



Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 03:05 PM JST

PDB ID : 5Y88
EMDB ID : EMD-6817
Title : Cryo-EM structure of the intron-lariat spliceosome ready for disassembly from *S.cerevisiae* at 3.5 angstrom
Authors : Wan, R.; Yan, C.; Bai, R.; Lei, J.; Shi, Y.
Deposited on : 2017-08-20
Resolution : 3.46 Å(reported)

This is a Full wwPDB EM Validation 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:

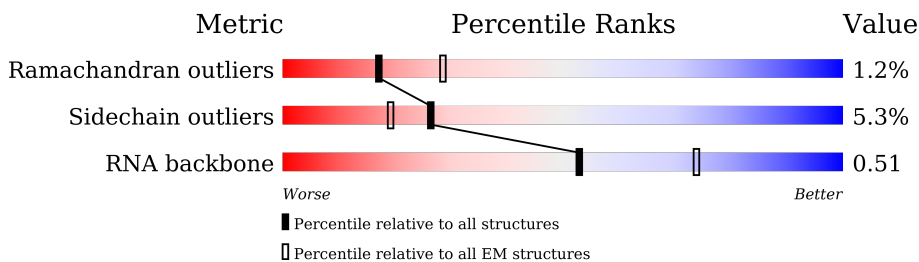
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.46 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
Sidechain outliers	154315	3826
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	A	2413	
2	B	214	
3	C	1008	
4	D	112	
5	E	38	
6	F	1175	
7	G	175	
8	H	859	

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Mol	Chain	Length	Quality of chain
9	I	687	48% 77% 21%
10	J	590	49% 69% 27%
11	K	215	21% 47% 53%
12	L	157	7% 97% ..
13	M	364	16% 48% 50%
14	N	339	8% 76% 23%
15	O	451	72% 25%
16	P	175	18% 37% 61%
17	Q	379	18% 49% 47%
18	R	278	16% 13% 83%
19	S	455	95%
20	T	283	30% 28% 6% 62%
21	U	708	61% 56% 6% 7% 31%
22	V	322	21% 18% 6% 72%
23	W	767	92% 91% 8%
24	a	196	37% 41% 59%
24	h	196	40% 40% 60%
25	b	94	79% 74% 5% 20%
25	i	94	80% 74% 5% 20%
26	c	86	80% 78% 19%
26	j	86	81% 78% 19%
27	d	77	83% 86% 10%
27	k	77	90% 86% 10%
28	e	101	44% 77% 19%
28	l	101	81% 77% 19%

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Mol	Chain	Length	Quality of chain
29	f	146	
29	m	146	
30	g	110	
30	n	110	
31	o	238	
32	p	111	
33	q	503	
33	r	503	
33	s	503	
33	t	503	
34	x	9	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 72347 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-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1903	15715	10107	2697	2854	57	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	117	2465	1104	414	830	117	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	913	7278	4696	1205	1347	30	0	0

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	101	2150	963	384	702	101	0	0

- Molecule 5 is a RNA chain called Intron lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	28	587	264	95	200	28	0	0

- Molecule 6 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	82	1727	772	286	587	82	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	155	921	582	159	179	1	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	601	3204	1958	611	634	1	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	541	3542	2200	667	667	8	0	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	431	2944	1824	544	568	8	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	102	822	504	152	165	1	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	157	1290	808	240	231	11	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	182	1298	805	235	243	15	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	261	2089	1320	369	388	12	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	337	2646	1669	466	501	10	0	0

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	68	554	348	111	94	1	0	0

- Molecule 17 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	201	1583	988	290	298	7	0	0

- Molecule 18 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	46	379	225	73	79	2	0	0

- Molecule 19 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	S	23	195	122	41	32	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	T	107	816	523	144	149	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP382.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	488	2690	1644	514	529	3	0	0

- Molecule 22 is a protein called Pre-mRNA-splicing factor NTR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	91	619	381	112	124	2	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	708	3505	2089	708	708	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	80	631	403	114	111	3	0	0
24	h	78	610	389	110	108	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	75	575	379	92	101	3	0	0
25	i	75	575	379	92	101	3	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	70	554	355	98	100	1	0	0
26	j	70	554	355	98	100	1	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	k	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
28	l	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	n	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	135	Total	C	N	O	0	0
			841	538	142	161		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	81	Total	C	N	O	0	0
			513	332	89	92		

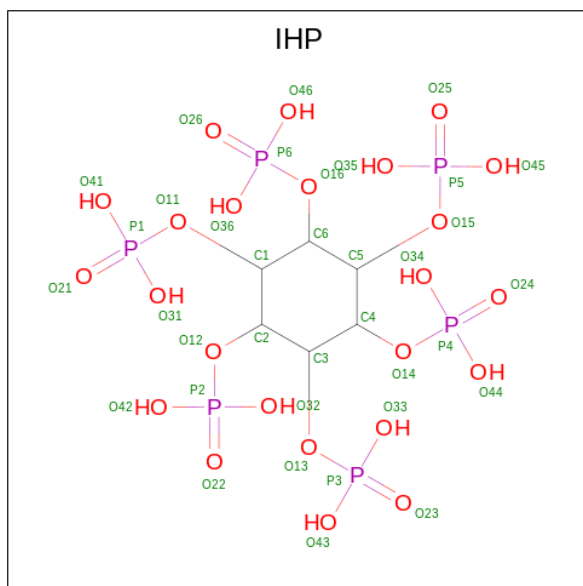
- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	q	126	Total 831	C 526	N 134	O 169	S 2	0	0
33	r	129	Total 849	C 536	N 137	O 174	S 2	0	0
33	s	129	Total 850	C 537	N 137	O 174	S 2	0	0
33	t	125	Total 823	C 521	N 133	O 167	S 2	0	0

- Molecule 34 is a RNA chain called RNA (intron or U6 snRNA).

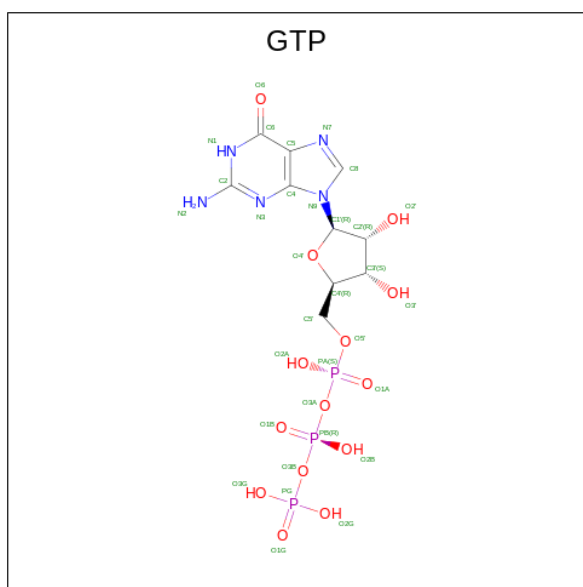
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	x	9	Total 177	C 81	N 18	O 70	P 8	0	0

- Molecule 35 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

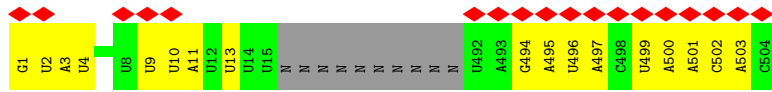
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	C	1	1	1	0
37	D	5	5	5	0

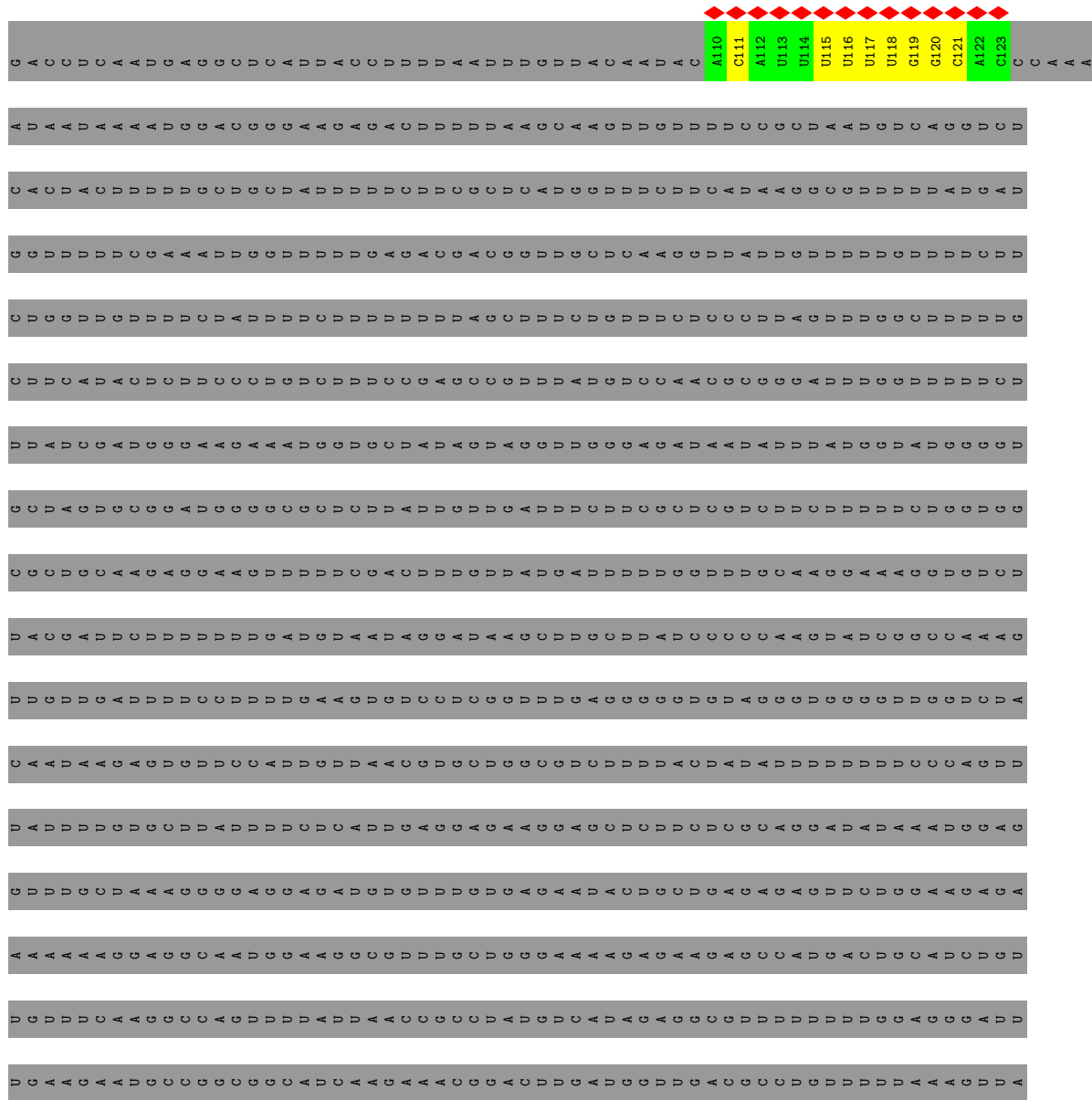
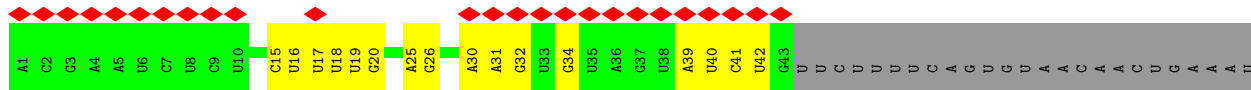
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

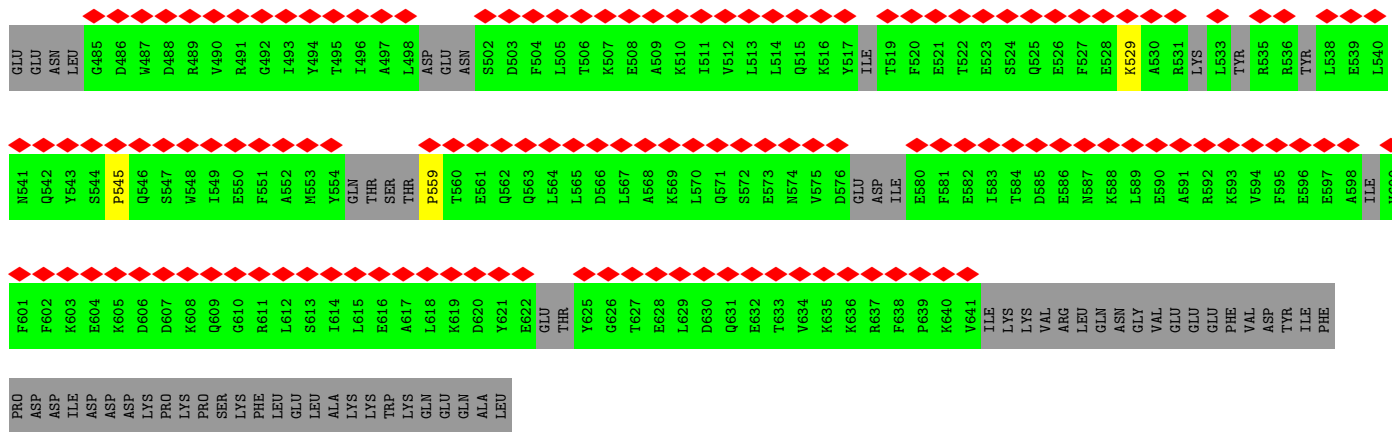
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	L	3	3	3	0
38	M	2	2	2	0
38	N	1	1	1	0

● Molecule 5: Intron lariat

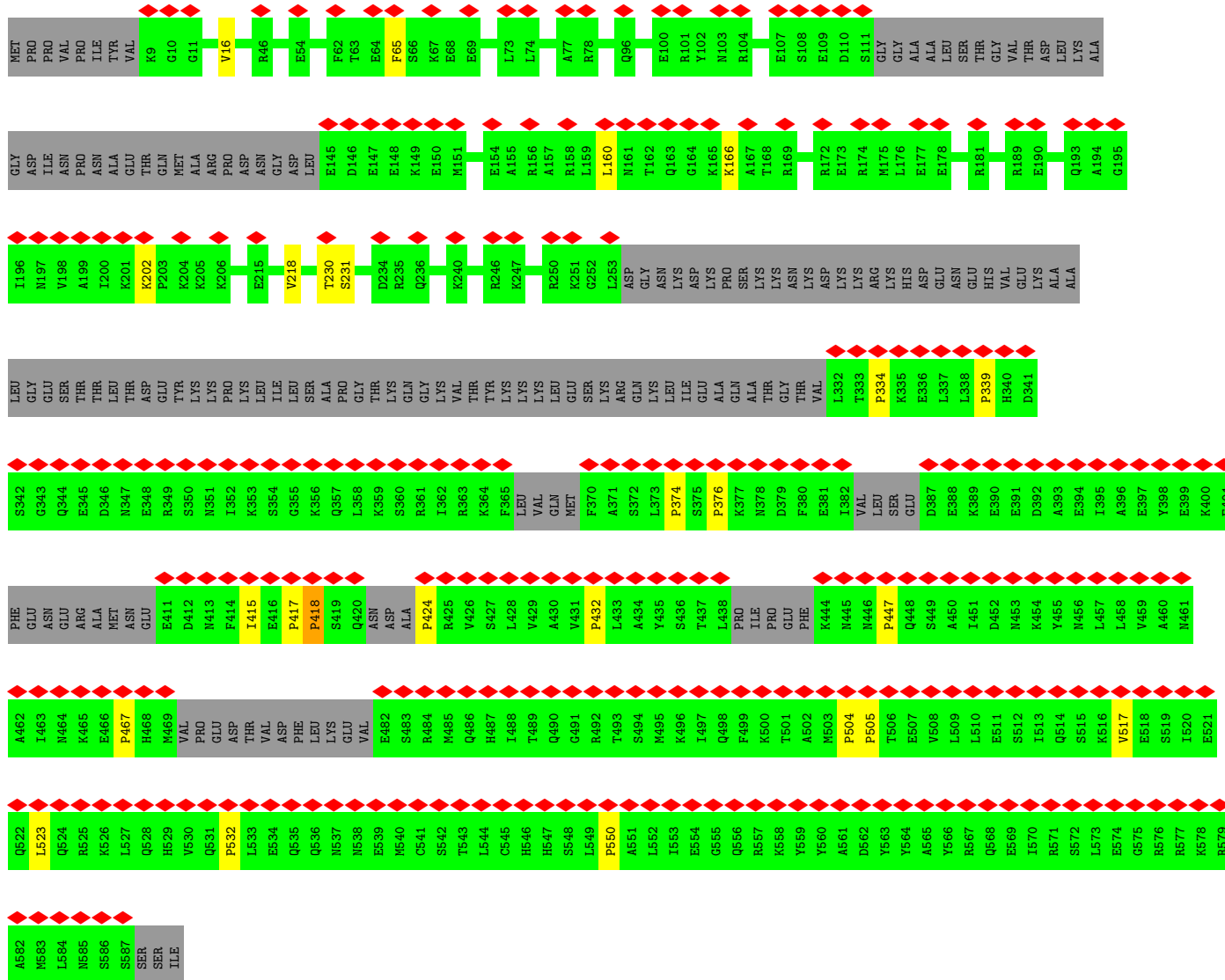


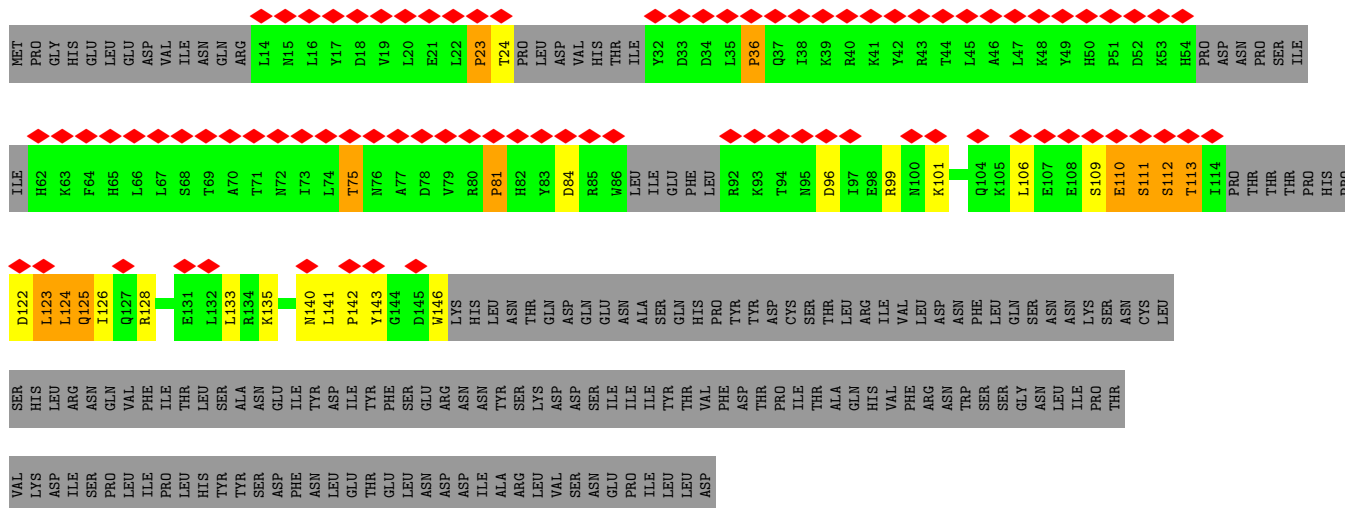
● Molecule 6: U2 snRNA



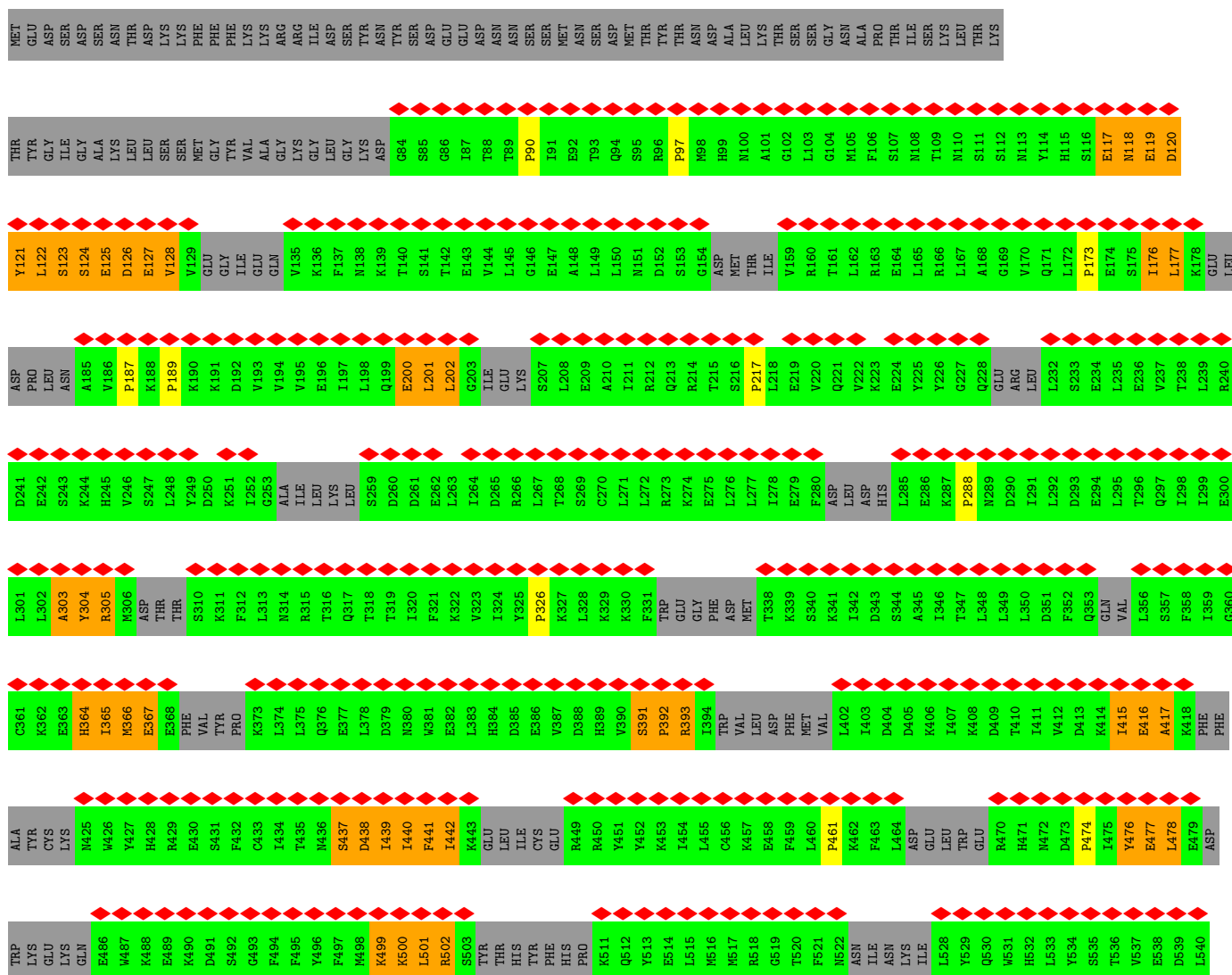


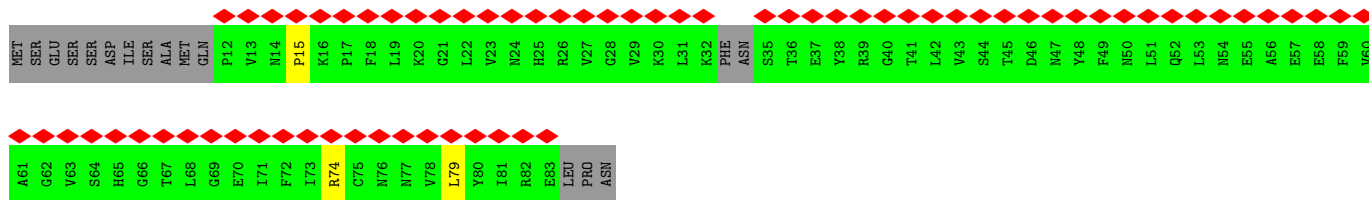
● Molecule 10: Pre-mRNA-splicing factor CEF1



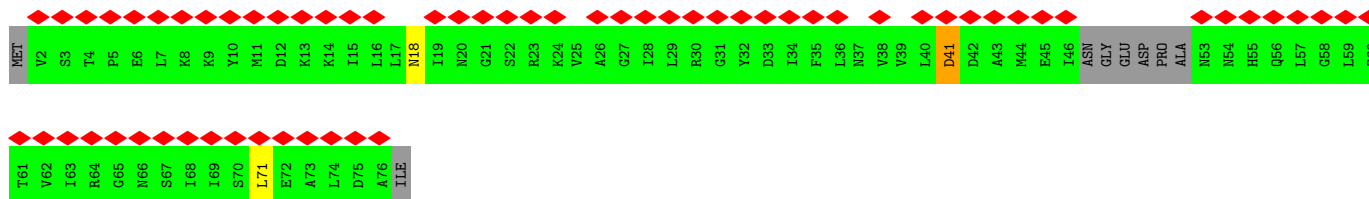
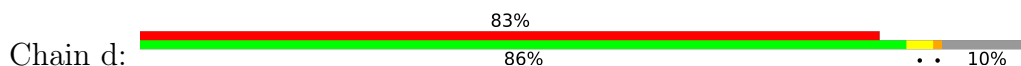


● Molecule 21: Pre-mRNA-splicing factor SPP382

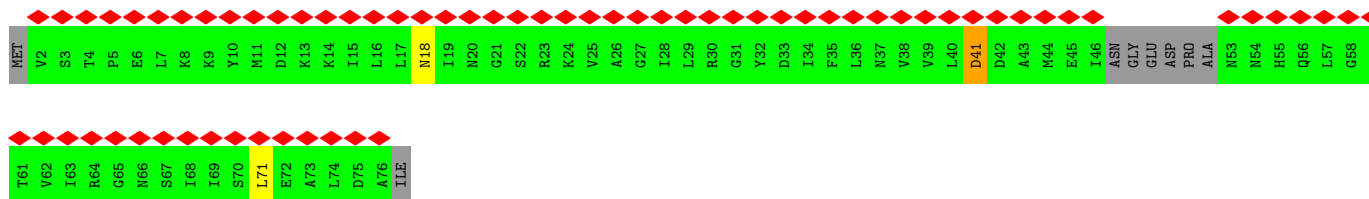
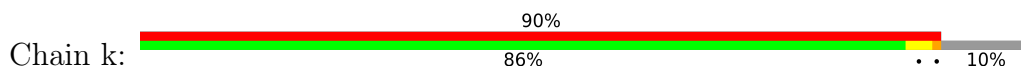




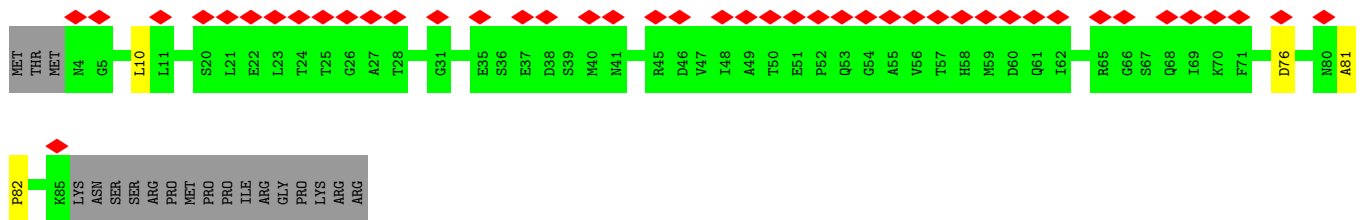
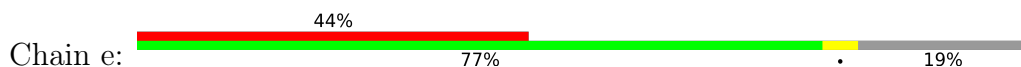
• Molecule 27: Small nuclear ribonucleoprotein G



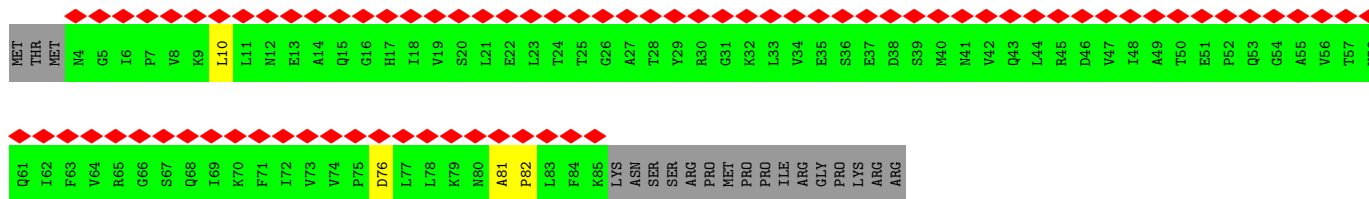
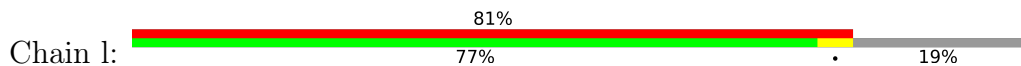
• Molecule 27: Small nuclear ribonucleoprotein G



• Molecule 28: Small nuclear ribonucleoprotein Sm D3



• Molecule 28: Small nuclear ribonucleoprotein Sm D3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.6	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	0.282	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	522.4, 522.4, 522.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3060001, 1.3060001, 1.3060001	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: IHP, ZN, GTP, MG

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	0.63	9/16117 (0.1%)	0.71	12/21848 (0.1%)
2	B	0.54	1/2747 (0.0%)	0.72	0/4267
3	C	0.70	7/7434 (0.1%)	0.78	12/10070 (0.1%)
4	D	0.53	1/2405 (0.0%)	0.72	0/3744
5	E	0.29	0/653	0.66	0/1010
6	F	0.77	11/1922 (0.6%)	1.13	18/2984 (0.6%)
7	G	0.42	0/919	0.56	2/1237 (0.2%)
8	H	0.65	8/3180 (0.3%)	0.62	23/4331 (0.5%)
9	I	0.55	1/3574 (0.0%)	0.61	8/4863 (0.2%)
10	J	0.45	1/2962 (0.0%)	0.59	9/3987 (0.2%)
11	K	0.51	0/826	0.64	0/1097
12	L	0.71	0/1314	0.78	1/1759 (0.1%)
13	M	0.59	0/1308	0.71	0/1758
14	N	0.61	0/2135	0.67	0/2871
15	O	0.79	0/2704	0.82	1/3676 (0.0%)
16	P	0.54	0/568	0.94	3/758 (0.4%)
17	Q	0.49	0/1604	0.63	0/2160
18	R	0.25	0/378	0.54	2/498 (0.4%)
19	S	0.57	0/200	0.85	0/264
20	T	0.64	1/825 (0.1%)	0.99	14/1100 (1.3%)
21	U	0.67	0/2684	1.23	58/3680 (1.6%)
22	V	0.51	0/622	1.36	18/843 (2.1%)
23	W	0.21	0/3502	0.47	2/4877 (0.0%)
24	a	0.37	0/636	0.62	0/856
24	h	0.37	0/615	0.61	0/829
25	b	0.42	0/585	0.62	0/795
25	i	0.42	0/585	0.62	0/795
26	c	0.44	0/564	0.65	1/761 (0.1%)
26	j	0.44	0/564	0.66	1/761 (0.1%)
27	d	0.37	0/532	0.60	0/715
27	k	0.37	0/532	0.60	0/715
28	e	0.40	0/634	0.70	0/859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	l	0.40	0/634	0.70	0/859
29	f	0.41	0/649	0.61	0/880
29	m	0.41	0/649	0.61	0/880
30	g	0.46	0/753	0.69	2/1013 (0.2%)
30	n	0.43	0/535	0.66	2/717 (0.3%)
31	o	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
32	p	0.82	4/514 (0.8%)	1.32	2/686 (0.3%)
33	q	0.40	0/837	0.52	0/1129
33	r	0.40	0/854	0.56	0/1151
33	s	0.40	0/856	0.54	0/1155
33	t	0.39	0/828	0.54	1/1117 (0.1%)
34	x	0.18	0/194	0.64	0/298
All	All	0.59	53/73972 (0.1%)	0.76	203/101780 (0.2%)

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	7
3	C	0	2
11	K	0	1
13	M	0	2
15	O	0	6
16	P	0	2
17	Q	0	1
19	S	0	2
20	T	0	9
21	U	0	47
22	V	0	14
23	W	0	1
27	d	0	1
27	k	0	1
28	e	0	2
28	l	0	2
30	g	0	2
30	n	0	2
All	All	0	104

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	712	CYS	CB-SG	-17.12	1.53	1.82
6	F	1096	C	O3'-P	-10.09	1.49	1.61
8	H	718	SER	CB-OG	8.66	1.53	1.42
8	H	723	SER	CB-OG	8.49	1.53	1.42
8	H	714	SER	CB-OG	7.89	1.52	1.42
8	H	681	SER	CB-OG	7.76	1.52	1.42
31	o	46	SER	CB-OG	7.51	1.52	1.42
6	F	1096	C	C1'-N1	7.45	1.59	1.48
6	F	1120	G	C1'-N9	-7.39	1.36	1.46
31	o	45	SER	CB-OG	7.35	1.51	1.42
6	F	1118	U	C1'-N1	7.30	1.59	1.48
1	A	217	TRP	CB-CG	-7.13	1.37	1.50
32	p	33	SER	CB-OG	7.10	1.51	1.42
31	o	69	ASP	CA-CB	-7.01	1.38	1.53
31	o	6	SER	CB-OG	6.97	1.51	1.42
8	H	633	SER	CB-OG	6.92	1.51	1.42
3	C	934	HIS	N-CA	-6.84	1.32	1.46
6	F	1111	U	C1'-N1	6.77	1.58	1.48
6	F	1101	C	C1'-N1	6.76	1.58	1.48
6	F	1119	C	C1'-N1	6.75	1.58	1.48
10	J	202	LYS	C-N	-6.63	1.21	1.34
6	F	1115	G	C1'-N9	-6.60	1.37	1.46
1	A	716	ARG	NE-CZ	-6.54	1.24	1.33
1	A	298	TYR	CE1-CZ	-6.15	1.30	1.38
6	F	1109	C	C1'-N1	6.08	1.57	1.48
31	o	42	SER	CB-OG	5.95	1.50	1.42
4	D	64	U	O3'-P	-5.83	1.54	1.61
31	o	102	THR	CB-OG1	5.76	1.54	1.43
8	H	640	SER	CB-OG	5.75	1.49	1.42
31	o	15	TYR	CB-CG	-5.70	1.43	1.51
6	F	1112	G	C1'-N9	-5.66	1.39	1.46
6	F	121	C	C1'-N1	5.63	1.57	1.48
3	C	415	TYR	CG-CD2	-5.59	1.31	1.39
9	I	102	TRP	CB-CG	-5.59	1.40	1.50
31	o	51	THR	CB-OG1	5.58	1.54	1.43
3	C	933	TRP	CA-C	-5.47	1.38	1.52
3	C	478	TYR	CG-CD2	-5.38	1.32	1.39
3	C	933	TRP	CB-CG	-5.30	1.40	1.50
8	H	685	GLU	CB-CG	-5.27	1.42	1.52
3	C	535	PRO	N-CD	5.25	1.55	1.47
1	A	872	PRO	N-CD	5.25	1.55	1.47
32	p	110	THR	CB-OG1	5.20	1.53	1.43
32	p	75	THR	CB-OG1	5.18	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	363	PRO	N-CD	5.18	1.55	1.47
2	B	104	G	O3'-P	-5.16	1.54	1.61
31	o	153	THR	CB-OG1	5.13	1.53	1.43
1	A	902	PRO	N-CD	5.12	1.55	1.47
1	A	1391	PRO	N-CD	5.12	1.55	1.47
1	A	1380	PRO	N-CD	5.09	1.54	1.47
1	A	947	PRO	N-CD	5.08	1.54	1.47
32	p	65	PHE	CB-CG	-5.06	1.42	1.51
20	T	142	PRO	N-CD	5.04	1.54	1.47
1	A	298	TYR	CG-CD2	-5.01	1.32	1.39

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	462	LEU	CA-C-N	-14.21	85.94	117.20
6	F	1110	U	C5-C4-O4	11.98	133.09	125.90
1	A	831	ARG	NE-CZ-NH2	-11.67	114.47	120.30
23	W	462	LEU	C-N-CA	-10.96	94.29	121.70
22	V	240	GLU	N-CA-CB	10.82	130.08	110.60
6	F	1107	C	N1-C2-O2	-10.10	112.84	118.90
16	P	12	ARG	NE-CZ-NH1	10.08	125.34	120.30
3	C	938	ARG	NE-CZ-NH2	-9.30	115.65	120.30
22	V	239	ASN	N-CA-C	9.17	135.76	111.00
31	o	44	PRO	N-CA-CB	8.87	113.94	103.30
6	F	1109	C	O4'-C1'-N1	8.79	115.23	108.20
3	C	363	PRO	CA-N-CD	-8.57	99.51	111.50
6	F	1112	G	P-O3'-C3'	8.37	129.75	119.70
6	F	1107	C	C5'-C4'-O4'	-8.32	99.11	109.10
16	P	6	ARG	C-N-CD	-8.32	102.30	120.60
6	F	1110	U	N3-C4-O4	-8.20	113.66	119.40
21	U	303	ALA	O-C-N	-8.16	109.65	122.70
20	T	113	THR	O-C-N	-8.15	109.66	122.70
21	U	119	GLU	O-C-N	-8.14	109.67	122.70
21	U	123	SER	O-C-N	-8.14	109.67	122.70
21	U	201	LEU	O-C-N	-8.14	109.67	122.70
21	U	499	LYS	O-C-N	-8.14	109.68	122.70
21	U	126	ASP	O-C-N	-8.14	109.68	122.70
21	U	393	ARG	O-C-N	-8.14	109.68	122.70
21	U	440	ILE	O-C-N	-8.13	109.69	122.70
21	U	478	LEU	O-C-N	-8.13	109.69	122.70
22	V	300	ALA	O-C-N	-8.13	109.69	122.70
20	T	110	GLU	O-C-N	-8.13	109.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	304	TYR	O-C-N	-8.13	109.70	122.70
20	T	123	LEU	O-C-N	-8.13	109.70	122.70
21	U	437	SER	O-C-N	-8.12	109.70	122.70
21	U	589	ASP	O-C-N	-8.12	109.71	122.70
22	V	298	LEU	O-C-N	-8.12	109.70	122.70
22	V	299	GLN	O-C-N	-8.12	109.70	122.70
22	V	290	GLN	O-C-N	-8.12	109.71	122.70
21	U	121	TYR	O-C-N	-8.12	109.71	122.70
21	U	365	ILE	O-C-N	-8.12	109.71	122.70
22	V	302	GLU	O-C-N	-8.12	109.71	122.70
22	V	295	GLU	O-C-N	-8.11	109.72	122.70
21	U	364	HIS	O-C-N	-8.11	109.72	122.70
21	U	558	SER	O-C-N	-8.11	109.72	122.70
21	U	117	GLU	O-C-N	-8.11	109.72	122.70
21	U	442	ILE	O-C-N	-8.11	109.73	122.70
21	U	118	ASN	O-C-N	-8.11	109.73	122.70
21	U	367	GLU	O-C-N	-8.11	109.73	122.70
22	V	301	LEU	O-C-N	-8.11	109.73	122.70
20	T	111	SER	O-C-N	-8.10	109.74	122.70
20	T	112	SER	O-C-N	-8.10	109.74	122.70
20	T	125	GLN	O-C-N	-8.10	109.74	122.70
21	U	366	MET	O-C-N	-8.10	109.74	122.70
21	U	502	ARG	O-C-N	-8.10	109.74	122.70
20	T	124	LEU	O-C-N	-8.10	109.74	122.70
21	U	177	LEU	O-C-N	-8.10	109.74	122.70
21	U	417	ALA	O-C-N	-8.10	109.74	122.70
21	U	556	GLU	O-C-N	-8.10	109.74	122.70
22	V	292	LYS	O-C-N	-8.10	109.74	122.70
22	V	293	LYS	O-C-N	-8.10	109.74	122.70
22	V	303	LYS	O-C-N	-8.10	109.74	122.70
21	U	122	LEU	O-C-N	-8.10	109.75	122.70
21	U	415	ILE	O-C-N	-8.10	109.75	122.70
22	V	291	ARG	O-C-N	-8.10	109.75	122.70
21	U	125	GLU	O-C-N	-8.09	109.75	122.70
21	U	441	PHE	O-C-N	-8.09	109.75	122.70
22	V	297	ARG	O-C-N	-8.09	109.75	122.70
21	U	127	GLU	O-C-N	-8.09	109.75	122.70
22	V	296	MET	O-C-N	-8.09	109.75	122.70
21	U	438	ASP	O-C-N	-8.09	109.76	122.70
21	U	439	ILE	O-C-N	-8.09	109.76	122.70
21	U	501	LEU	O-C-N	-8.09	109.75	122.70
21	U	557	HIS	O-C-N	-8.09	109.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	128	VAL	O-C-N	-8.09	109.76	122.70
21	U	176	ILE	O-C-N	-8.09	109.76	122.70
21	U	124	SER	O-C-N	-8.08	109.77	122.70
21	U	476	TYR	O-C-N	-8.08	109.77	122.70
21	U	200	GLU	O-C-N	-8.08	109.77	122.70
21	U	305	ARG	O-C-N	-8.08	109.78	122.70
21	U	120	ASP	O-C-N	-8.07	109.78	122.70
22	V	294	VAL	O-C-N	-8.07	109.78	122.70
21	U	416	GLU	O-C-N	-8.07	109.78	122.70
21	U	392	PRO	O-C-N	-8.07	109.79	122.70
21	U	500	LYS	O-C-N	-8.07	109.79	122.70
21	U	477	GLU	O-C-N	-8.07	109.79	122.70
21	U	202	LEU	O-C-N	-7.90	109.77	123.20
6	F	1107	C	P-O3'-C3'	7.57	128.78	119.70
1	A	1384	PRO	C-N-CD	-7.57	103.95	120.60
6	F	1110	U	N1-C2-O2	7.55	128.08	122.80
6	F	1107	C	N3-C2-O2	7.48	127.13	121.90
1	A	716	ARG	NE-CZ-NH2	-7.29	116.66	120.30
31	o	5	PRO	N-CA-CB	7.25	112.00	103.30
31	o	42	SER	N-CA-CB	-7.20	99.71	110.50
6	F	1111	U	P-O5'-C5'	-7.12	109.51	120.90
6	F	1110	U	N3-C2-O2	-6.99	117.31	122.20
6	F	1108	A	O4'-C1'-N9	-6.90	102.68	108.20
31	o	12	PRO	N-CA-CB	6.70	111.34	103.30
16	P	12	ARG	NE-CZ-NH2	-6.70	116.95	120.30
8	H	617	PRO	CA-CB-CG	6.63	117.39	104.80
3	C	884	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	A	831	ARG	NE-CZ-NH1	6.54	123.57	120.30
8	H	613	PRO	N-CA-CB	6.52	111.12	103.30
8	H	722	PRO	N-CA-CB	6.47	111.07	103.30
10	J	334	PRO	N-CA-CB	6.40	110.98	103.30
31	o	4	THR	N-CA-CB	-6.33	98.28	110.30
31	o	57	LEU	N-CA-CB	6.33	123.05	110.40
1	A	1383	PHE	C-N-CD	6.29	141.62	128.40
8	H	479	PRO	N-CA-CB	6.21	110.75	103.30
22	V	234	VAL	C-N-CD	6.16	141.33	128.40
1	A	1882	LEU	C-N-CA	-6.14	106.35	121.70
8	H	443	PRO	N-CA-CB	6.07	110.59	103.30
8	H	223	PRO	N-CA-CB	6.07	110.58	103.30
8	H	161	PRO	N-CA-CB	5.99	110.49	103.30
8	H	150	PRO	N-CA-CB	5.97	110.47	103.30
8	H	515	PRO	N-CA-CB	5.97	110.47	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	774	PRO	N-CA-CB	5.97	110.46	103.30
8	H	477	PRO	N-CA-CB	5.97	110.46	103.30
8	H	641	PRO	CA-CB-CG	5.97	116.14	104.80
21	U	391	SER	O-C-N	-5.96	109.78	121.10
3	C	938	ARG	NE-CZ-NH1	5.96	123.28	120.30
10	J	418	PRO	N-CA-CB	5.96	110.45	103.30
8	H	616	PRO	N-CA-CB	5.96	110.45	103.30
8	H	267	PRO	N-CA-CB	5.95	110.44	103.30
8	H	299	PRO	N-CA-CB	5.95	110.44	103.30
9	I	397	PRO	N-CA-CB	5.94	110.43	103.30
3	C	884	ARG	NE-CZ-NH2	5.94	123.27	120.30
8	H	262	PRO	N-CA-CB	5.93	110.42	103.30
8	H	437	PRO	N-CA-CB	5.93	110.41	103.30
21	U	97	PRO	N-CA-CB	5.93	110.41	103.30
8	H	533	PRO	N-CA-CB	5.92	110.41	103.30
31	o	141	ARG	CD-NE-CZ	5.91	131.88	123.60
3	C	933	TRP	CA-C-N	-5.90	104.22	117.20
8	H	557	PRO	N-CA-CB	5.90	110.38	103.30
31	o	7	ILE	CA-CB-CG1	5.90	122.21	111.00
21	U	217	PRO	N-CA-CB	5.87	110.34	103.30
9	I	435	PRO	N-CA-CB	5.86	110.33	103.30
6	F	1107	C	C5-C4-N4	-5.86	116.10	120.20
8	H	252	PRO	N-CA-CB	5.84	110.31	103.30
6	F	1111	U	C5'-C4'-C3'	-5.83	106.67	116.00
3	C	463	THR	C-N-CD	5.83	140.63	128.40
9	I	468	PRO	N-CA-CB	5.82	110.29	103.30
20	T	141	LEU	C-N-CD	5.81	140.60	128.40
6	F	1110	U	O3'-P-O5'	-5.81	92.97	104.00
1	A	901	PRO	C-N-CD	5.80	140.58	128.40
1	A	1390	THR	C-N-CD	5.79	140.56	128.40
20	T	23	PRO	N-CA-CB	5.79	110.25	103.30
1	A	946	ASN	C-N-CD	5.79	140.56	128.40
7	G	105	PRO	CA-CB-CG	5.78	115.78	104.80
9	I	559	PRO	N-CA-CB	5.77	110.23	103.30
9	I	545	PRO	N-CA-CB	5.77	110.22	103.30
9	I	351	PRO	N-CA-CB	5.77	110.22	103.30
8	H	773	PRO	N-CA-CB	5.75	110.20	103.30
8	H	518	PRO	N-CA-CB	5.75	110.20	103.30
10	J	376	PRO	N-CA-CB	5.74	110.19	103.30
31	o	68	PRO	N-CA-CB	5.73	110.17	103.30
1	A	622	MET	CB-CG-SD	-5.70	95.30	112.40
9	I	421	PRO	N-CA-CB	5.65	110.08	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	534	THR	C-N-CD	5.65	140.26	128.40
1	A	1379	MET	C-N-CD	5.63	140.22	128.40
21	U	461	PRO	N-CA-CB	5.62	110.05	103.30
1	A	871	GLY	C-N-CD	5.61	140.19	128.40
21	U	187	PRO	N-CA-CB	5.61	110.03	103.30
21	U	173	PRO	N-CA-CB	5.60	110.02	103.30
21	U	288	PRO	N-CA-CB	5.58	110.00	103.30
21	U	189	PRO	N-CA-CB	5.56	109.97	103.30
21	U	326	PRO	N-CA-CB	5.55	109.96	103.30
30	n	81	GLY	CA-C-N	-5.55	104.98	117.20
30	g	81	GLY	CA-C-N	-5.51	105.08	117.20
21	U	474	PRO	N-CA-CB	5.50	109.90	103.30
3	C	927	MET	CG-SD-CE	-5.44	91.49	100.20
20	T	23	PRO	CA-CB-CG	5.41	115.07	104.80
10	J	424	PRO	N-CA-CB	5.38	109.75	103.30
10	J	467	PRO	N-CA-CB	5.36	109.73	103.30
10	J	339	PRO	N-CA-CB	5.35	109.72	103.30
10	J	447	PRO	N-CA-CB	5.34	109.71	103.30
26	j	74	ARG	NE-CZ-NH1	5.34	122.97	120.30
10	J	432	PRO	N-CA-CB	5.33	109.70	103.30
12	L	59	ARG	NE-CZ-NH2	-5.31	117.64	120.30
6	F	1113	U	O4'-C1'-C2'	-5.31	100.49	105.80
7	G	77	PRO	CA-CB-CG	5.29	114.86	104.80
15	O	155	PHE	CB-CA-C	-5.29	99.82	110.40
3	C	656	LEU	CA-CB-CG	-5.27	103.17	115.30
18	R	180	ASP	CB-CG-OD2	5.27	123.04	118.30
20	T	81	PRO	CA-CB-CG	5.24	114.75	104.80
20	T	36	PRO	N-CA-CB	5.24	109.58	103.30
3	C	684	GLU	N-CA-C	5.22	125.10	111.00
31	o	71	SER	N-CA-CB	-5.21	102.68	110.50
33	t	62	LEU	CA-CB-CG	-5.21	103.31	115.30
6	F	1119	C	OP1-P-OP2	-5.20	111.81	119.60
18	R	179	ASP	CB-CG-OD2	5.17	122.96	118.30
8	H	617	PRO	N-CA-CB	5.16	109.50	103.30
9	I	36	ASP	CB-CG-OD2	5.16	122.94	118.30
10	J	374	PRO	N-CA-CB	5.14	109.47	103.30
20	T	122	ASP	CB-CG-OD2	5.14	122.92	118.30
21	U	90	PRO	N-CA-CB	5.13	109.46	103.30
20	T	75	THR	O-C-N	-5.12	114.51	122.70
32	p	46	VAL	CA-CB-CG2	5.09	118.54	110.90
31	o	107	SER	N-CA-CB	-5.08	102.87	110.50
30	n	82	LYS	N-CA-C	5.08	124.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	171	GLY	N-CA-C	5.07	125.76	113.10
30	g	82	LYS	N-CA-C	5.06	124.65	111.00
22	V	268	PRO	N-CA-CB	5.05	109.36	103.30
21	U	392	PRO	N-CA-CB	5.05	109.36	103.30
32	p	33	SER	N-CA-CB	5.05	118.07	110.50
26	c	74	ARG	NE-CZ-NH1	5.04	122.82	120.30
6	F	1096	C	OP2-P-O3'	5.03	116.27	105.20

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1375	LEU	Peptide
1	A	1377	SER	Peptide
1	A	239	PHE	Peptide,Mainchain
1	A	539	PRO	Peptide
1	A	772	GLU	Peptide
3	C	170	LEU	Peptide
3	C	885	GLY	Peptide
11	K	92	ARG	Peptide
13	M	103	GLU	Peptide
13	M	45	HIS	Peptide
15	O	123	PRO	Peptide
15	O	278	ASP	Peptide
15	O	351	GLY	Peptide,Mainchain
15	O	436	SER	Peptide
15	O	437	GLU	Peptide
16	P	6	ARG	Peptide,Mainchain
17	Q	85	SER	Peptide
19	S	67	GLY	Peptide,Mainchain
20	T	110	GLU	Mainchain
20	T	111	SER	Mainchain
20	T	112	SER	Mainchain
20	T	113	THR	Mainchain
20	T	123	LEU	Mainchain
20	T	124	LEU	Mainchain
20	T	125	GLN	Mainchain
20	T	126	ILE	Mainchain
20	T	75	THR	Mainchain
21	U	117	GLU	Mainchain
21	U	118	ASN	Mainchain

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Mol	Chain	Res	Type	Group
21	U	119	GLU	Mainchain
21	U	120	ASP	Mainchain
21	U	121	TYR	Mainchain
21	U	122	LEU	Mainchain
21	U	123	SER	Mainchain
21	U	124	SER	Mainchain
21	U	125	GLU	Mainchain
21	U	126	ASP	Mainchain
21	U	127	GLU	Mainchain
21	U	128	VAL	Mainchain
21	U	176	ILE	Mainchain
21	U	177	LEU	Mainchain
21	U	200	GLU	Mainchain
21	U	201	LEU	Mainchain
21	U	202	LEU	Mainchain
21	U	303	ALA	Mainchain
21	U	304	TYR	Mainchain
21	U	305	ARG	Mainchain
21	U	364	HIS	Mainchain
21	U	365	ILE	Mainchain
21	U	366	MET	Mainchain
21	U	367	GLU	Mainchain
21	U	391	SER	Mainchain
21	U	392	PRO	Mainchain
21	U	393	ARG	Mainchain
21	U	415	ILE	Mainchain
21	U	416	GLU	Mainchain
21	U	417	ALA	Mainchain
21	U	437	SER	Mainchain
21	U	438	ASP	Mainchain
21	U	439	ILE	Mainchain
21	U	440	ILE	Mainchain
21	U	441	PHE	Mainchain
21	U	442	ILE	Mainchain
21	U	476	TYR	Mainchain
21	U	477	GLU	Mainchain
21	U	478	LEU	Mainchain
21	U	499	LYS	Mainchain
21	U	500	LYS	Mainchain
21	U	501	LEU	Mainchain
21	U	502	ARG	Mainchain
21	U	556	GLU	Mainchain

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Mol	Chain	Res	Type	Group
21	U	557	HIS	Mainchain
21	U	558	SER	Mainchain
21	U	589	ASP	Mainchain
22	V	290	GLN	Mainchain
22	V	291	ARG	Mainchain
22	V	292	LYS	Mainchain
22	V	293	LYS	Mainchain
22	V	294	VAL	Mainchain
22	V	295	GLU	Mainchain
22	V	296	MET	Mainchain
22	V	297	ARG	Mainchain
22	V	298	LEU	Mainchain
22	V	299	GLN	Mainchain
22	V	300	ALA	Mainchain
22	V	301	LEU	Mainchain
22	V	302	GLU	Mainchain
22	V	303	LYS	Mainchain
23	W	462	LEU	Mainchain
27	d	41	ASP	Peptide
28	e	81	ALA	Peptide,Mainchain
30	g	81	GLY	Peptide,Mainchain
27	k	41	ASP	Peptide
28	l	81	ALA	Peptide,Mainchain
30	n	81	GLY	Peptide,Mainchain

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1895/2413 (78%)	1750 (92%)	125 (7%)	20 (1%)	14	50
3	C	907/1008 (90%)	820 (90%)	70 (8%)	17 (2%)	8	38
7	G	149/175 (85%)	134 (90%)	12 (8%)	3 (2%)	7	37
8	H	529/859 (62%)	505 (96%)	18 (3%)	6 (1%)	14	50
9	I	500/687 (73%)	468 (94%)	30 (6%)	2 (0%)	34	70
10	J	413/590 (70%)	384 (93%)	22 (5%)	7 (2%)	9	40
11	K	98/215 (46%)	96 (98%)	2 (2%)	0	100	100
12	L	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	12	46
13	M	172/364 (47%)	151 (88%)	19 (11%)	2 (1%)	13	48
14	N	259/339 (76%)	241 (93%)	18 (7%)	0	100	100
15	O	335/451 (74%)	295 (88%)	34 (10%)	6 (2%)	8	39
16	P	62/175 (35%)	56 (90%)	4 (6%)	2 (3%)	4	28
17	Q	193/379 (51%)	175 (91%)	13 (7%)	5 (3%)	5	32
18	R	44/278 (16%)	44 (100%)	0	0	100	100
19	S	21/455 (5%)	19 (90%)	1 (5%)	1 (5%)	2	19
20	T	97/283 (34%)	93 (96%)	4 (4%)	0	100	100
21	U	442/708 (62%)	430 (97%)	5 (1%)	7 (2%)	9	42
22	V	87/322 (27%)	82 (94%)	4 (5%)	1 (1%)	14	50
23	W	702/767 (92%)	657 (94%)	39 (6%)	6 (1%)	17	54
24	a	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
24	h	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
25	b	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
25	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
26	c	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	43
26	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	43
27	d	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
28	e	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	46
28	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	46
29	f	78/146 (53%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
30	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	14	50
30	n	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9	42
31	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9	42
32	p	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
33	q	120/503 (24%)	114 (95%)	4 (3%)	2 (2%)	9	40
33	r	123/503 (24%)	117 (95%)	6 (5%)	0	100	100
33	s	125/503 (25%)	115 (92%)	6 (5%)	4 (3%)	4	28
33	t	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5	32
All	All	8774/14606 (60%)	8126 (93%)	544 (6%)	104 (1%)	17	48

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1347	ARG
1	A	1359	ILE
1	A	1385	PRO
1	A	1403	SER
3	C	363	PRO
3	C	366	ASN
3	C	431	GLN
3	C	464	PRO
3	C	466	GLY
3	C	683	ASN
3	C	685	SER
7	G	77	PRO
8	H	616	PRO
8	H	797	TYR
9	I	315	ASN
10	J	417	PRO
10	J	418	PRO
16	P	7	PRO
21	U	633	PHE
21	U	634	LYS
21	U	661	GLY
22	V	213	ASP
23	W	463	SER
23	W	599	ILE
31	o	68	PRO

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Mol	Chain	Res	Type
33	s	53	ILE
33	s	77	ILE
33	t	64	GLU
1	A	483	PRO
1	A	1358	ASP
3	C	357	GLY
3	C	532	ASP
7	G	110	GLU
8	H	601	VAL
8	H	618	GLU
10	J	230	THR
10	J	415	ILE
13	M	99	VAL
13	M	236	ASN
16	P	9	LEU
17	Q	36	LYS
17	Q	86	ASN
17	Q	112	ILE
23	W	734	GLY
33	q	56	SER
1	A	540	THR
1	A	645	ASP
1	A	741	ILE
3	C	116	THR
3	C	829	VAL
7	G	80	ASN
8	H	634	HIS
8	H	752	GLU
15	O	124	GLU
19	S	61	LYS
23	W	453	SER
23	W	598	GLY
33	q	17	PRO
33	t	20	ARG
1	A	377	VAL
1	A	1384	PRO
1	A	1628	ASP
3	C	994	SER
9	I	529	LYS
10	J	231	SER
12	L	104	CYS
15	O	278	ASP

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Mol	Chain	Res	Type
15	O	279	PRO
15	O	391	GLU
21	U	697	THR
28	e	82	PRO
30	g	82	LYS
28	l	82	PRO
30	n	82	LYS
1	A	1327	THR
3	C	649	GLU
3	C	655	LEU
3	C	690	PRO
3	C	884	ARG
12	L	120	CYS
15	O	435	GLU
17	Q	102	ALA
21	U	651	ILE
33	s	60	ALA
1	A	240	PRO
1	A	261	LEU
1	A	407	VAL
1	A	875	THR
1	A	1015	PRO
21	U	659	PRO
23	W	709	THR
1	A	259	GLU
10	J	218	VAL
21	U	676	GLY
26	c	15	PRO
31	o	52	LYS
26	j	15	PRO
33	s	36	GLY
3	C	975	GLY
15	O	277	VAL
1	A	264	ILE
10	J	16	VAL
17	Q	34	ILE
33	t	36	GLY

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	A	1727/2182 (79%)	1661 (96%)	66 (4%)	33	64
3	C	822/910 (90%)	785 (96%)	37 (4%)	27	60
7	G	40/165 (24%)	29 (72%)	11 (28%)	0	2
8	H	59/786 (8%)	49 (83%)	10 (17%)	2	11
9	I	219/633 (35%)	217 (99%)	2 (1%)	78	91
10	J	213/525 (41%)	204 (96%)	9 (4%)	30	61
11	K	92/193 (48%)	92 (100%)	0	100	100
12	L	141/141 (100%)	138 (98%)	3 (2%)	53	78
13	M	121/332 (36%)	116 (96%)	5 (4%)	30	62
14	N	224/296 (76%)	221 (99%)	3 (1%)	69	86
15	O	295/397 (74%)	295 (100%)	0	100	100
16	P	55/151 (36%)	54 (98%)	1 (2%)	59	81
17	Q	173/328 (53%)	163 (94%)	10 (6%)	20	52
18	R	40/256 (16%)	31 (78%)	9 (22%)	1	3
19	S	20/413 (5%)	13 (65%)	7 (35%)	0	1
20	T	75/272 (28%)	59 (79%)	16 (21%)	1	4
21	U	76/663 (12%)	48 (63%)	28 (37%)	0	1
22	V	47/296 (16%)	34 (72%)	13 (28%)	0	2
24	a	70/176 (40%)	70 (100%)	0	100	100
24	h	67/176 (38%)	67 (100%)	0	100	100
25	b	65/83 (78%)	60 (92%)	5 (8%)	13	42
25	i	65/83 (78%)	60 (92%)	5 (8%)	13	42
26	c	61/77 (79%)	60 (98%)	1 (2%)	62	83
26	j	61/77 (79%)	60 (98%)	1 (2%)	62	83
27	d	58/66 (88%)	55 (95%)	3 (5%)	23	55
27	k	58/66 (88%)	55 (95%)	3 (5%)	23	55
28	e	69/89 (78%)	67 (97%)	2 (3%)	42	71
28	l	69/89 (78%)	67 (97%)	2 (3%)	42	71
29	f	77/129 (60%)	71 (92%)	6 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	m	77/129 (60%)	71 (92%)	6 (8%)	12	41
30	g	79/103 (77%)	74 (94%)	5 (6%)	18	50
30	n	59/103 (57%)	55 (93%)	4 (7%)	16	47
31	o	47/219 (22%)	44 (94%)	3 (6%)	17	49
32	p	25/100 (25%)	24 (96%)	1 (4%)	31	63
33	q	62/451 (14%)	55 (89%)	7 (11%)	6	25
33	r	62/451 (14%)	54 (87%)	8 (13%)	4	20
33	s	63/451 (14%)	56 (89%)	7 (11%)	6	26
33	t	60/451 (13%)	55 (92%)	5 (8%)	11	38
All	All	5693/12508 (46%)	5389 (95%)	304 (5%)	26	54

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	PHE
1	A	365	ASN
1	A	376	ARG
1	A	380	ARG
1	A	382	GLU
1	A	488	ARG
1	A	489	THR
1	A	495	ARG
1	A	588	LEU
1	A	612	LYS
1	A	689	TYR
1	A	693	LYS
1	A	874	ILE
1	A	893	ARG
1	A	903	LEU
1	A	928	ARG
1	A	936	GLU
1	A	937	LEU
1	A	941	GLU
1	A	1011	ASN
1	A	1045	GLN
1	A	1046	SER
1	A	1049	LEU
1	A	1050	LEU
1	A	1068	ARG

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Mol	Chain	Res	Type
1	A	1130	ARG
1	A	1171	LEU
1	A	1172	PHE
1	A	1174	PHE
1	A	1181	GLU
1	A	1290	ASP
1	A	1292	ARG
1	A	1295	GLN
1	A	1296	ARG
1	A	1326	THR
1	A	1328	PHE
1	A	1337	THR
1	A	1339	LEU
1	A	1356	LEU
1	A	1360	LEU
1	A	1361	VAL
1	A	1362	LYS
1	A	1370	ARG
1	A	1390	THR
1	A	1392	LYS
1	A	1393	GLU
1	A	1394	LEU
1	A	1405	ILE
1	A	1415	SER
1	A	1416	LYS
1	A	1418	THR
1	A	1441	PHE
1	A	1442	ARG
1	A	1443	TYR
1	A	1448	GLU
1	A	1464	LYS
1	A	1465	ARG
1	A	1474	ARG
1	A	1475	LEU
1	A	1477	PHE
1	A	1479	GLU
1	A	1480	LEU
1	A	1536	LEU
1	A	1539	LEU
1	A	1545	ASP
1	A	1571	GLU
3	C	117	ARG

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Mol	Chain	Res	Type
3	C	205	SER
3	C	208	ARG
3	C	272	ARG
3	C	274	ILE
3	C	275	LEU
3	C	276	ASP
3	C	356	LYS
3	C	360	ARG
3	C	361	THR
3	C	362	LYS
3	C	363	PRO
3	C	364	PHE
3	C	368	GLU
3	C	430	ARG
3	C	458	ILE
3	C	461	LYS
3	C	463	THR
3	C	465	GLU
3	C	510	ARG
3	C	530	GLU
3	C	638	GLU
3	C	685	SER
3	C	686	PHE
3	C	693	ASN
3	C	883	ARG
3	C	884	ARG
3	C	887	ARG
3	C	888	ILE
3	C	890	LYS
3	C	919	ARG
3	C	932	PHE
3	C	973	ARG
3	C	982	MET
3	C	997	LEU
3	C	1000	GLN
3	C	1002	ARG
7	G	5	SER
7	G	7	VAL
7	G	13	PRO
7	G	77	PRO
7	G	96	PRO
7	G	100	THR

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Mol	Chain	Res	Type
7	G	105	PRO
7	G	108	SER
7	G	133	PRO
7	G	136	VAL
7	G	150	THR
8	H	616	PRO
8	H	617	PRO
8	H	641	PRO
8	H	706	LEU
8	H	712	CYS
8	H	722	PRO
8	H	723	SER
8	H	725	THR
8	H	726	ARG
8	H	733	ILE
9	I	155	LEU
9	I	205	TRP
10	J	65	PHE
10	J	160	LEU
10	J	166	LYS
10	J	504	PRO
10	J	505	PRO
10	J	517	VAL
10	J	523	LEU
10	J	532	PRO
10	J	550	PRO
12	L	104	CYS
12	L	120	CYS
12	L	122	CYS
13	M	51	ARG
13	M	53	ASN
13	M	87	ARG
13	M	118	VAL
13	M	126	THR
14	N	8	SER
14	N	10	LYS
14	N	146	LEU
16	P	7	PRO
17	Q	202	MET
17	Q	204	LEU
17	Q	206	GLU
17	Q	209	GLU

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Mol	Chain	Res	Type
17	Q	212	ASP
17	Q	213	LYS
17	Q	216	ARG
17	Q	217	GLN
17	Q	220	ARG
17	Q	222	LYS
18	R	167	GLU
18	R	168	LYS
18	R	170	LEU
18	R	177	GLN
18	R	191	LEU
18	R	193	MET
18	R	196	ARG
18	R	198	GLU
18	R	202	ARG
19	S	51	PHE
19	S	55	GLU
19	S	57	LYS
19	S	58	ARG
19	S	59	ARG
19	S	62	THR
19	S	66	ASP
20	T	23	PRO
20	T	24	THR
20	T	36	PRO
20	T	81	PRO
20	T	84	ASP
20	T	96	ASP
20	T	99	ARG
20	T	101	LYS
20	T	106	LEU
20	T	109	SER
20	T	128	ARG
20	T	133	LEU
20	T	135	LYS
20	T	140	ASN
20	T	143	TYR
20	T	146	TRP
21	U	634	LYS
21	U	641	CYS
21	U	642	LEU
21	U	646	TYR

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Mol	Chain	Res	Type
21	U	648	ILE
21	U	650	LYS
21	U	653	ASN
21	U	656	THR
21	U	657	GLN
21	U	658	LEU
21	U	665	ASP
21	U	667	ILE
21	U	668	VAL
21	U	670	LEU
21	U	671	PHE
21	U	672	GLU
21	U	674	ARG
21	U	677	LYS
21	U	678	LYS
21	U	680	MET
21	U	681	GLU
21	U	684	LEU
21	U	689	LEU
21	U	691	VAL
21	U	693	ASP
21	U	699	LYS
21	U	703	LEU
21	U	707	ASP
22	V	201	MET
22	V	205	GLN
22	V	206	ASP
22	V	208	MET
22	V	209	LEU
22	V	215	GLN
22	V	219	GLN
22	V	229	LYS
22	V	233	GLU
22	V	236	TYR
22	V	237	ARG
22	V	241	GLU
22	V	245	GLN
25	b	16	CYS
25	b	18	PHE
25	b	25	THR
25	b	79	LYS
25	b	81	LEU

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Mol	Chain	Res	Type
26	c	79	LEU
27	d	18	ASN
27	d	41	ASP
27	d	71	LEU
28	e	10	LEU
28	e	76	ASP
29	f	20	LYS
29	f	26	TRP
29	f	30	GLN
29	f	77	ASP
29	f	99	ASP
29	f	104	ASP
30	g	24	PHE
30	g	49	ARG
30	g	77	THR
30	g	99	ASP
30	g	100	SER
31	o	4	THR
31	o	44	PRO
31	o	71	SER
32	p	38	LYS
25	i	16	CYS
25	i	18	PHE
25	i	25	THR
25	i	79	LYS
25	i	81	LEU
26	j	79	LEU
27	k	18	ASN
27	k	41	ASP
27	k	71	LEU
28	l	10	LEU
28	l	76	ASP
29	m	20	LYS
29	m	26	TRP
29	m	30	GLN
29	m	77	ASP
29	m	99	ASP
29	m	104	ASP
30	n	49	ARG
30	n	77	THR
30	n	99	ASP
30	n	100	SER

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Mol	Chain	Res	Type
33	q	17	PRO
33	q	26	SER
33	q	44	PRO
33	q	63	THR
33	q	96	PHE
33	q	109	LEU
33	q	134	SER
33	r	17	PRO
33	r	44	PRO
33	r	63	THR
33	r	80	LEU
33	r	85	GLN
33	r	93	LEU
33	r	99	ARG
33	r	109	LEU
33	s	17	PRO
33	s	44	PRO
33	s	55	PRO
33	s	56	SER
33	s	61	SER
33	s	102	LEU
33	s	126	LEU
33	t	17	PRO
33	t	44	PRO
33	t	63	THR
33	t	93	LEU
33	t	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	265	ASN
1	A	344	ASN
1	A	365	ASN
1	A	405	ASN
1	A	429	ASN
1	A	658	ASN
1	A	659	HIS
1	A	662	GLN
1	A	705	GLN
1	A	848	ASN

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Mol	Chain	Res	Type
1	A	864	GLN
1	A	868	GLN
1	A	948	HIS
1	A	1011	ASN
1	A	1033	ASN
1	A	1045	GLN
1	A	1099	ASN
1	A	1156	HIS
1	A	1173	HIS
1	A	1376	ASN
1	A	1417	GLN
1	A	1424	HIS
1	A	1529	ASN
1	A	1532	HIS
1	A	1718	HIS
1	A	1737	GLN
1	A	1863	HIS
1	A	1947	HIS
1	A	2018	ASN
3	C	82	ASN
3	C	101	GLN
3	C	158	HIS
3	C	251	GLN
3	C	289	ASN
3	C	403	ASN
3	C	683	ASN
3	C	764	ASN
3	C	794	GLN
3	C	817	GLN
3	C	830	ASN
3	C	869	HIS
3	C	1000	GLN
3	C	1004	ASN
9	I	79	HIS
10	J	82	ASN
10	J	214	ASN
11	K	200	ASN
12	L	54	GLN
12	L	116	ASN
12	L	143	HIS
13	M	53	ASN
13	M	106	ASN

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Mol	Chain	Res	Type
14	N	58	HIS
14	N	91	HIS
14	N	92	HIS
14	N	150	HIS
14	N	191	ASN
14	N	201	ASN
14	N	248	ASN
15	O	126	HIS
15	O	215	GLN
15	O	382	HIS
16	P	8	GLN
16	P	34	HIS
16	P	173	HIS
17	Q	37	ASN
17	Q	198	ASN
17	Q	217	GLN
20	T	50	HIS
20	T	138	HIS
21	U	664	GLN
21	U	686	HIS
25	b	34	GLN
25	b	86	ASN
27	d	66	ASN
28	e	41	ASN
29	f	30	GLN
25	i	34	GLN
25	i	86	ASN
26	j	52	GLN
27	k	66	ASN
28	l	41	ASN
29	m	30	GLN
30	n	71	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	114/214 (53%)	30 (26%)	3 (2%)
34	x	8/9 (88%)	5 (62%)	0
4	D	100/112 (89%)	35 (35%)	8 (8%)
5	E	27/38 (71%)	15 (55%)	7 (25%)
6	F	79/1175 (6%)	30 (37%)	11 (13%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	328/1548 (21%)	115 (35%)	29 (8%)

All (115) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	29	G
2	B	31	G
2	B	32	G
2	B	33	U
2	B	42	A
2	B	44	A
2	B	74	U
2	B	75	A
2	B	76	U
2	B	77	A
2	B	79	C
2	B	80	G
2	B	81	A
2	B	82	A
2	B	84	A
2	B	90	C
2	B	92	U
2	B	94	C
2	B	101	C
2	B	104	G
2	B	127	U
2	B	164	C
2	B	165	A
2	B	166	U
2	B	170	U
2	B	171	U
2	B	172	U
2	B	173	U
2	B	174	G
2	B	175	G
4	D	12	A
4	D	13	A
4	D	14	C
4	D	15	C
4	D	16	C
4	D	33	C
4	D	36	U

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Mol	Chain	Res	Type
4	D	37	U
4	D	39	G
4	D	43	C
4	D	50	G
4	D	51	A
4	D	52	G
4	D	54	U
4	D	57	U
4	D	58	C
4	D	59	A
4	D	60	G
4	D	62	A
4	D	65	U
4	D	66	C
4	D	67	C
4	D	68	C
4	D	73	A
4	D	74	U
4	D	75	A
4	D	80	U
4	D	81	G
4	D	85	C
4	D	86	G
4	D	87	U
4	D	88	U
4	D	90	U
4	D	91	A
4	D	92	C
5	E	2	U
5	E	3	A
5	E	4	U
5	E	9	U
5	E	10	U
5	E	11	A
5	E	13	U
5	E	494	G
5	E	495	A
5	E	496	U
5	E	497	A
5	E	500	A
5	E	501	A
5	E	502	C

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Mol	Chain	Res	Type
5	E	503	A
6	F	15	C
6	F	16	U
6	F	17	U
6	F	18	U
6	F	19	U
6	F	20	G
6	F	25	A
6	F	26	G
6	F	30	A
6	F	31	A
6	F	32	G
6	F	34	G
6	F	39	A
6	F	40	U
6	F	41	C
6	F	42	U
6	F	111	C
6	F	115	U
6	F	116	U
6	F	117	U
6	F	118	U
6	F	119	G
6	F	120	G
6	F	1099	G
6	F	1107	C
6	F	1108	A
6	F	1111	U
6	F	1112	G
6	F	1114	G
6	F	1120	G
34	x	2	U
34	x	3	U
34	x	4	U
34	x	8	U
34	x	9	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	78	A
2	B	83	C

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Mol	Chain	Res	Type
2	B	172	U
4	D	14	C
4	D	42	A
4	D	51	A
4	D	56	A
4	D	57	U
4	D	58	C
4	D	64	U
4	D	66	C
5	E	1	G
5	E	2	U
5	E	3	A
5	E	9	U
5	E	494	G
5	E	499	U
5	E	500	A
6	F	15	C
6	F	16	U
6	F	17	U
6	F	18	U
6	F	19	U
6	F	30	A
6	F	40	U
6	F	41	C
6	F	117	U
6	F	1107	C
6	F	1111	U

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 14 ligands modelled in this entry, 12 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
36	GTP	C	1500	37	26,34,34	1.11	1 (3%)	32,54,54	2.03	7 (21%)
35	IHP	A	3000	-	36,36,36	0.69	0	54,60,60	0.93	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
36	GTP	C	1500	37	-	5/18/38/38	0/3/3/3
35	IHP	A	3000	-	-	11/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C6-N1	-3.01	1.33	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	1500	GTP	PB-O3B-PG	-5.75	113.11	132.83
36	C	1500	GTP	O6-C6-C5	-4.28	116.02	124.37
36	C	1500	GTP	PA-O3A-PB	-3.61	120.45	132.83
36	C	1500	GTP	C5-C6-N1	3.25	119.69	113.95
36	C	1500	GTP	O6-C6-N1	3.08	124.29	120.65
36	C	1500	GTP	C2-N1-C6	-2.49	120.51	125.10
36	C	1500	GTP	C3'-C2'-C1'	2.26	104.38	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	3000	IHP	C1-C6-O16-P6

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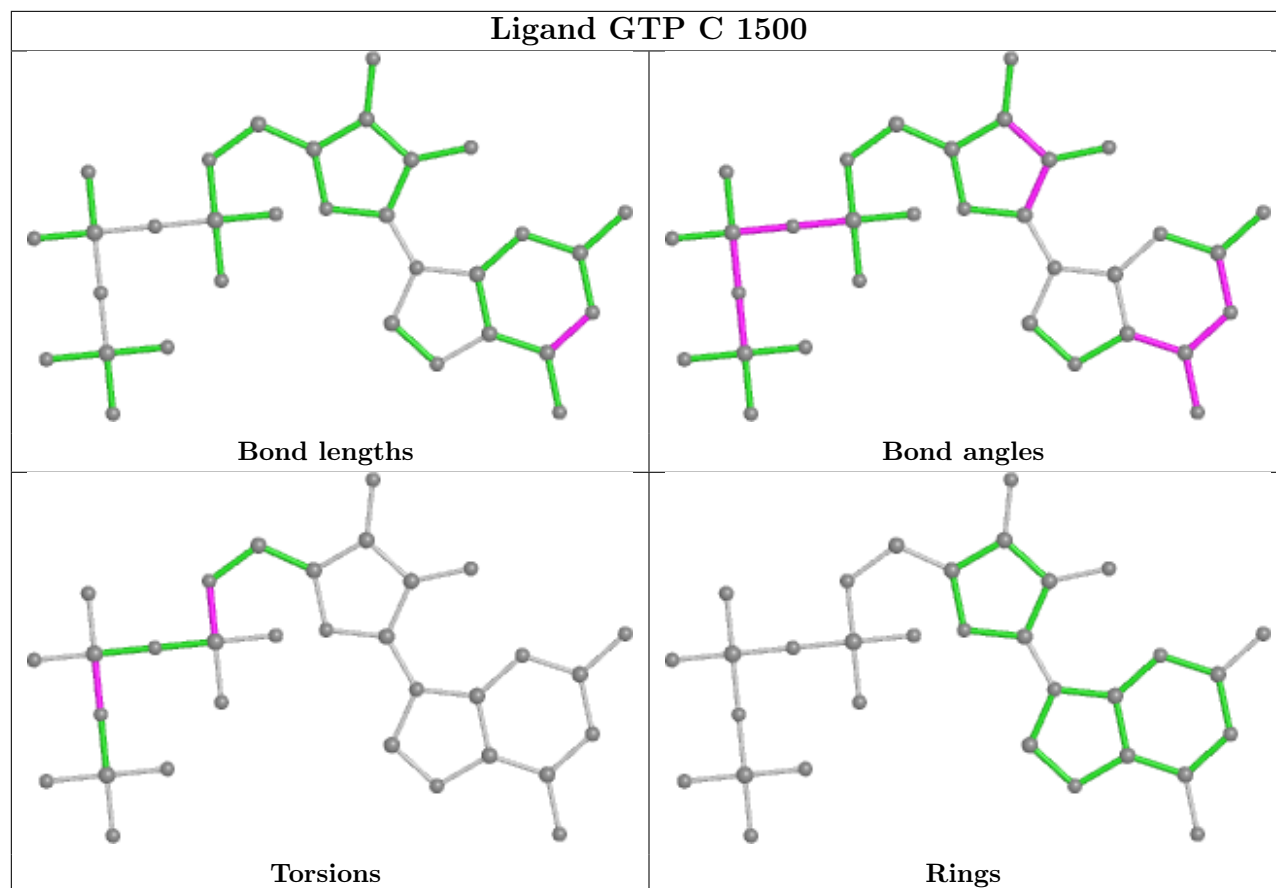
Continued from previous page...

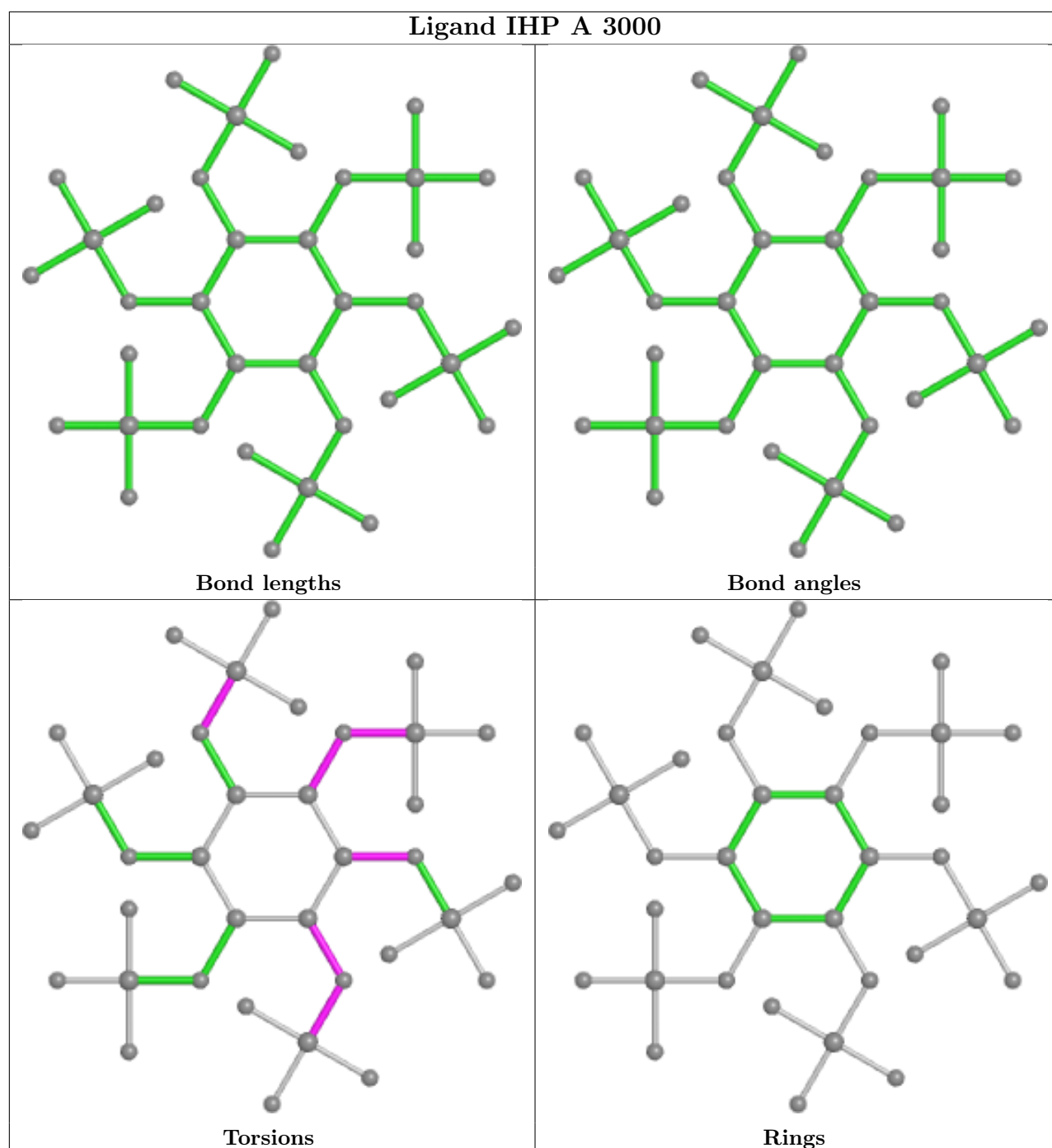
Mol	Chain	Res	Type	Atoms
35	A	3000	IHP	C5-C6-O16-P6
35	A	3000	IHP	C4-O14-P4-O24
36	C	1500	GTP	C5'-O5'-PA-O3A
36	C	1500	GTP	C5'-O5'-PA-O1A
36	C	1500	GTP	C5'-O5'-PA-O2A
35	A	3000	IHP	C4-C5-O15-P5
35	A	3000	IHP	C6-C5-O15-P5
35	A	3000	IHP	C3-C4-O14-P4
36	C	1500	GTP	PG-O3B-PB-O1B
35	A	3000	IHP	C6-O16-P6-O26
35	A	3000	IHP	C3-O13-P3-O33
35	A	3000	IHP	C4-O14-P4-O34
35	A	3000	IHP	C6-O16-P6-O36
35	A	3000	IHP	C6-O16-P6-O46
36	C	1500	GTP	PG-O3B-PB-O2B

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](#)

There are no chain breaks in this entry.

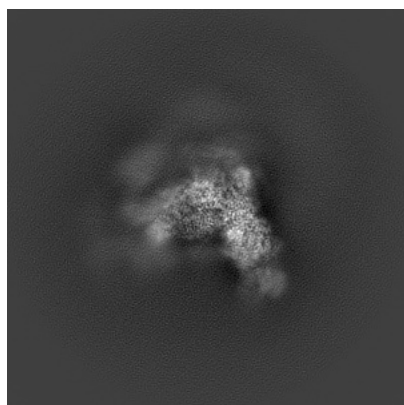
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6817. These allow visual inspection of the internal detail of the map and identification of artifacts.

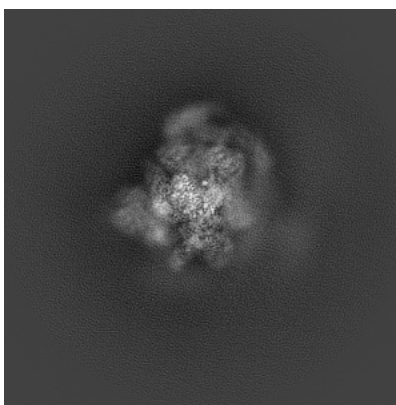
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

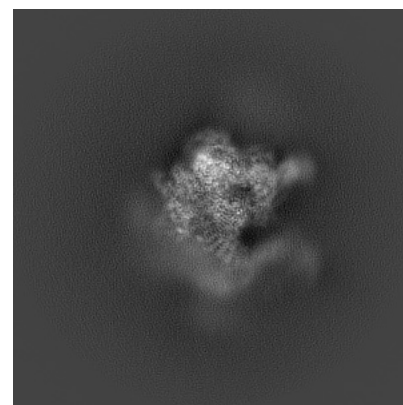
6.1.1 Primary map



X



Y

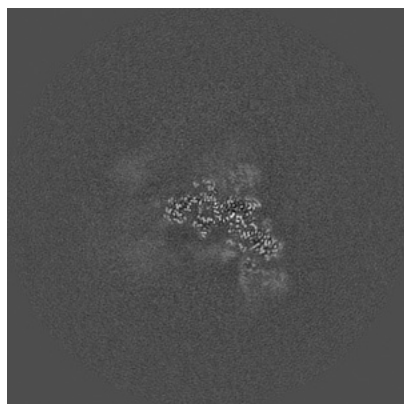


Z

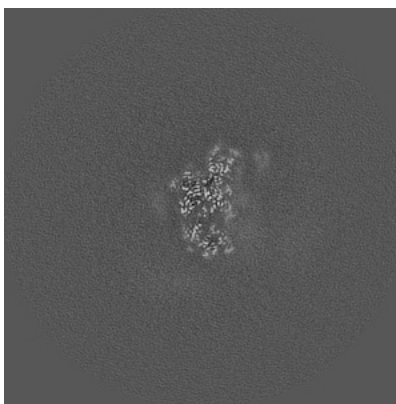
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

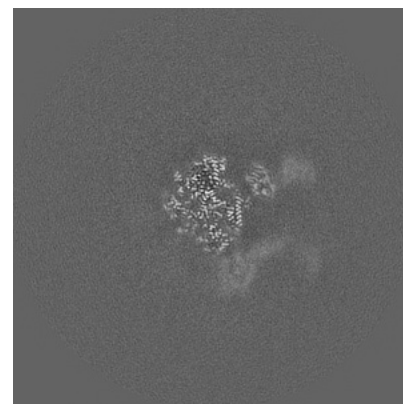
6.2.1 Primary map



X Index: 200



Y Index: 200

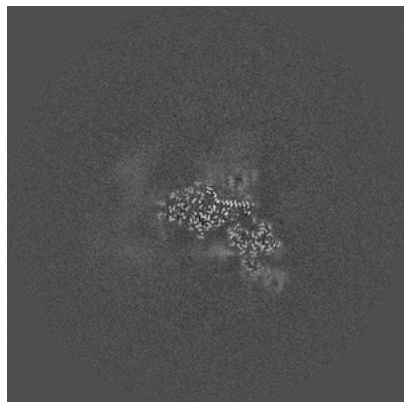


Z Index: 200

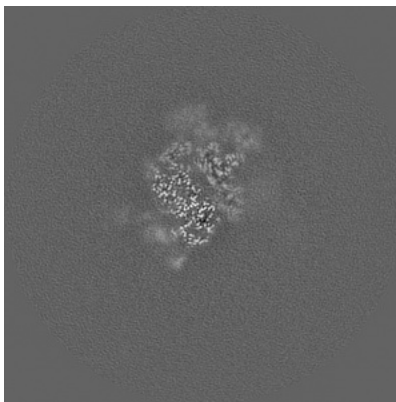
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

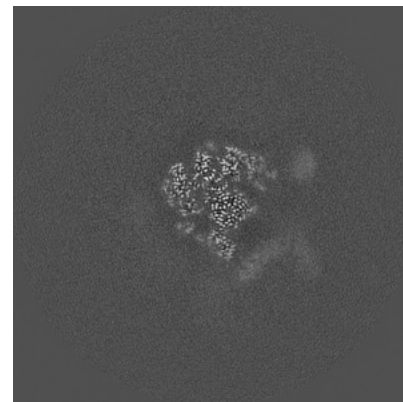
6.3.1 Primary map



X Index: 204



Y Index: 230

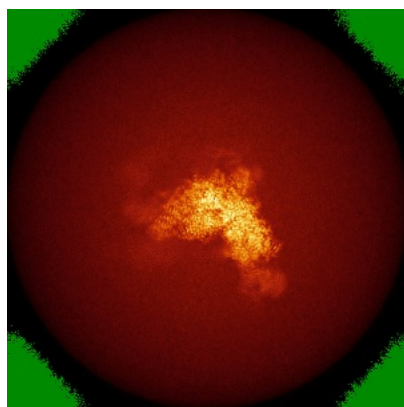


Z Index: 186

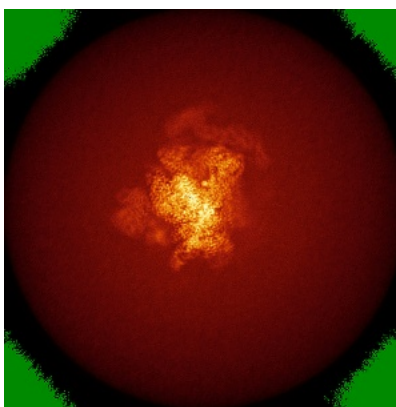
The images above show the largest variance slices of the map in three orthogonal directions.

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

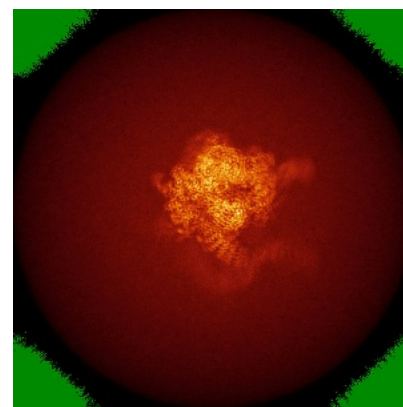
6.4.1 Primary map



X



Y

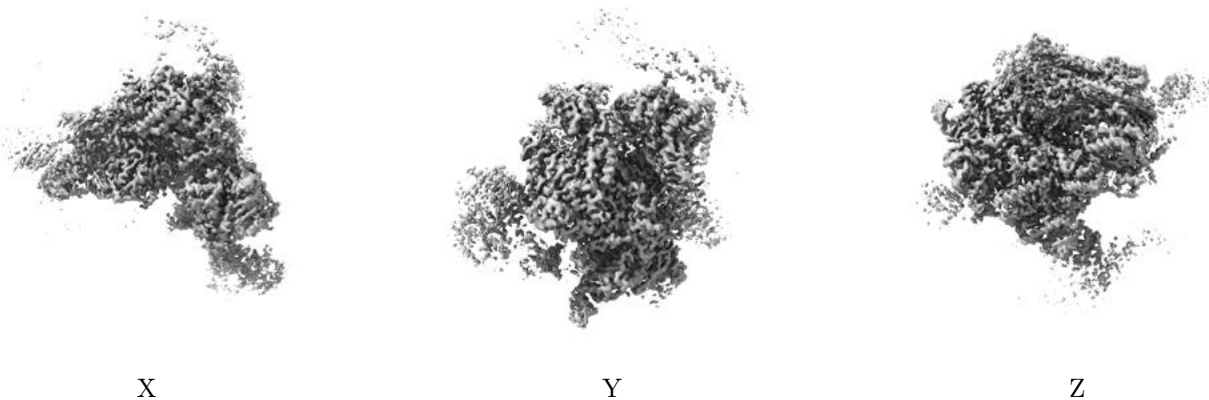


Z

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

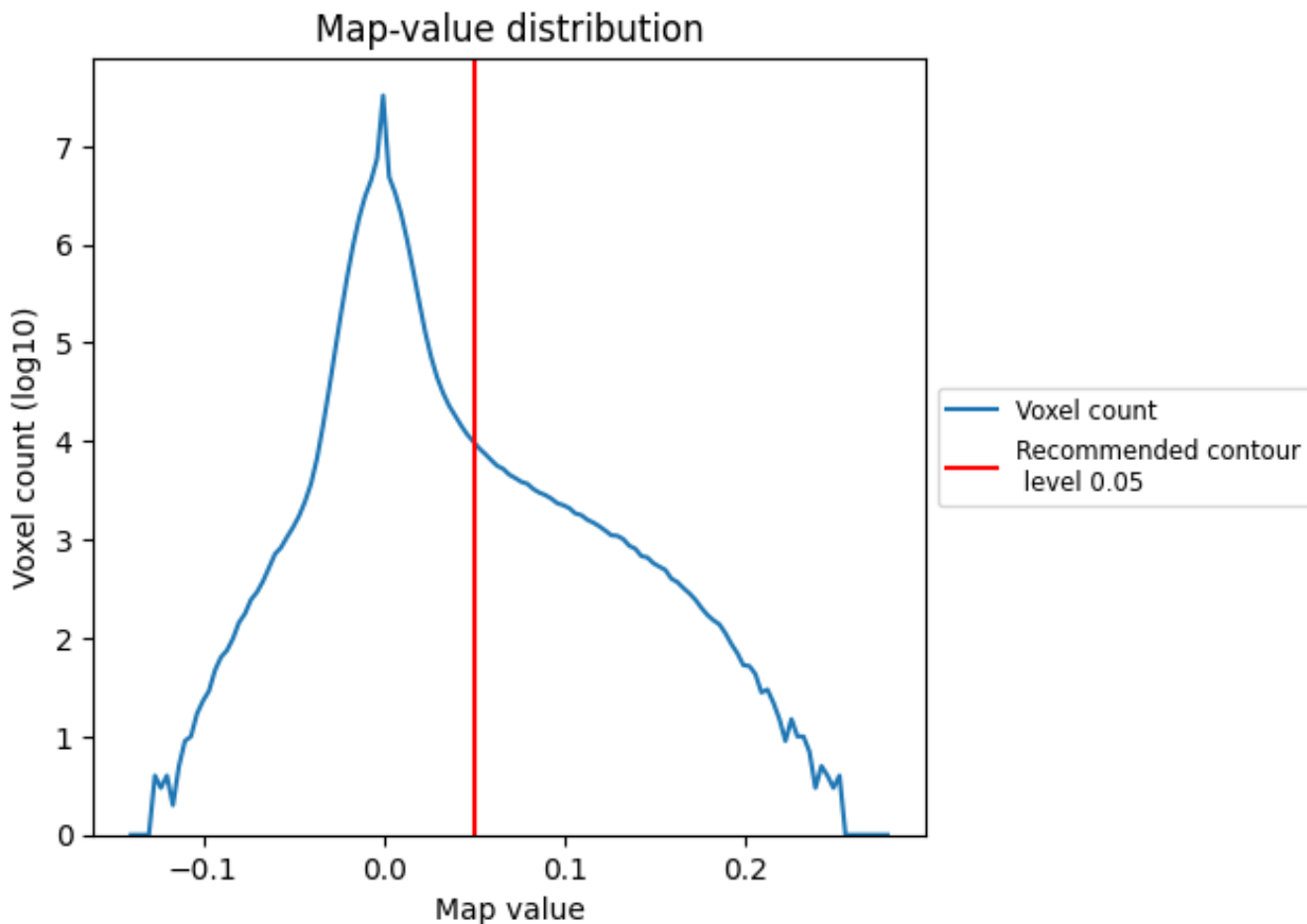
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

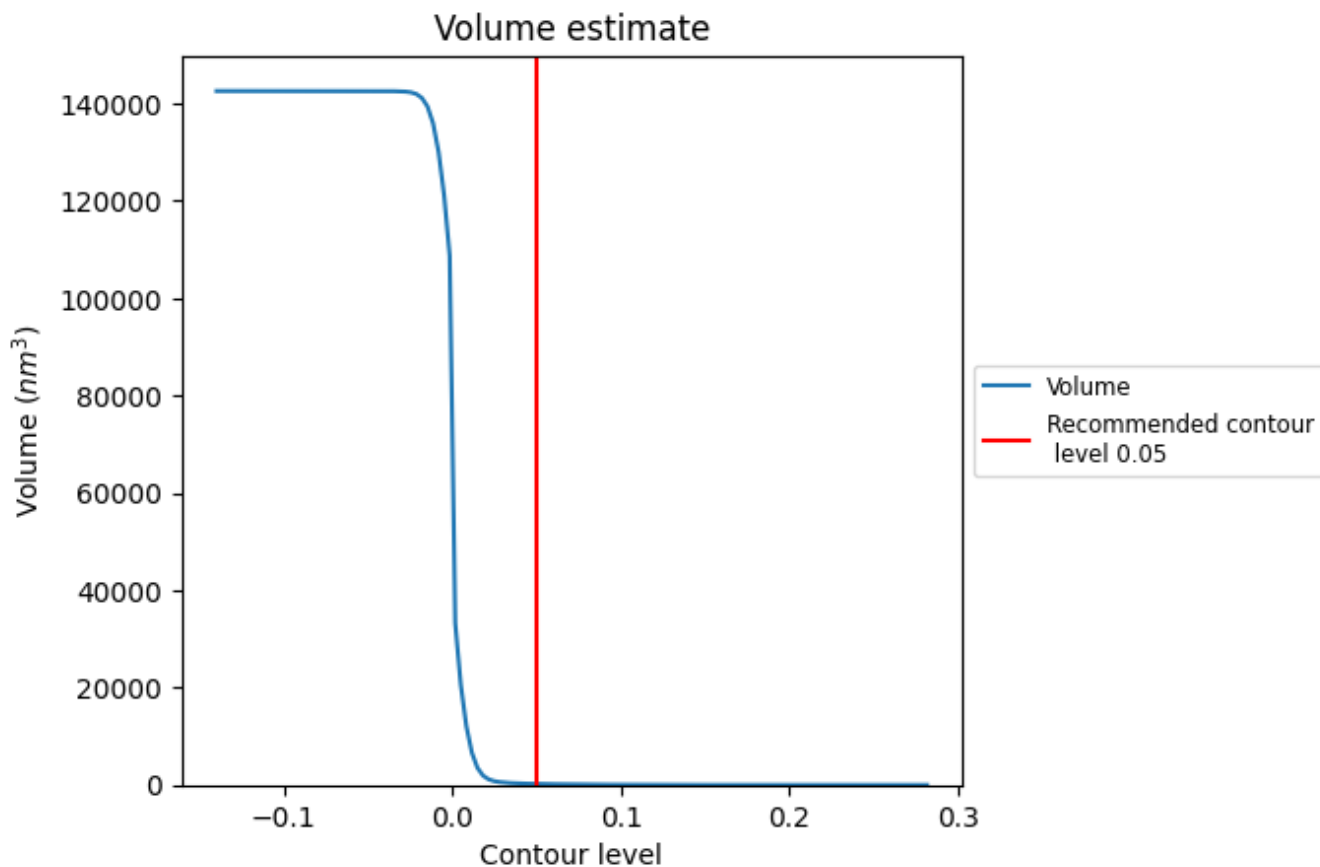
This section contains the results of statistical analysis of the map.

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.

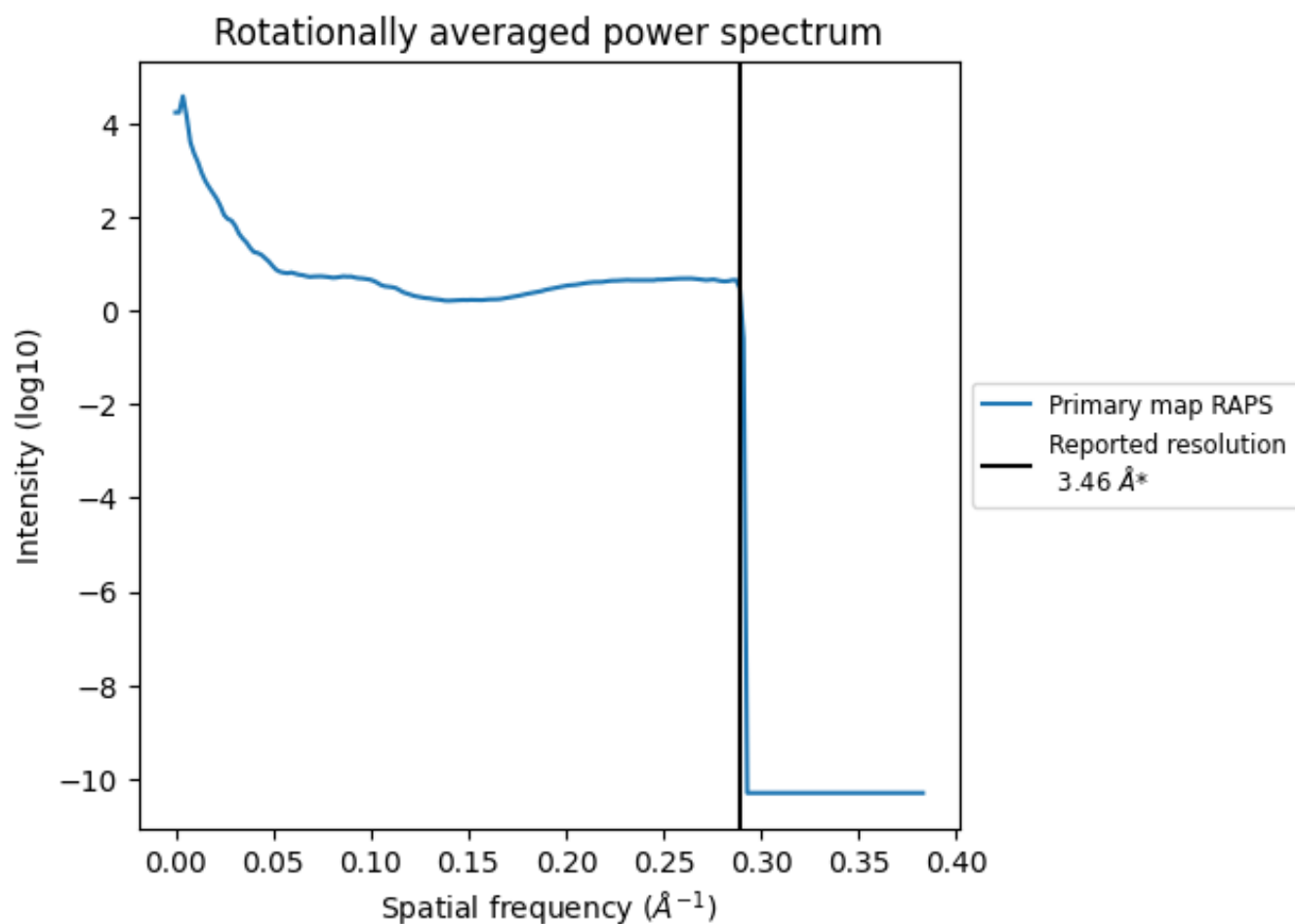
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm^3 ; this corresponds to an approximate mass of 193 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 0.289 Å⁻¹

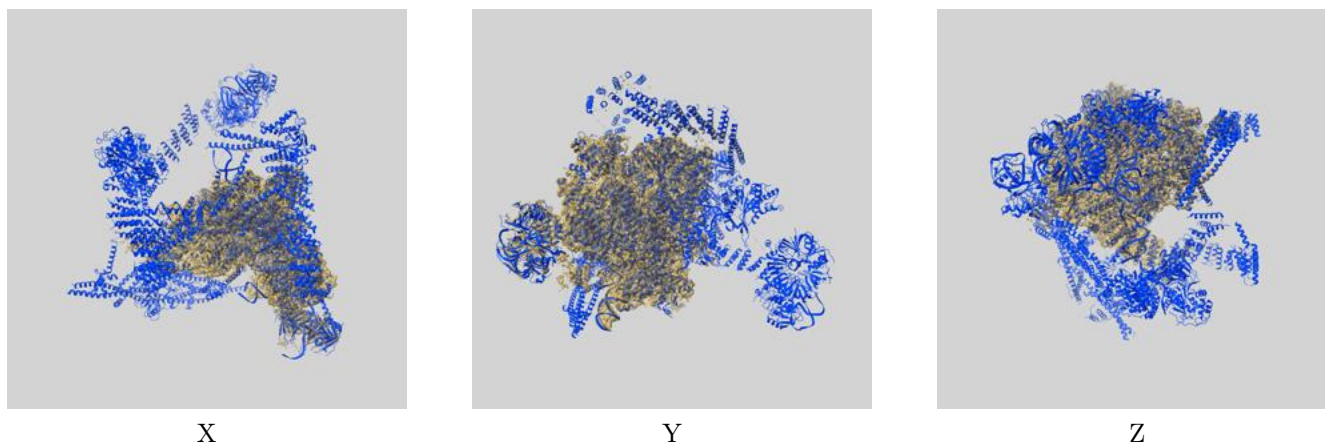
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

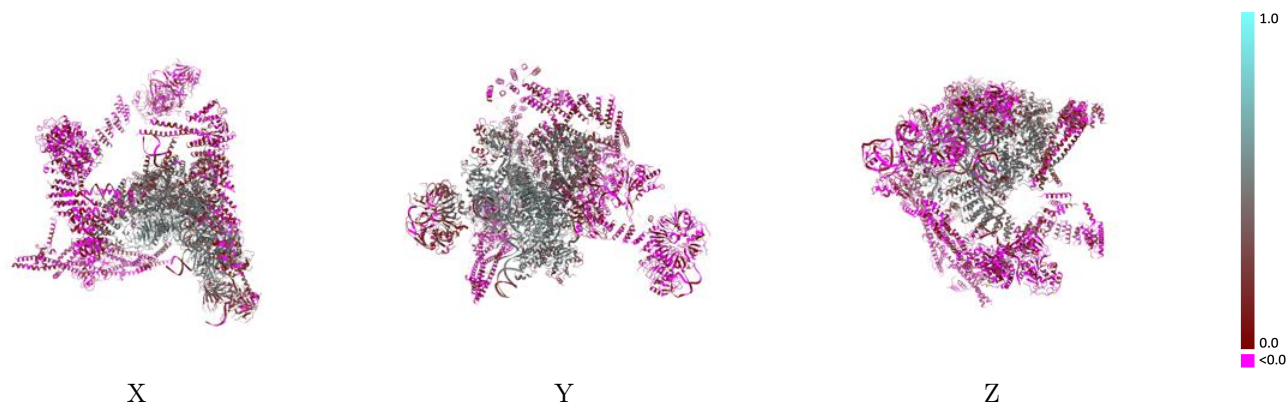
This section contains information regarding the fit between EMDB map EMD-6817 and PDB model 5Y88. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



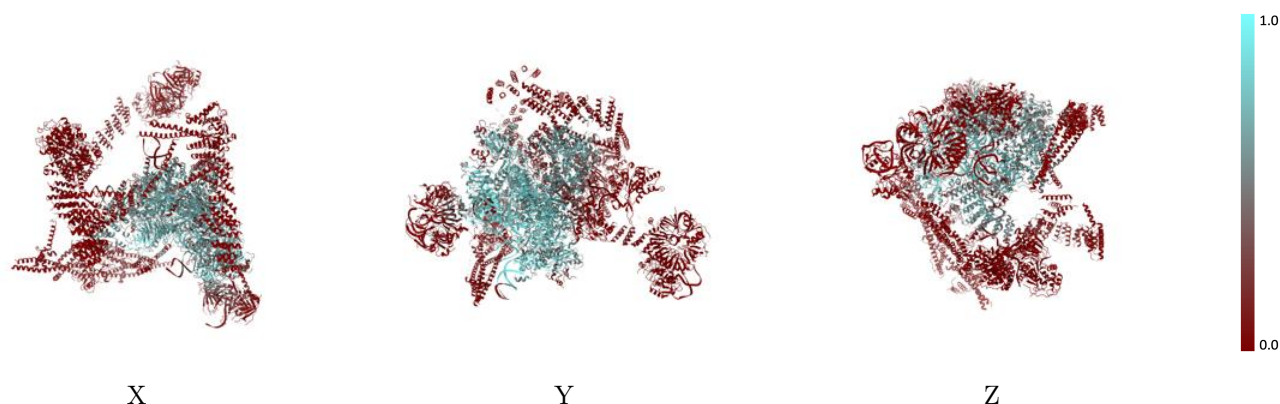
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



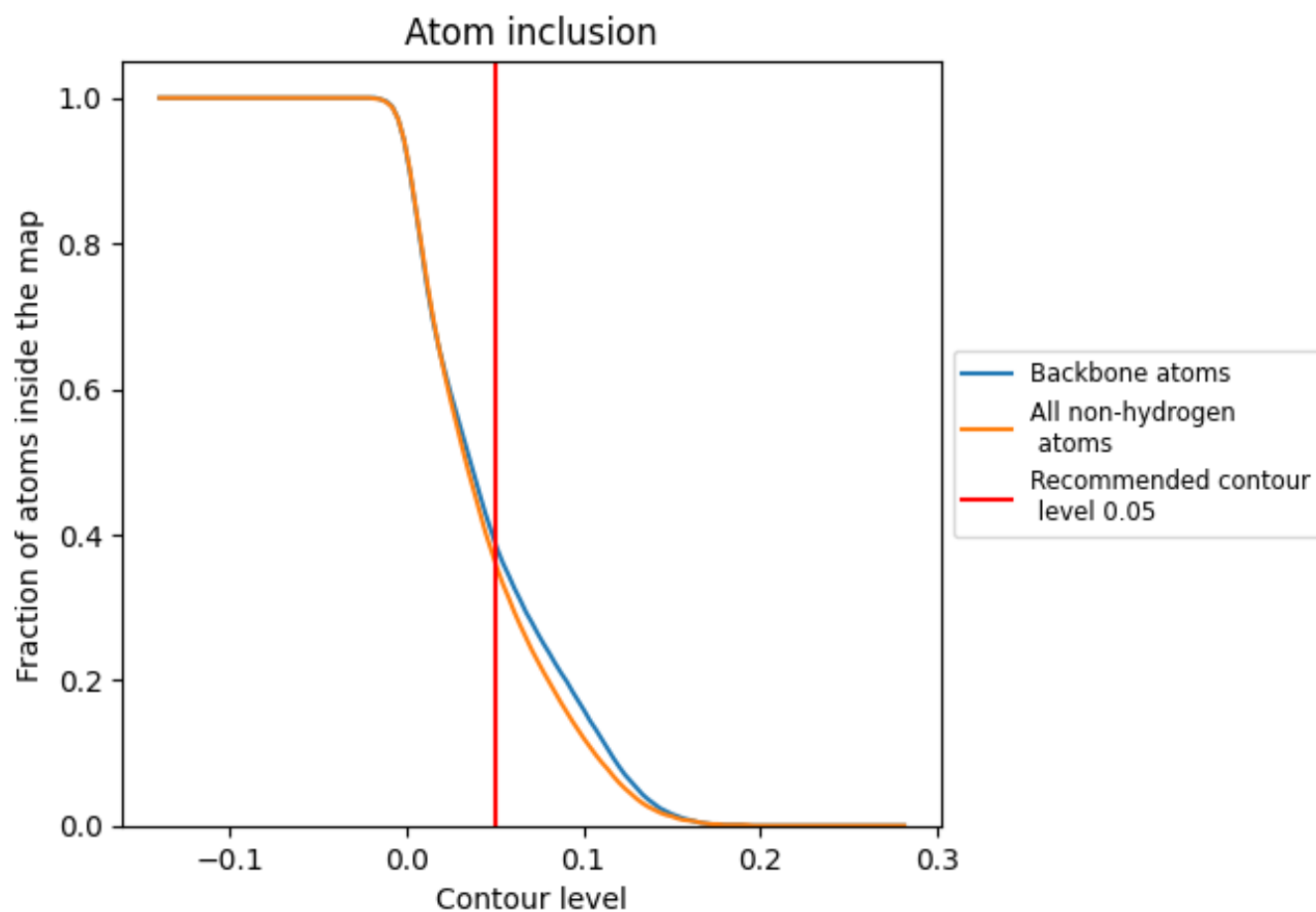
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 36% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3620	 0.2640
A	 0.4920	 0.3410
B	 0.6360	 0.3930
C	 0.6660	 0.4500
D	 0.7370	 0.4380
E	 0.2590	 0.1780
F	 0.1930	 0.1400
G	 0.0000	 0.0050
H	 0.0110	 0.0250
I	 0.3750	 0.2640
J	 0.2990	 0.2320
K	 0.3900	 0.3570
L	 0.7300	 0.4710
M	 0.5540	 0.4190
N	 0.6640	 0.4310
O	 0.7480	 0.5060
P	 0.4470	 0.4480
Q	 0.4960	 0.4030
R	 0.0920	 0.2520
S	 0.6430	 0.4470
T	 0.1840	 0.1710
U	 0.1330	 0.1710
V	 0.2630	 0.2790
W	 0.0000	 0.0080
a	 0.1670	 0.3050
b	 0.0380	 0.1550
c	 0.0370	 0.0920
d	 0.1570	 0.2530
e	 0.3560	 0.3730
f	 0.0770	 0.1570
g	 0.0500	 0.1510
h	 0.0000	 -0.0100
i	 0.0000	 -0.0110
j	 0.0000	 0.0030
k	 0.0000	 0.0180



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Chain	Atom inclusion	Q-score
l	0.0000	0.0080
m	0.0000	0.0270
n	0.0000	0.0050
o	0.0000	-0.0210
p	0.0000	0.0010
q	0.0000	0.0350
r	0.0000	-0.0090
s	0.0000	0.0000
t	0.0000	-0.0040
x	0.0000	-0.0440