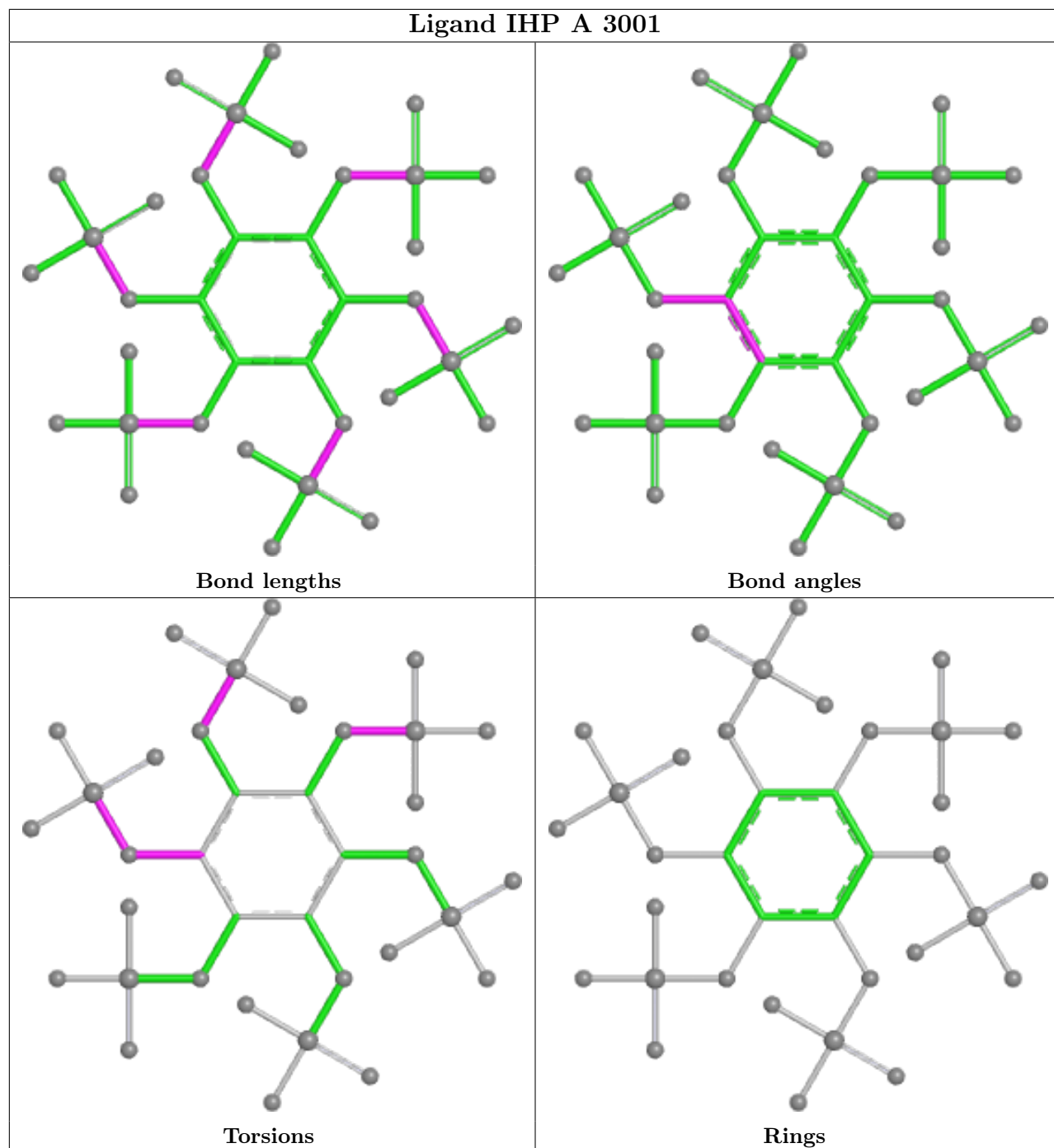
Mol	Chain	Res	Type	Atoms
53	A	3001	IHP	C1-C2-O12-P2
53	A	3001	IHP	C4-O14-P4-O24
54	B	1500	GTP	C5'-O5'-PA-O3A
55	r	2201	ADP	PA-O3A-PB-O2B
55	r	2201	ADP	C5'-O5'-PA-O1A

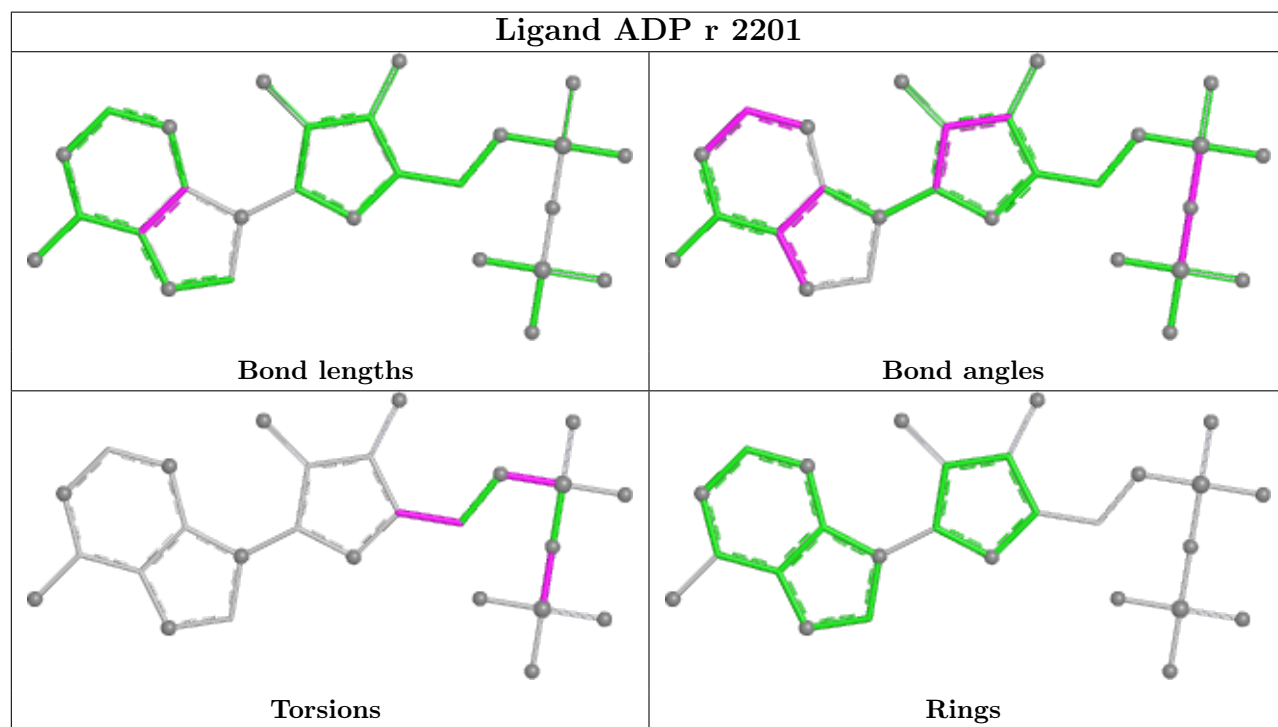
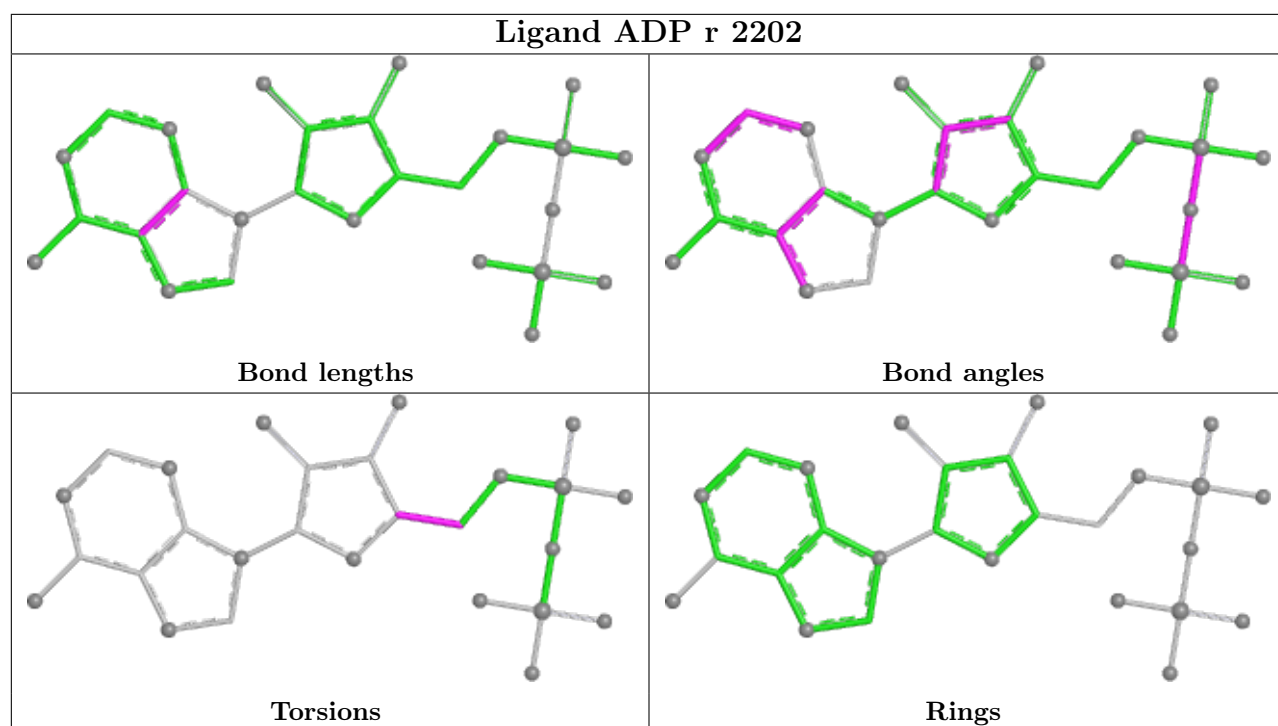
There are no ring outliers.

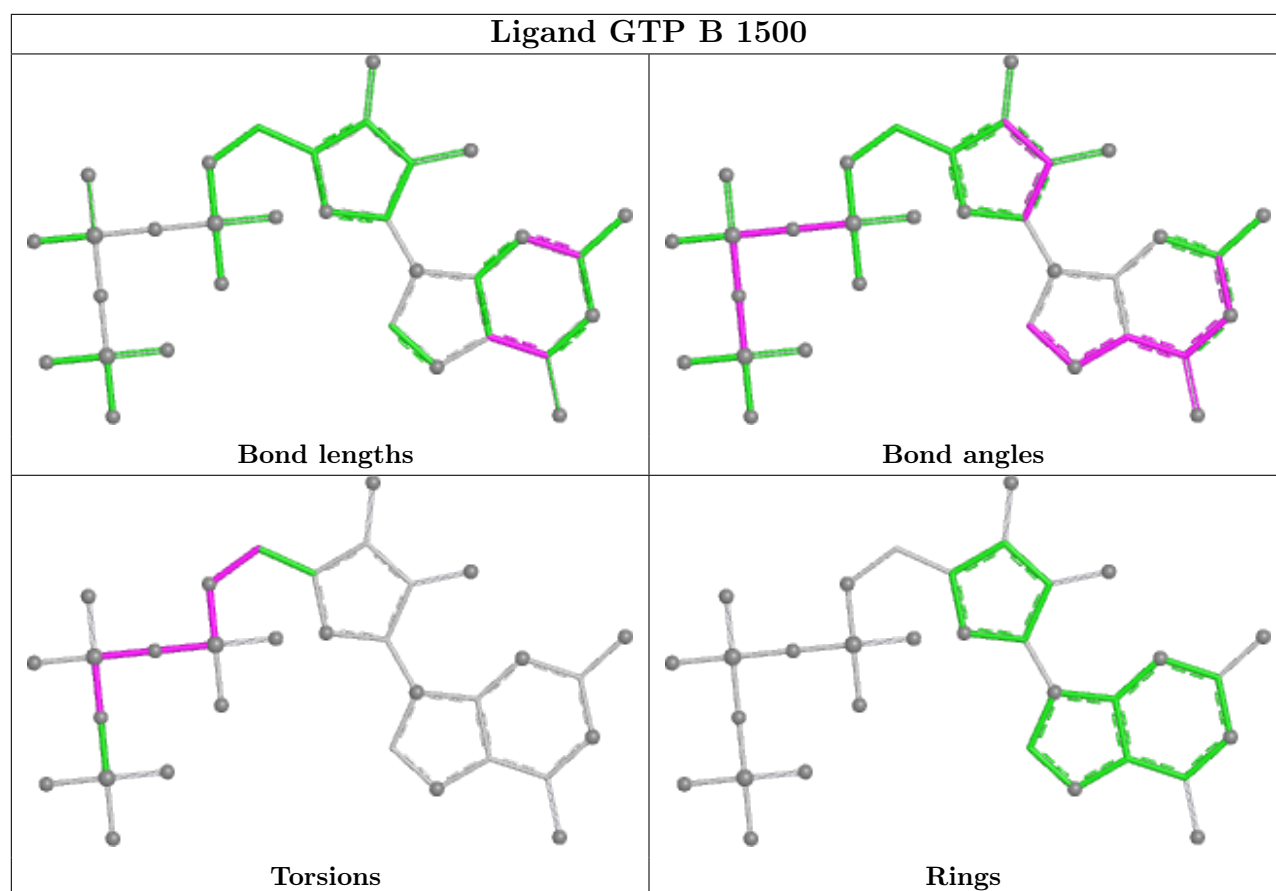
No monomer is involved in short contacts.

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
30	9	5
34	M	3
38	X	1
36	U	1
2	2	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	124:ALA	C	125:GLN	N	48.62
1	X	163:ASN	C	164:GLU	N	43.68

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	96:ARG	C	97:LYS	N	22.97
1	9	30:LYS	C	31:SER	N	15.71
1	9	172:ASP	C	173:ILE	N	11.06

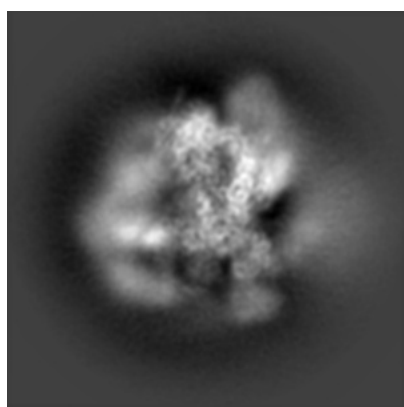
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4240. These allow visual inspection of the internal detail of the map and identification of artifacts.

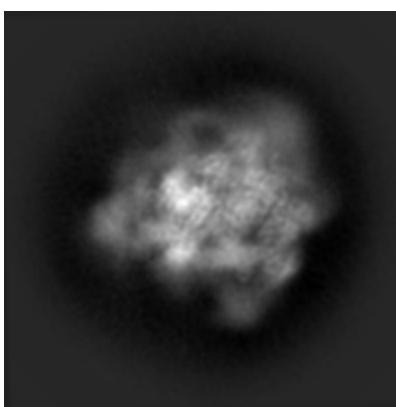
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

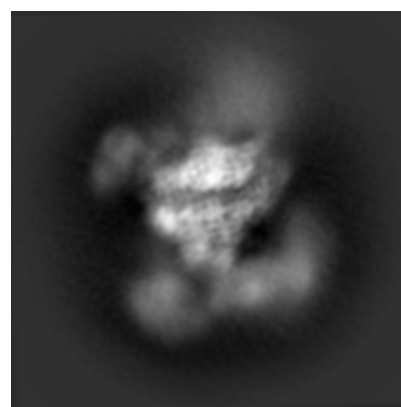
6.1.1 Primary map



X



Y

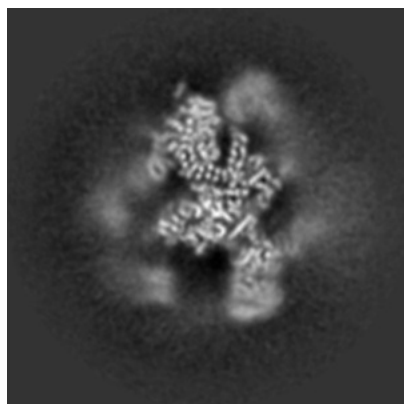


Z

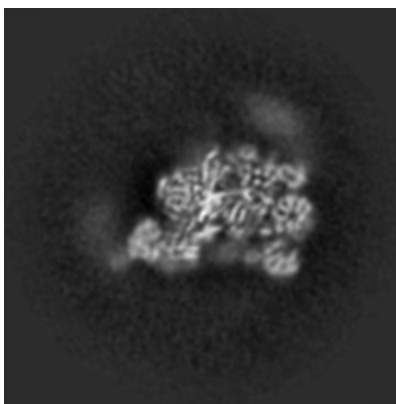
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

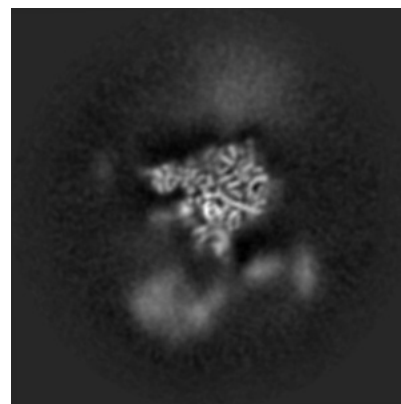
6.2.1 Primary map



X Index: 210



Y Index: 210

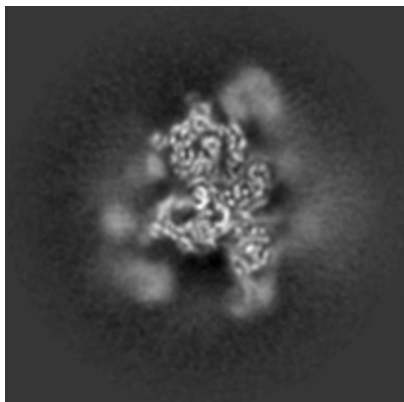


Z Index: 210

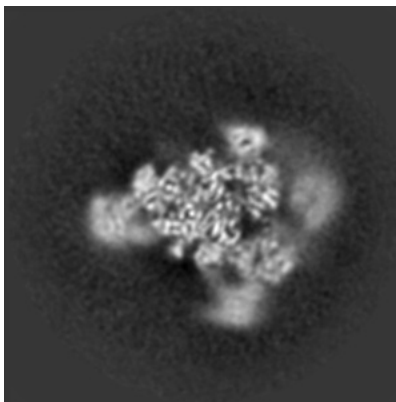
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

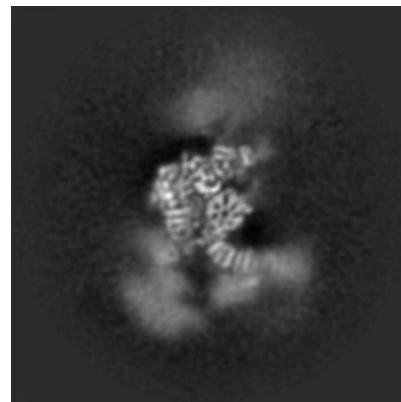
6.3.1 Primary map



X Index: 218



Y Index: 249

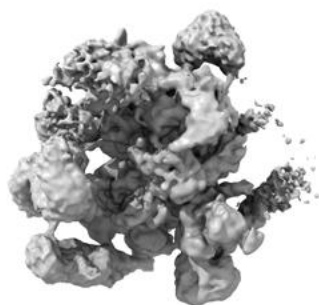


Z Index: 184

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

6.4 Orthogonal surface views [i](#)

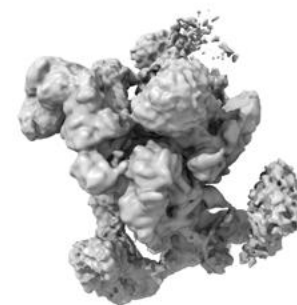
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

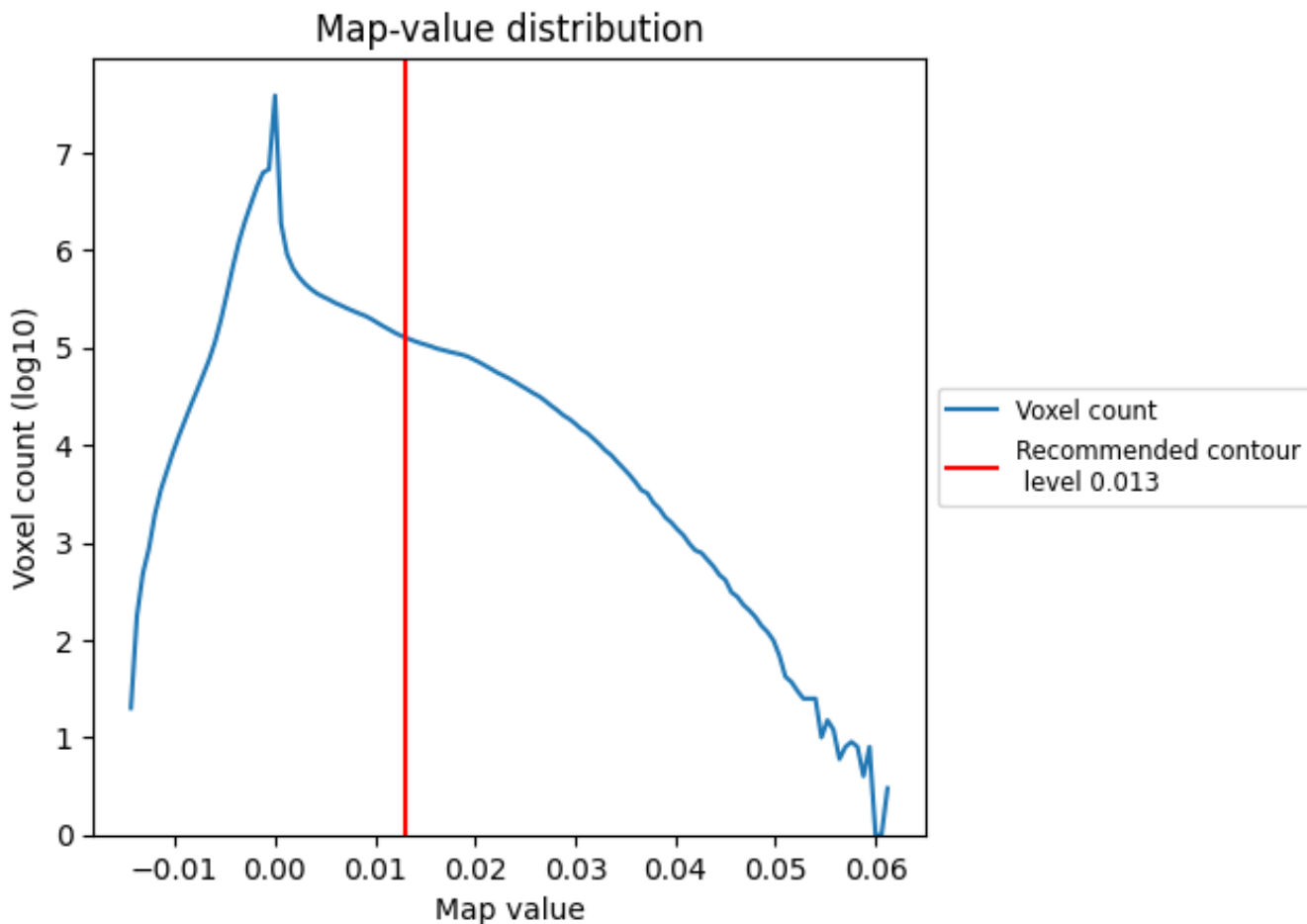
6.5 Mask visualisation

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

7 Map analysis [i](#)

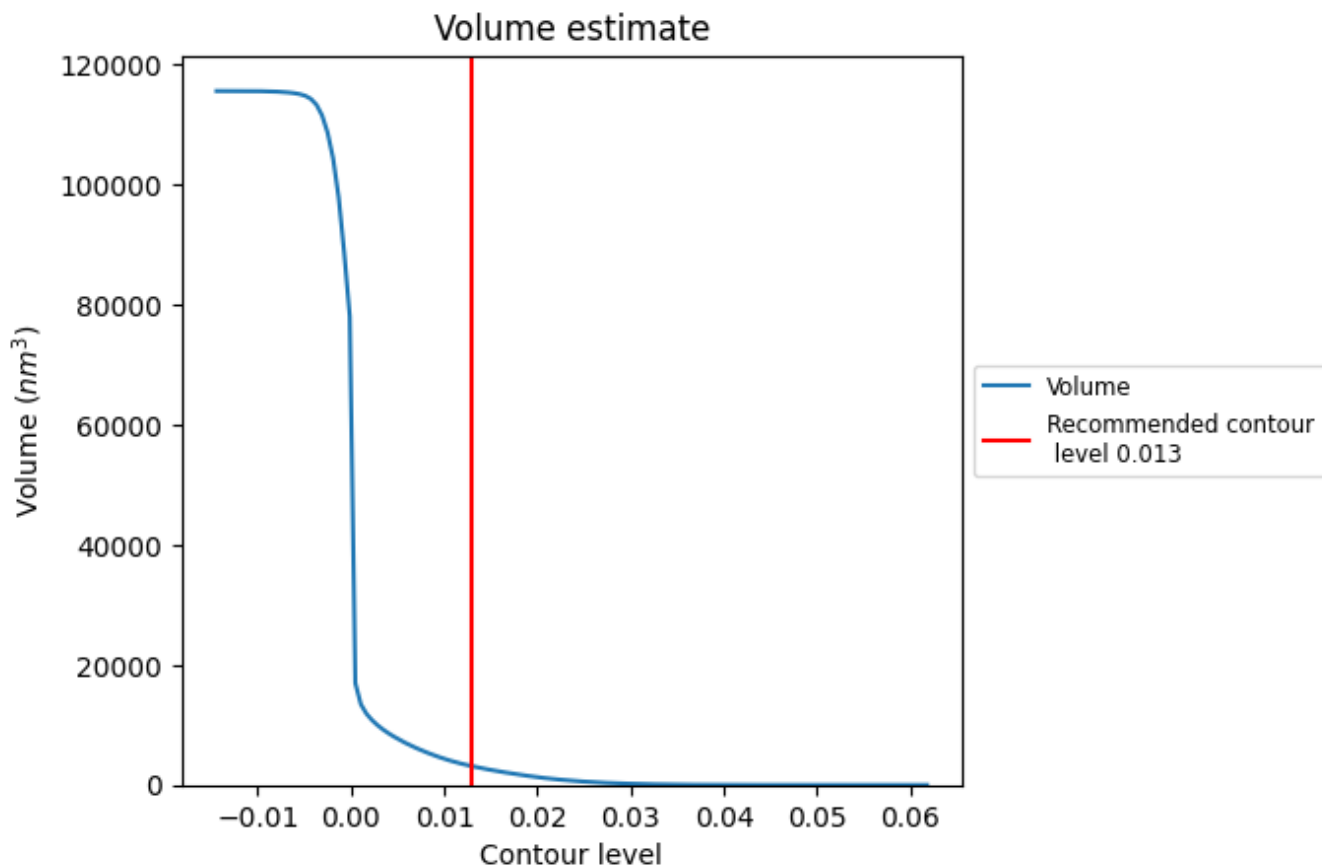
This section contains the results of statistical analysis of the map.

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.

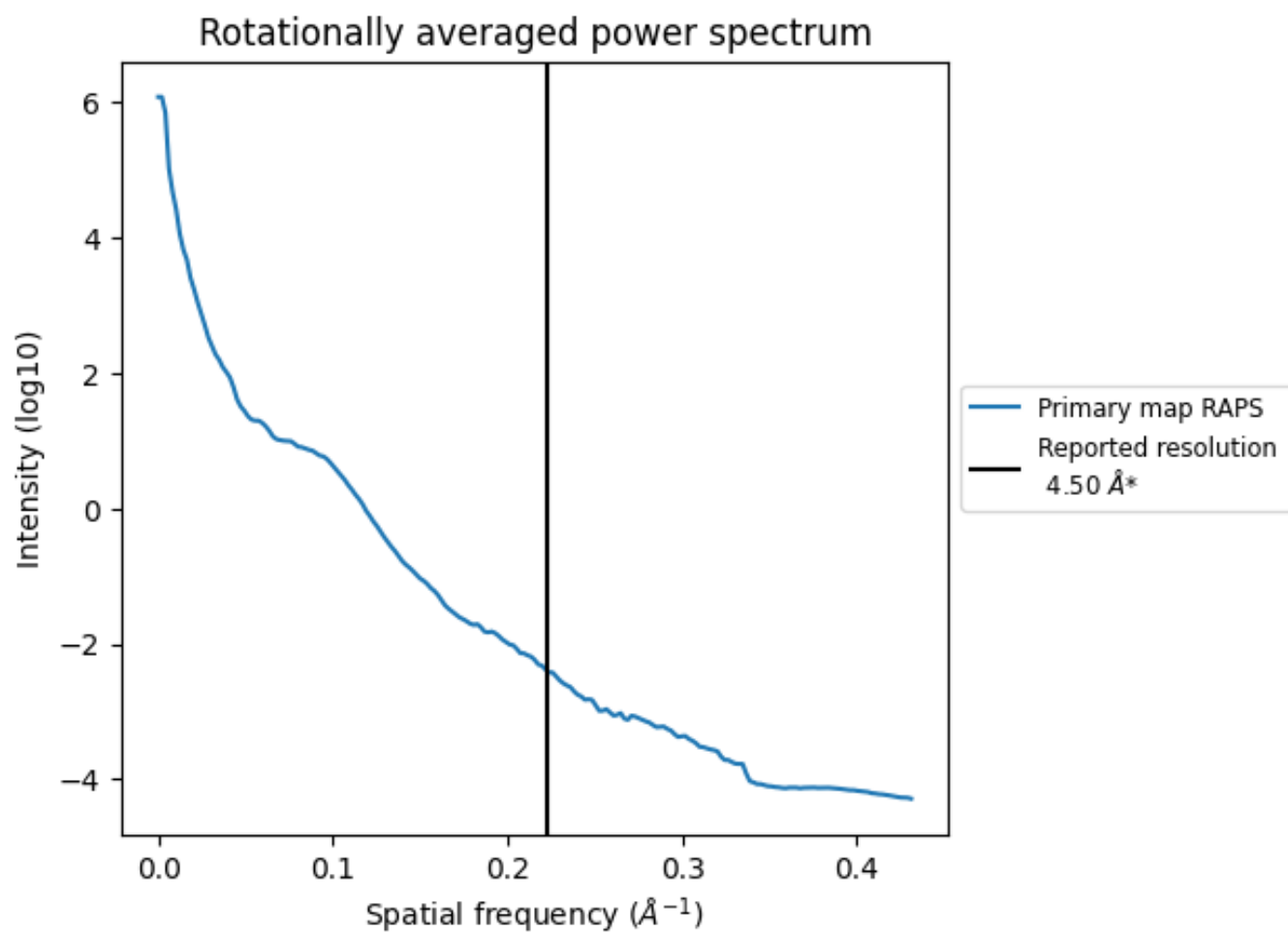
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3127 nm³; this corresponds to an approximate mass of 2825 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

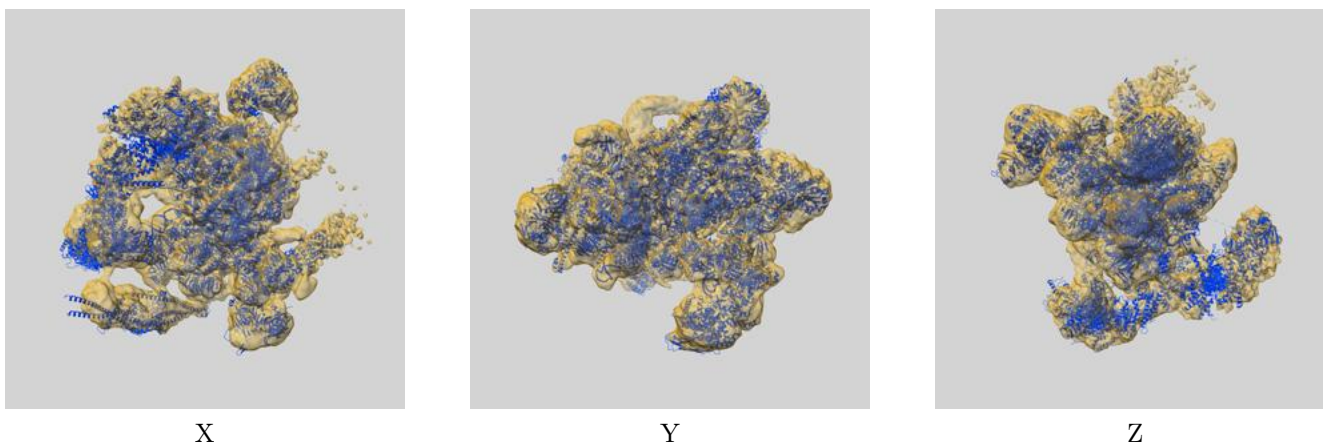
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

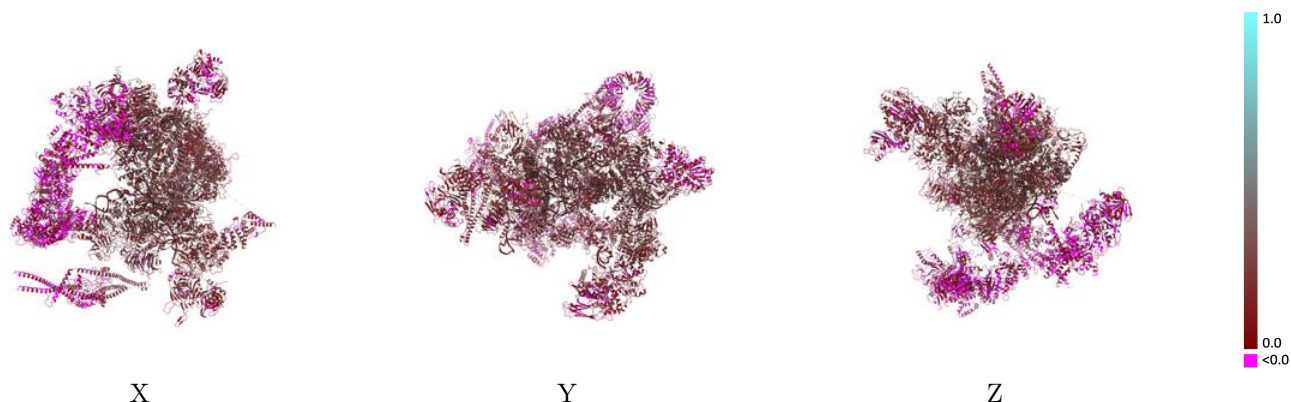
This section contains information regarding the fit between EMDB map EMD-4240 and PDB model 6FF7. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



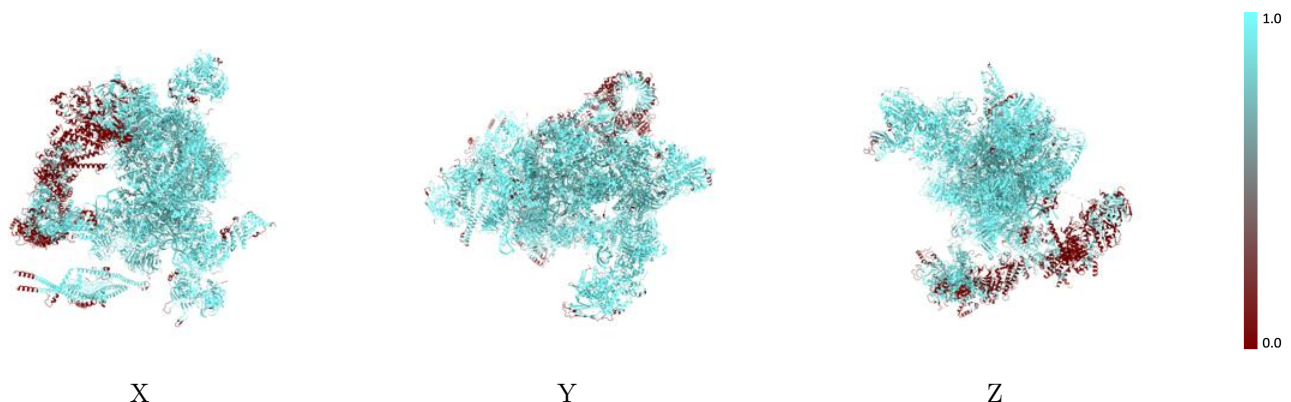
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



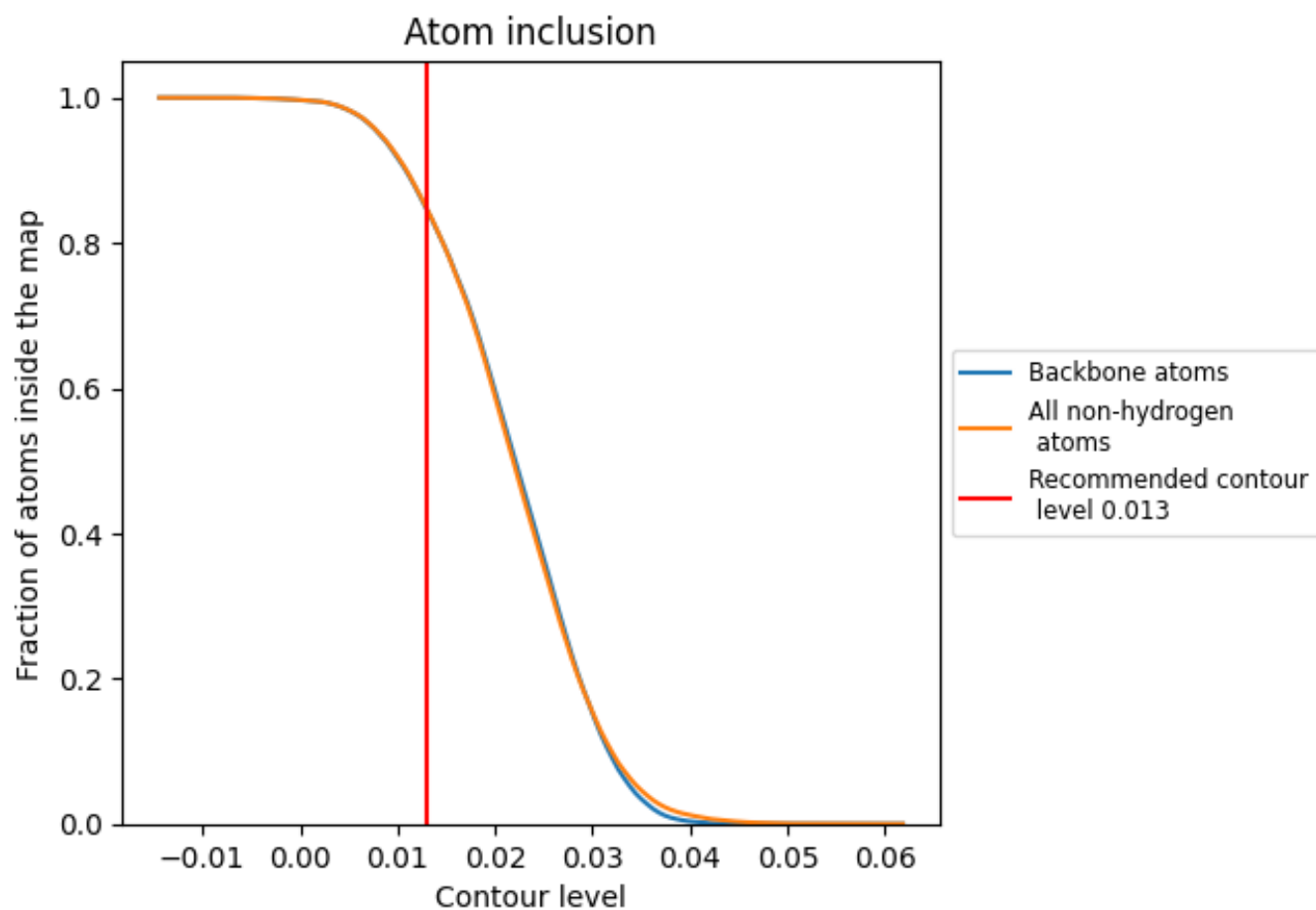
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8473	 0.1670
0	 0.9191	 0.1610
1	 0.9468	 0.2430
2	 0.9818	 0.2000
3	 0.8579	 0.2320
5	 0.9905	 0.2150
6	 0.9931	 0.2100
7	 0.9234	 0.2390
8	 0.9846	 0.2750
9	 0.1753	 0.0230
A	 0.9757	 0.2600
B	 0.9806	 0.2160
C	 0.9083	 0.2540
D	 0.9930	 0.2600
E	 0.9829	 0.1800
F	 0.9721	 0.1660
G	 0.7481	 0.0420
H	 0.7804	 0.0320
I	 0.9656	 0.1100
J	 0.6944	 0.0850
K	 0.6827	 0.0980
L	 0.9785	 0.2650
M	 0.5645	 0.0120
N	 0.9780	 0.2510
O	 0.9817	 0.2320
P	 0.9336	 0.1790
Q	 0.9971	 0.2310
R	 0.9448	 0.2360
S	 0.7362	 0.1640
T	 0.8669	 0.1900
U	 0.6885	 0.0370
V	 0.9923	 0.1600
W	 0.0846	 -0.0140
X	 0.3685	 0.0470
Y	 0.9979	 0.2330



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Chain	Atom inclusion	Q-score
Z	 0.9961	 0.2180
a	 0.9159	 0.1150
b	 0.9466	 0.0820
c	 0.9326	 0.0960
d	 0.8966	 0.1460
e	 0.8917	 0.1560
f	 0.7995	 0.1180
g	 0.9631	 0.1490
h	 0.3134	 0.0120
i	 0.6648	 0.0260
j	 0.6317	 0.0420
k	 0.6529	 0.0480
l	 0.5061	 0.0720
m	 0.1433	 0.0170
n	 0.2759	 -0.0040
o	 0.2109	 0.0070
p	 0.2552	 0.0250
q	 0.8997	 0.0760
r	 0.9412	 0.1590
s	 0.9802	 0.2590
t	 0.9270	 0.2440
u	 0.9793	 0.2660
v	 0.9922	 0.2410
w	 0.0000	 0.0580
x	 0.9872	 0.2510
y	 0.9858	 0.2370
z	 0.9660	 0.3160