



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 09:35 am BST

PDB ID : 6G90
EMDB ID : EMD-4364
Title : Prespliceosome structure provides insight into spliceosome assembly and regulation (map A2)
Authors : Plaschka, C.; Lin, P.-C.; Charenton, C.; Nagai, K.
Deposited on : 2018-04-10
Resolution : 4.00 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:

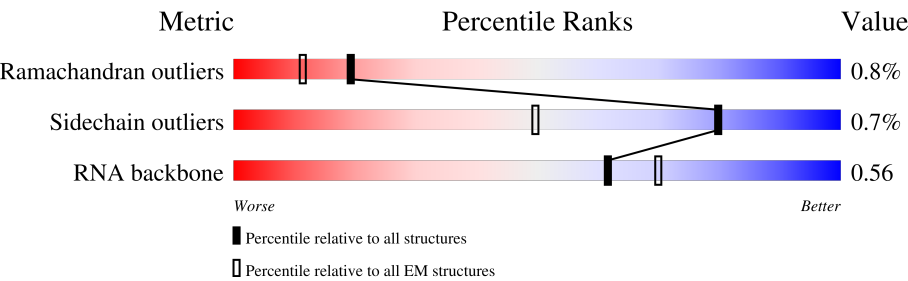
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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.






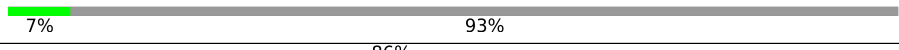



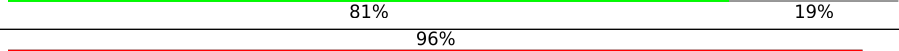
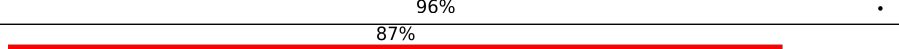



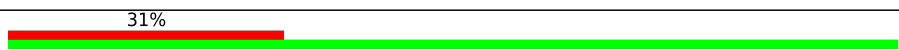

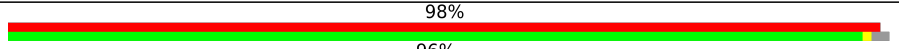






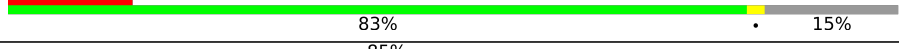

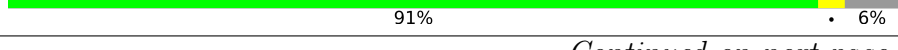

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	407	
2	2	143	
3	A	298	
4	B	300	
5	C	231	
6	D	629	
7	E	544	
8	F	523	

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Mol	Chain	Length	Quality of chain
9	G	492	
10	H	261	
11	I	38	
12	J	620	
13	O	971	
14	P	1361	
15	Q	435	
16	R	213	
17	S	107	
18	T	530	
19	U	266	
20	V	280	
21	W	238	
22	X	51	
23	Y	111	
24	Z	85	
25	b	196	
25	s	196	
26	d	101	
26	v	101	
27	e	94	
27	w	94	
28	f	86	
28	x	86	
29	g	77	

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Mol	Chain	Length	Quality of chain
29	y	77	
30	h	146	
30	t	146	
31	i	110	
31	u	110	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	327	Total	C	N	O	P	0	0
			6625	2951	1072	2275	327		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	143	Total	C	N	O	P	0	0
			3025	1352	513	1017	143		

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	99	Total	C	N	O	0	0
			492	294	99	99		

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	193	Total	C	N	O	S	0	0
			1450	929	261	258	2		

- Molecule 5 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	177	Total	C	N	O	S	0	0
			1323	832	246	240	5		

- Molecule 6 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	509	Total	C	N	O	S	0	0
			3462	2188	608	659	7		

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	541	Total	C	N	O	S	0	0
			4574	2996	723	836	19		

- Molecule 8 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	175	Total	C	N	O	S	0	0
			1337	840	232	255	10		

- Molecule 9 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	216	Total	C	N	O	S	0	0
			1684	1098	274	301	11		

- Molecule 10 is a protein called Protein LUC7,Protein LUC7,Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	158	Total	C	N	O	S	0	0
			1083	675	198	201	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	83	VAL	GLU	conflict	UNP Q07508
H	84	GLU	VAL	conflict	UNP Q07508

- Molecule 11 is a RNA chain called Yeast UBC4 pre-mRNA (mutant).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	38	Total	C	N	O	P	0	0
			789	355	132	264	38		

- Molecule 12 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	42	Total	C	N	O	0	0
			324	210	55	59		

- Molecule 13 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	833	Total	C	N	O	S	0	0
			6612	4258	1121	1192	41		

- Molecule 14 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	1186	Total	C	N	O	S	0	0
			9437	6034	1589	1763	51		

- Molecule 15 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	220	Total	C	N	O	S	0	0
			1786	1157	307	313	9		

- Molecule 16 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	173	Total	C	N	O	S	0	0
			1429	930	239	258	2		

- Molecule 17 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 18 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	462	Total	C	N	O	S	0	0
			3915	2487	677	735	16		

- Molecule 19 is a protein called Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	196	Total	C	N	O	S	0	0
			1489	934	258	291	6		

- Molecule 20 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	170	Total	C	N	O	S	0	0
			1383	866	253	257	7		

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	51	Total	C	N	O	0	0
			255	153	51	51		

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	84	Total	C	N	O	S	0	0
			683	439	119	122	3		

- Molecule 24 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	83	Total	C	N	O	S	0	0
			685	424	129	131	1		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	121	Total	C	N	O	S	0	0
			972	613	183	173	3		
25	s	65	Total	C	N	O	S	0	0
			518	331	91	93	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	93	Total	C	N	O	S	0	0
			714	453	125	133	3		
26	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	77	Total	C	N	O	S	0	0
			600	395	96	106	3		
27	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
28	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	72	Total	C	N	O	S	0	0
			556	352	97	105	2		
29	y	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	107	Total	C	N	O	S	0	0
			834	525	149	157	3		
30	t	72	Total	C	N	O	S	0	0
			569	364	99	104	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	99	Total	C	N	O	S	0	0
			805	514	148	139	4		


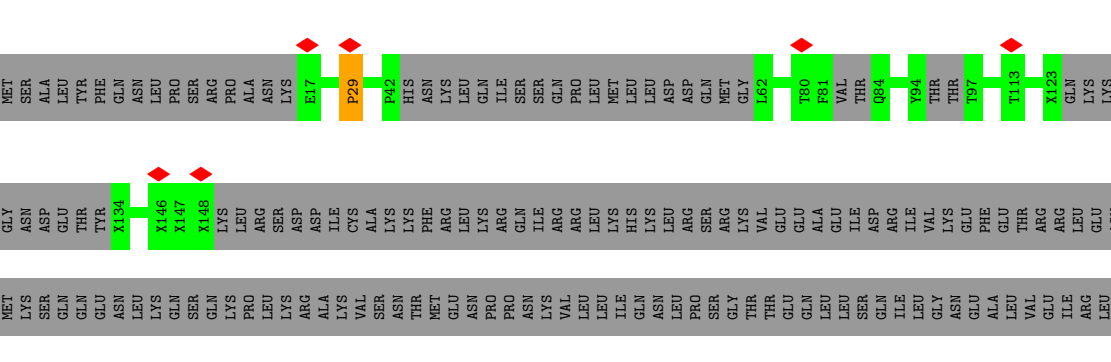
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Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

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

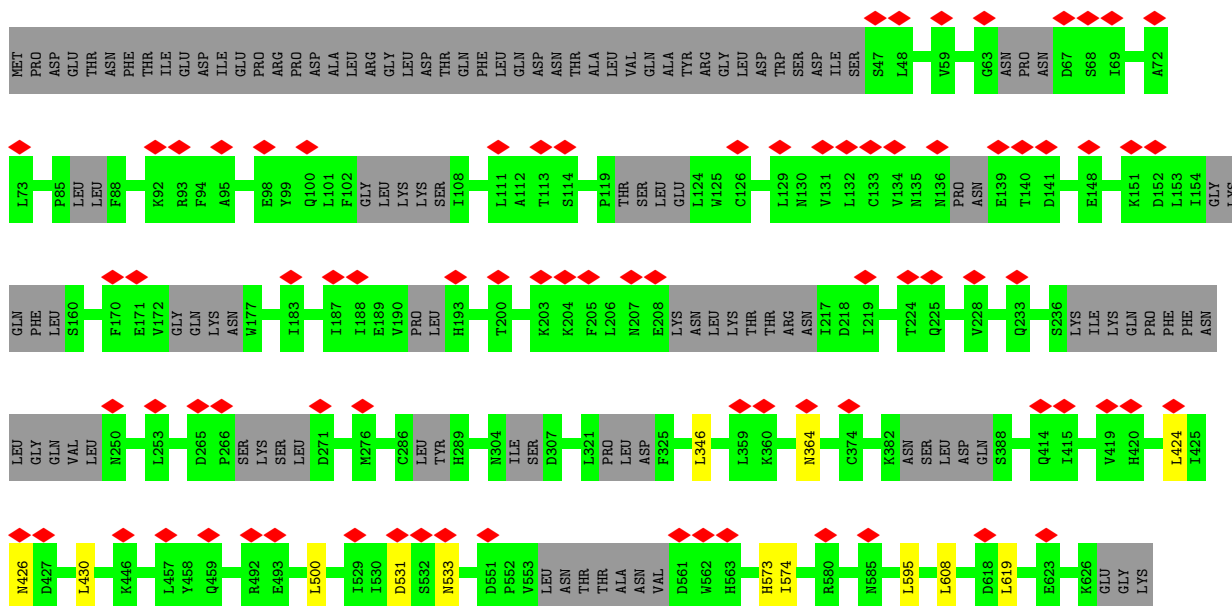
Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total	Zn	0
			1	1	
32	H	2	Total	Zn	0
			2	2	
32	S	3	Total	Zn	0
			3	3	
32	T	2	Total	Zn	0
			2	2	
32	U	1	Total	Zn	0
			1	1	

- Chain A:  33% 67%
- 
- | Position | Amino Acid | Frequency (approx.) |
|----------|------------|---------------------|
| 1 | GLY | 0.25 |
| 2 | ASP | 0.25 |
| 3 | ASN | 0.25 |
| 4 | ASP | 0.25 |
| 5 | GLN | 0.25 |
| 6 | THR | 0.25 |
| 7 | THR | 0.25 |
| 8 | TYR | 0.25 |
| 9 | PHE | 0.25 |
| 10 | GLN | 0.25 |
| 11 | ASN | 0.25 |
| 12 | LEU | 0.25 |
| 13 | LEU | 0.25 |
| 14 | PRO | 0.25 |
| 15 | ARG | 0.25 |
| 16 | LYS | 0.25 |
| 17 | E17 | 0.25 |
| 18 | LYS | 0.25 |
| 19 | P29 | 0.25 |
| 20 | CYS | 0.25 |
| 21 | ILE | 0.25 |
| 22 | ASP | 0.25 |
| 23 | P42 | 0.25 |
| 24 | LYS | 0.25 |
| 25 | ASN | 0.25 |
| 26 | ASN | 0.25 |
| 27 | LEU | 0.25 |
| 28 | LEU | 0.25 |
| 29 | GLN | 0.25 |
| 30 | ILE | 0.25 |
| 31 | GLN | 0.25 |
| 32 | SER | 0.25 |
| 33 | SER | 0.25 |
| 34 | GLN | 0.25 |
| 35 | PRO | 0.25 |
| 36 | LEU | 0.25 |
| 37 | LEU | 0.25 |
| 38 | MET | 0.25 |
| 39 | LEU | 0.25 |
| 40 | LEU | 0.25 |
| 41 | LEU | 0.25 |
| 42 | ASP | 0.25 |
| 43 | ASP | 0.25 |
| 44 | GLN | 0.25 |
| 45 | MET | 0.25 |
| 46 | GLY | 0.25 |
| 47 | L62 | 0.25 |
| 48 | VAL | 0.25 |
| 49 | GLU | 0.25 |
| 50 | GLU | 0.25 |
| 51 | ALA | 0.25 |
| 52 | VAL | 0.25 |
| 53 | THR | 0.25 |
| 54 | THR | 0.25 |
| 55 | THR | 0.25 |
| 56 | THR | 0.25 |
| 57 | THR | 0.25 |
| 58 | THR | 0.25 |
| 59 | THR | 0.25 |
| 60 | THR | 0.25 |
| 61 | THR | 0.25 |
| 62 | THR | 0.25 |
| 63 | THR | 0.25 |
| 64 | THR | 0.25 |
| 65 | THR | 0.25 |
| 66 | THR | 0.25 |
| 67 | THR | 0.25 |
| 68 | THR | 0.25 |
| 69 | THR | 0.25 |
| 70 | THR | 0.25 |
| 71 | THR | 0.25 |
| 72 | THR | 0.25 |
| 73 | THR | 0.25 |
| 74 | THR | 0.25 |
| 75 | THR | 0.25 |
| 76 | THR | 0.25 |
| 77 | THR | 0.25 |
| 78 | T80 | 0.25 |
| 79 | F81 | 0.25 |
| 80 | VAL | 0.25 |
| 81 | THR | 0.25 |
| 82 | THR | 0.25 |
| 83 | THR | 0.25 |
| 84 | THR | 0.25 |
| 85 | THR | 0.25 |
| 86 | THR | 0.25 |
| 87 | THR | 0.25 |
| 88 | THR | 0.25 |
| 89 | THR | 0.25 |
| 90 | THR | 0.25 |
| 91 | THR | 0.25 |
| 92 | THR | 0.25 |
| 93 | THR | 0.25 |
| 94 | T94 | 0.25 |
| 95 | THR | 0.25 |
| 96 | THR | 0.25 |
| 97 | THR | 0.25 |
| 98 | THR | 0.25 |
| 99 | THR | 0.25 |
| 100 | THR | 0.25 |
| 101 | T113 | 0.25 |
| 102 | THR | 0.25 |
| 103 | THR | 0.25 |
| 104 | THR | 0.25 |
| 105 | THR | 0.25 |
| 106 | THR | 0.25 |
| 107 | THR | 0.25 |
| 108 | THR | 0.25 |
| 109 | THR | 0.25 |
| 110 | THR | 0.25 |
| 111 | THR | 0.25 |
| 112 | THR | 0.25 |
| 113 | T113 | 0.25 |
| 114 | THR | 0.25 |
| 115 | THR | 0.25 |
| 116 | THR | 0.25 |
| 117 | THR | 0.25 |
| 118 | THR | 0.25 |
| 119 | THR | 0.25 |
| 120 | THR | 0.25 |
| 121 | THR | 0.25 |
| 122 | THR | 0.25 |
| 123 | X123 | 0.25 |
| 124 | GLN | 0.25 |
| 125 | LYS | 0.25 |
| 126 | LYS | 0.25 |
| 127 | LYS | 0.25 |
| 128 | LYS | 0.25 |
| 129 | LYS | 0.25 |
| 130 | LYS | 0.25 |
| 131 | LYS | 0.25 |
| 132 | LYS | 0.25 |
| 133 | LYS | 0.25 |
| 134 | LYS | 0.25 |
| 135 | LYS | 0.25 |
| 136 | LYS | 0.25 |
| 137 | LYS | 0.25 |
| 138 | LYS | 0.25 |
| 139 | LYS | 0.25 |
| 140 | LYS | 0.25 |
| 141 | LYS | 0.25 |
| 142 | LYS | 0.25 |
| 143 | LYS | 0.25 |
| 144 | LYS | 0.25 |
| 145 | LYS | 0.25 |
| 146 | LYS | |

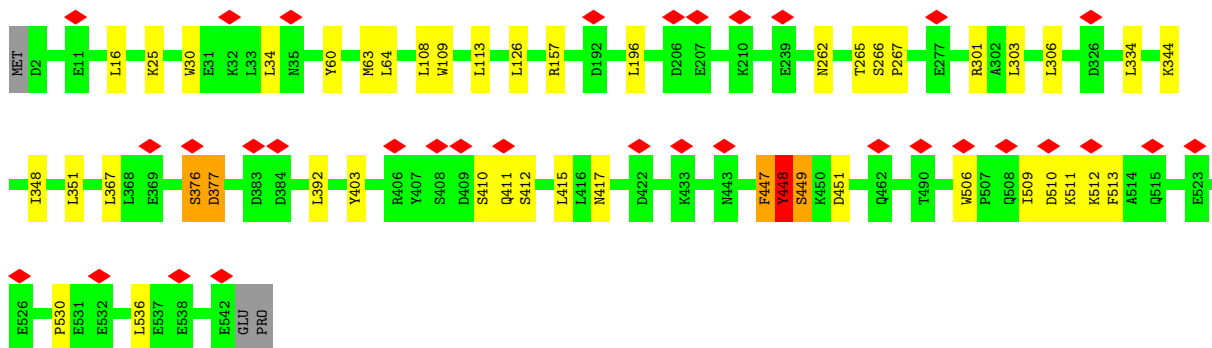
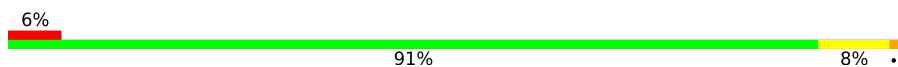
- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 128. A bar at the top indicates the percentage of positions with conservation: 38% (red), 62% (green), and 36% (grey).
- Conserved positions (bits > 0.05):
- Position 1: MET (0.18 bits)
 - Position 2: ASN (0.18 bits)
 - Position 3: TYR (0.18 bits)
 - Position 4: ASN (0.18 bits)
 - Position 5: L5 (0.18 bits)
 - Position 6: S6 (0.18 bits)
 - Position 7: K7 (0.18 bits)
 - Position 8: D10 (0.18 bits)
 - Position 9: S13 (0.18 bits)
 - Position 10: R14 (0.18 bits)
 - Position 11: K17 (0.18 bits)
 - Position 12: P18 (0.18 bits)
 - Position 13: R19 (0.18 bits)
 - Position 14: D29 (0.18 bits)
 - Position 15: N38 (0.18 bits)
 - Position 16: G43 (0.18 bits)
 - Position 17: V44 (0.18 bits)
 - Position 18: Y55 (0.18 bits)
 - Position 19: MET (0.18 bits)
 - Position 20: GLU (0.18 bits)
 - Position 21: Y58 (0.18 bits)
 - Position 22: X82 (0.18 bits)
 - Position 23: X83 (0.18 bits)
 - Position 24: X84 (0.18 bits)
 - Position 25: X85 (0.18 bits)
 - Position 26: X86 (0.18 bits)
 - Position 27: X87 (0.18 bits)
 - Position 28: X88 (0.18 bits)
 - Position 29: LEU (0.18 bits)
 - Position 30: GLN (0.18 bits)
 - Position 31: ASN (0.18 bits)
 - Position 32: TRP (0.18 bits)
 - Position 33: ASN (0.18 bits)
 - Position 34: P94 (0.18 bits)
 - Position 35: N95 (0.18 bits)
 - Position 36: V96 (0.18 bits)
 - Position 37: D97 (0.18 bits)
 - Position 38: P98 (0.18 bits)
 - Position 39: H99 (0.18 bits)
 - Position 40: I100 (0.18 bits)
 - Position 41: K101 (0.18 bits)
 - Position 42: D102 (0.18 bits)
 - Position 43: T103 (0.18 bits)
 - Position 44: D104 (0.18 bits)
 - Position 45: P105 (0.18 bits)
 - Position 46: Y106 (0.18 bits)
 - Position 47: T107 (0.18 bits)
 - Position 48: T108 (0.18 bits)
 - Position 49: I109 (0.18 bits)
 - Position 50: F110 (0.18 bits)
 - Position 51: I111 (0.18 bits)
 - Position 52: G112 (0.18 bits)
 - Position 53: R113 (0.18 bits)
 - Position 54: L114 (0.18 bits)
 - Position 55: P115 (0.18 bits)
 - Position 56: Y116 (0.18 bits)
 - Position 57: D117 (0.18 bits)
 - Position 58: L118 (0.18 bits)
 - Position 59: D119 (0.18 bits)
 - Position 60: E120 (0.18 bits)
 - Position 61: I121 (0.18 bits)
 - Position 62: E122 (0.18 bits)
 - Position 63: Q123 (0.18 bits)
 - Position 64: Q124 (0.18 bits)
 - Position 65: K125 (0.18 bits)
 - Position 66: Y126 (0.18 bits)
 - Position 67: F127 (0.18 bits)
 - Position 68: V128 (0.18 bits)
 - Position 69: K129 (0.18 bits)
 - Position 70: F130 (0.18 bits)
 - Position 71: G131 (0.18 bits)
 - Position 72: E132 (0.18 bits)
 - Position 73: I133 (0.18 bits)
 - Position 74: E134 (0.18 bits)
 - Position 75: K135 (0.18 bits)
 - Position 76: I136 (0.18 bits)
 - Position 77: R137 (0.18 bits)
 - Position 78: V138 (0.18 bits)
 - Position 79: V139 (0.18 bits)
 - Position 80: K140 (0.18 bits)
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 - Position 87: S147 (0.18 bits)
 - Position 88: K148 (0.18 bits)
 - Position 89: G149 (0.18 bits)
 - Position 90: Y150 (0.18 bits)
 - Position 91: I153 (0.18 bits)
 - Position 92: V154 (0.18 bits)
 - Position 93: F155 (0.18 bits)
 - Position 94: K156 (0.18 bits)
 - Position 95: D157 (0.18 bits)
 - Position 96: P158 (0.18 bits)
 - Position 97: I159 (0.18 bits)
 - Position 98: S160 (0.18 bits)
 - Position 99: S161 (0.18 bits)
 - Position 100: K162 (0.18 bits)
 - Position 101: M163 (0.18 bits)
 - Position 102: A164 (0.18 bits)
 - Position 103: F165 (0.18 bits)
 - Position 104: K166 (0.18 bits)
 - Position 105: E167 (0.18 bits)
 - Position 106: I168 (0.18 bits)
 - Position 107: G169 (0.18 bits)
 - Position 108: V170 (0.18 bits)
 - Position 109: H171 (0.18 bits)
 - Position 110: G172 (0.18 bits)
 - Position 111: R173 (0.18 bits)
 - Position 112: I174 (0.18 bits)
 - Position 113: Q175 (0.18 bits)
 - Position 114: K177 (0.18 bits)
 - Position 115: D178 (0.18 bits)
 - Position 116: R179 (0.18 bits)
 - Position 117: I180 (0.18 bits)
 - Position 118: C181 (0.18 bits)
 - Position 119: I182 (0.18 bits)
 - Position 120: V183 (0.18 bits)
 - Position 121: D184 (0.18 bits)
 - Position 122: I185 (0.18 bits)
 - Position 123: E186 (0.18 bits)
 - Position 124: R187 (0.18 bits)
 - Position 125: G188 (0.18 bits)
 - Position 126: R189 (0.18 bits)
 - Position 127: T190 (0.18 bits)
 - Position 128: V191 (0.18 bits)
 - Position 129: K192 (0.18 bits)
 - Position 130: F194 (0.18 bits)
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 - Position 132: K195 (0.18 bits)
 - Position 133: P196 (0.18 bits)
 - Position 134: R197 (0.18 bits)
 - Position 135: R198 (0.18 bits)
 - Position 136: L199 (0.18 bits)
 - Position 137: G200 (0.18 bits)
 - Position 138: L203 (0.18 bits)
 - Position 139: G204 (0.18 bits)
 - Position 140: GLY (0.18 bits)
 - Position 141: ARG (0.18 bits)
 - Position 142: GLY (0.18 bits)
 - Position 143: THR (0.18 bits)
 - Position 144: VAL (0.18 bits)
 - Position 145: THR (0.18 bits)
 - Position 146: SER (0.18 bits)
 - Position 147: THR (0.18 bits)
 - Position 148: VAL (0.18 bits)
 - Position 149: ASP (0.18 bits)
 - Position 150: LYS (0.18 bits)
 - Position 151: SER (0.18 bits)
 - Position 152: ARG (0.18 bits)
 - Position 153: ASN (0.18 bits)
 - Position 154: PRO (0.18 bits)
 - Position 155: GLY (0.18 bits)
 - Position 156: ARG (0.18 bits)
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 - Position 158: ALA (0.18 bits)
 - Position 159: SER (0.18 bits)
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 - Position 161: SER (0.18 bits)
 - Position 162: GLN (0.18 bits)
 - Position 163: PRO (0.18 bits)
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 - Position 166: THR (0.18 bits)
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 - Position 170: PRO (0.18 bits)
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 - Position 172: GLU (0.18 bits)
 - Position 173: ALA (0.18 bits)
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 - Position 175: ASP (0.18 bits)
 - Position 176: ASP (0.18 bits)
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 - Position 179: THR (0.18 bits)
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 - Position 189: THR (0.18 bits)
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 - Position 193: THR (0.18 bits)
 - Position 194: ARG (0.18 bits)
 - Position 195: GLY (0.18 bits)
 - Position 196: ASN (0.18 bits)
 - Position 197: ARG (0.18 bits)
 - Position 198: PRO (0.18 bits)
 - Position 199: LEU (0.18 bits)
 - Position 200: LEU (0.18 bits)
 - Position 201: SER (0.18 bits)
 - Position 202: ALA (0.

- Chain C: 
- 

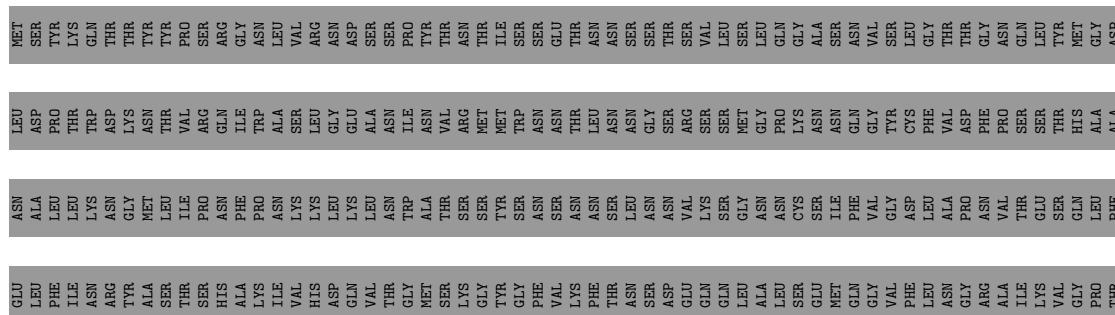
Chain D:

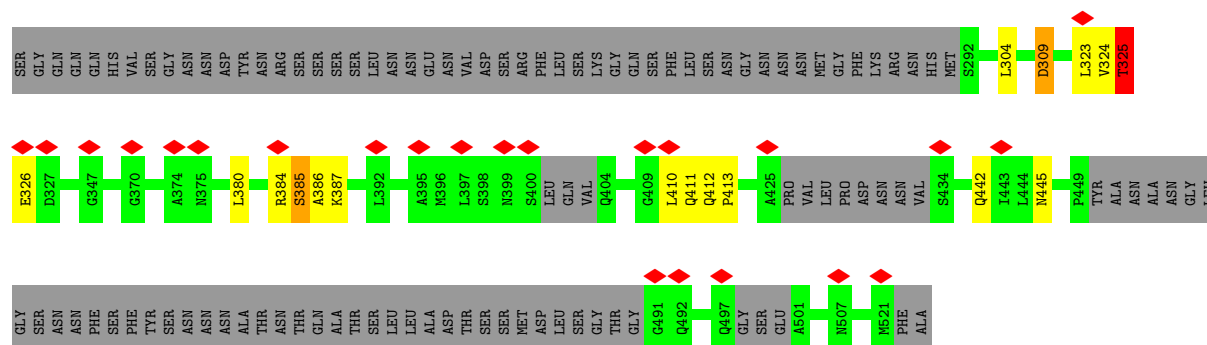


Chain E:



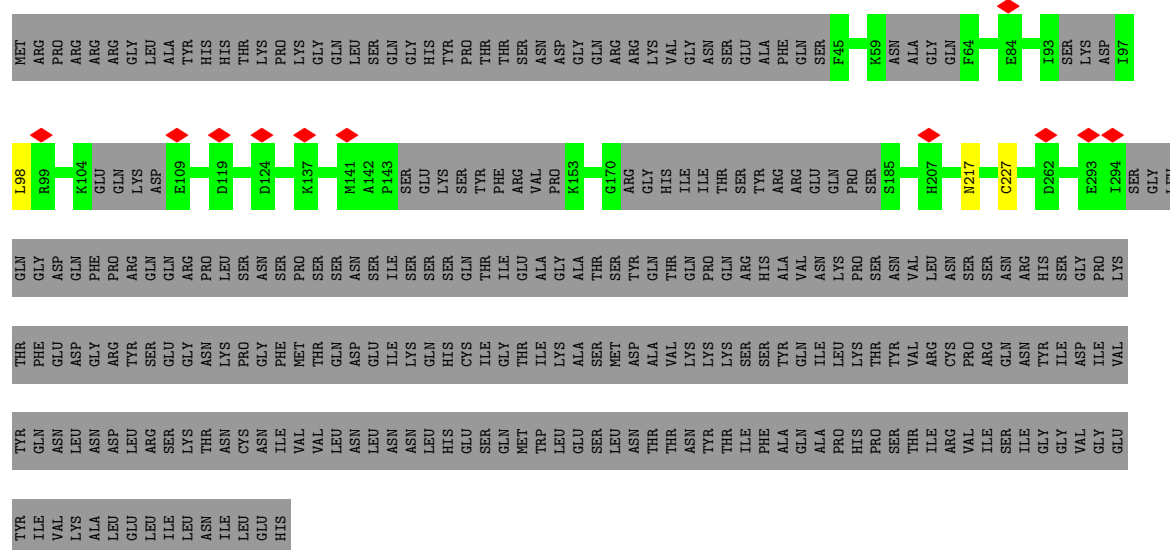
Chain F:





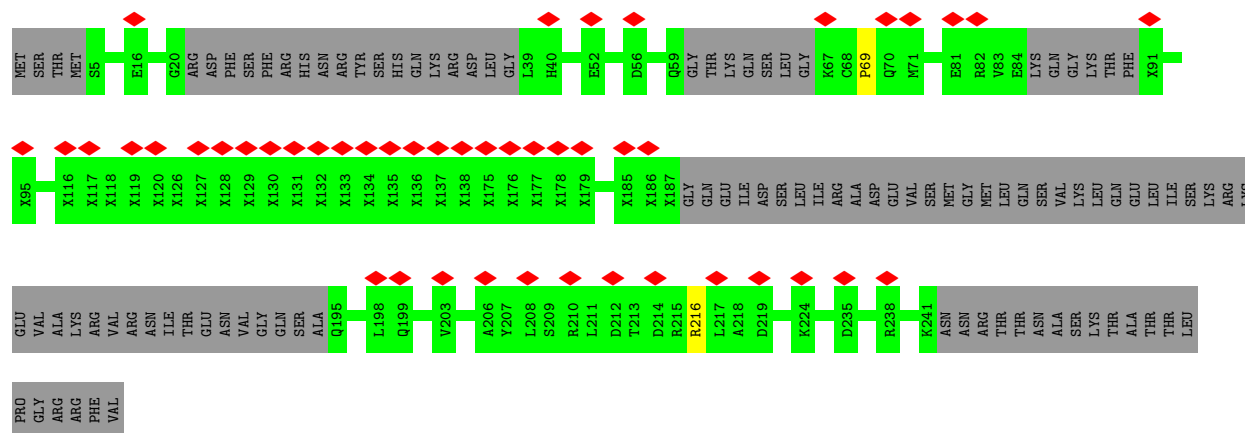
- Molecule 9: 56 kDa U1 small nuclear ribonucleoprotein component

Chain G: 43% 56%



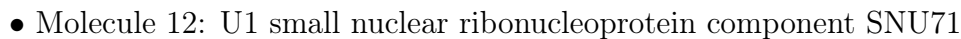
- Molecule 10: Protein LUC7,Protein LUC7,Protein LUC7

Chain H: 18% 60% 39%



- Molecule 11: Yeast UBC4 pre-mRNA (mutant)

Chain I:



Chain J:

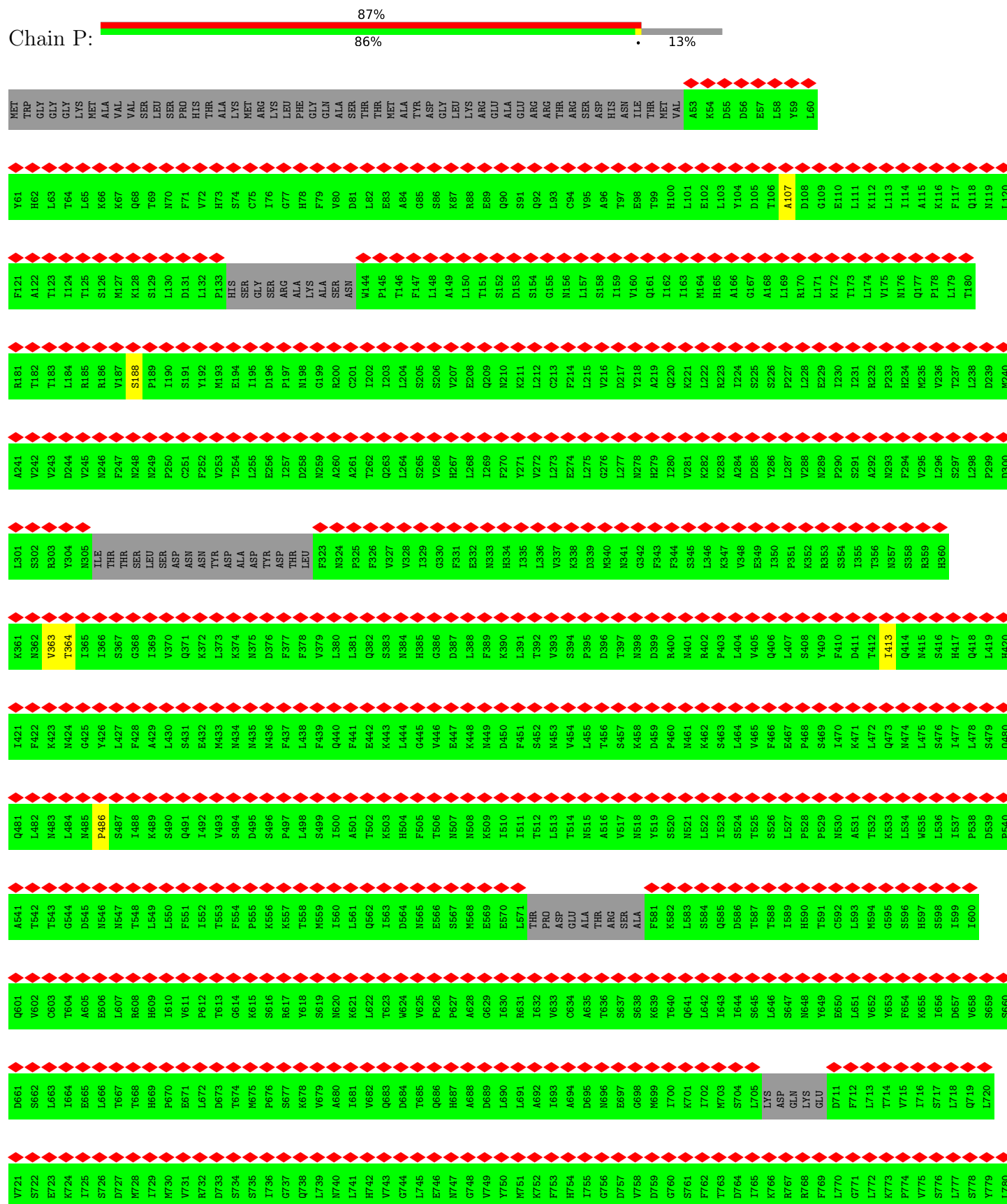
- Molecule 13: U2 snRNP component HSH155

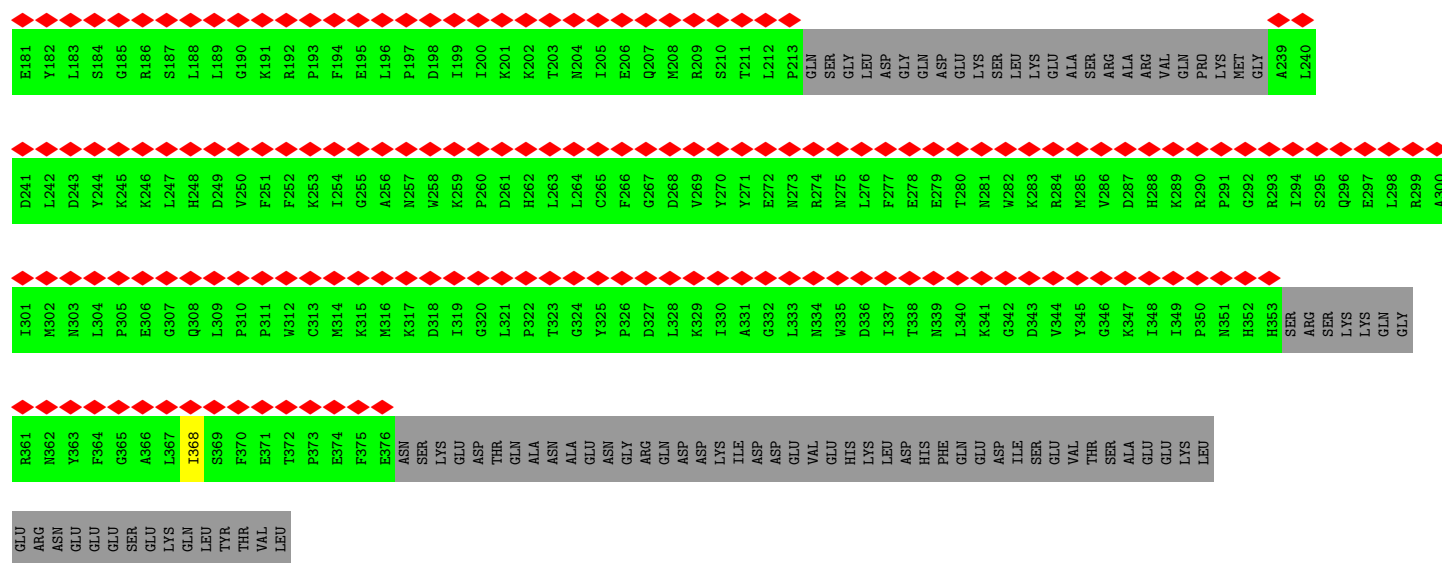
Chain 0

R181	H241	A301	D361	S421	P481	V541	I601	S661	P721	T781	L841	E901
R182	K242	A302	C362	M422	E482	T542	V602	T662	K722	A782	L842	G902
T183	K243	V303	L363	I423	F483	R543	S603	L663	E723	V783	E843	L903
S184	L244	V304	M364	P424	F484	T544	T604	N664	W724	A784	D844	E904
M185	V245	A305	D365	L425	K485	V545	L605	A665	W725	T785	A845	A905
R186	V246	K306	D366	M426	K486	N546	L606	M666	R726	G786	L846	L906
L187	A247	A307	H367	D427	F487	L547	N607	V667	L727	L787	T847	S907
L188	A248	L308	V368	P428	N488	L548	H608	C668	C728	V788	D848	Q908
L189	P249	G309	P369	E429	N489	G549	L609	L669	F729	A789	R849	A909
D190	L250	V310	V370	N430	R490	T550	K610	T670	E730	K790	D850	L910
K191	L251	N311	R371	A431	R491	A551	H611	S671	L731	V791	L851	G911
A192	I252	Q312	I372	G432	V492	D552	K612	V672	L732	C792	V852	P912
V193	D253	L313	V373	Y433	A493	L553	T613	M673	E733	G793	H853	G913
L194	E254	L314	T374	Y434	L494	D554	P614	D674	L734	P794	R854	L914
F195	D255	P315	A375	T435	D495	E555	L615	L675	L735	Y795	Q855	F915
G196	P256	F316	H376	T436	R496	R556	V616	D676	K736	N796	T856	N916
P197	M257	L317	T377	E437	P497	L557	R617	K677	S737	V797	A857	N917
E198	V258	N318	L378	A438	L498	E558	Q618	L678	T738	L798	S858	Y918
M199	R259	A319	S379	M439	N499	T559	H619	Q679	W739	P799	R859	I919
I200	S260	A320	T380	R440	K500	R560	A620	P680	K740	V800	V860	W920
F201	L261	C321	L381	I441	V501	L561	A621	P681	E741	L801	L861	A921
N202	G262	H322	A382	I442	V502	I562	D622	T682	L742	M802	T862	Q922
R203	Q263	S323	E383	R443	T503	D563	L623	N683	K743	H803	H863	L923
L204	E264	R324	N384	R444	Y504	A564	C624	Q684	R744	E804	L864	F924
L205	I265	K325	S385	E445	T505	L565	A625	L685	S745	Y805	A865	H925
P206	I266	S326	Y386	F446	V506	L566	I626	L686	A746	T806	L866	P926
L207	T267	W327	P387	D447	V507	I567	L627	P687	W747	T807	R867	A927
L208	N268	K328	Y388	S448	T508	A568	I628	T688	A748	P808	C868	K928
L209	L269	A329	G389	P449	L509	F569	P629	L689	T749	E809	S869	N929
D210	S270	R330	I390	D450	A510	Q570	V630	T690	F750	T810	O870	V930
R211	T271	H331	E391	D451	K511	E571	I631	P691	G751	N811	T871	R931
S212	V272	T332	V392	E452	K512	Q572	K632	T692	F752	W812	O872	K932
E213	A273	G333	F393	M453	L513	T573	N633	L693	L753	Q813	H873	A933
L214	G274	I334	N394	K454	G514	N574	C634	R694	A754	R814	E874	F934
D215	L275	K335	V395	K455	C515	S575	H635	N695	E755	G815	D875	W935
Q216	K276	I336	V396	T456	S516	D576	E636	K696	A756	W816	A876	R936
E217	T277	L337	L397	I457	Y517	S577	F637	H697	L757	L817	F877	Y937
R218	I278	Q338	E398	L458	T518	L578	E638	R698	G758	K818	T878	Y938
H219	L279	Q339	P399	L459	L519	I579	M639	K699	P759	A819	R879	N939
L220	T280	I340	L400	V460	D520	F580	L640	W700	H760	M820	L880	N940
M221	V281	G341	W401	L461	K521	K581	N641	E701	D761	S821	M881	M941
I222	M282	I342	K402	Q462	L522	G582	K642	W702	V762	F822	H882	Y942
K223	R283	L343	G403	K463	L523	F583	L643	N703	L763	H823	L883	Y943
T224	P284	L344	I404	C464	T524	G584	N644	T704	V764	F824	L884	N944
I225	D285	G345	R405	S465	P525	A585	I645	L705	A765	E825	T885	Y945
D226	I286	I346	S406	A466	L526	V586	I646	K706	L766	W826	P886	Q946
R227	E287	G347	H407	V467	R527	T587	L647	F707	L767	L827	R887	D947
V228	N288	V348	R408	E468	D528	V588	Y648	W708	N768	G828	T888	A948
L229	E289	L349	G409	S469	E529	S589	E649	G709	N769	M829	F889	N949
Y230	D290	N350	K410	I470	A530	L590	S650	L710	L770	M830	V890	V950
Q231	E291	H351	V411	T471	E531	D591	L651	T711	K771	S831	T891	P951
L232	Y292	L352	L412	P472	P532	I592	G652	G712	V772	K832	S892	F952
G233	V293	T353	S413	K473	F533	R593	E653	K713	Q773	D833	P893	Y953
D234	R294	G354	S414	F474	R534	N594	L654	L714	E774	Y834	H894	P954
L235	N295	L355	F415	L475	T535	K595	Y655	A715	R775	T835	A895	Y955
T236	V296	M356	L416	R476	M536	P596	P656	P716	Q776	Y836	T896	T956
K237	T297	K357	K417	E477	A537	F597	E657	T717	L777	F837	H897	P957
P238	S298	C358	A418	E478	V538	L598	L658	Y718	R778	T838	R898	D958
Y239	R299	I359	V419	I479	H539	A599	L659	A719	V779	T839	T899	N959
V240	A300	K360	G420	A480	A540	P600	G660	P720	C780	P840	L900	N960
E961												
E962												
Y963												
E964												
E965												
E966												
L967												
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L969												
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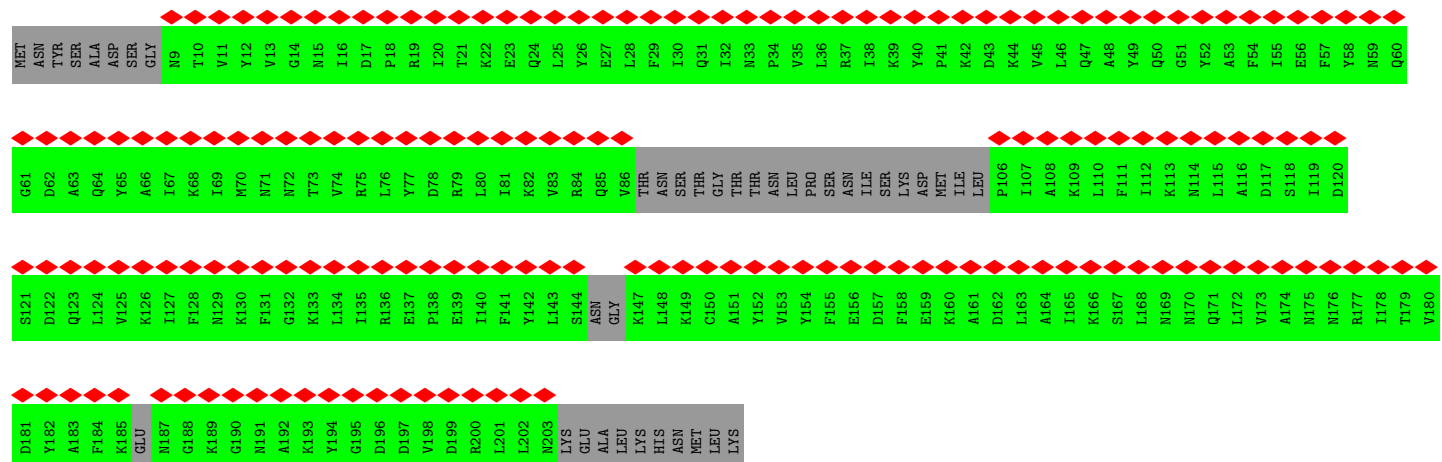
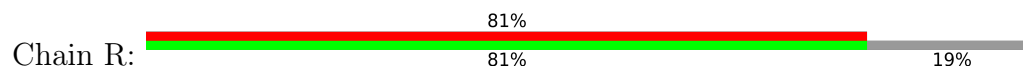
● Molecule 14: Pre-mRNA-splicing factor RSE1

Chain P:

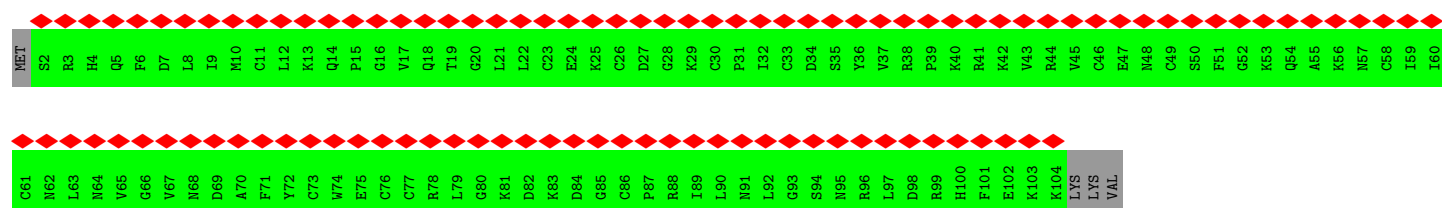




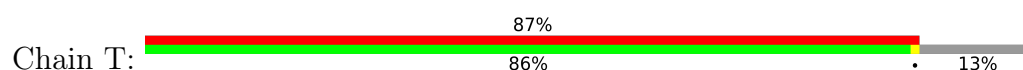
● Molecule 16: Protein HSH49



● Molecule 17: Pre-mRNA-splicing factor RDS3

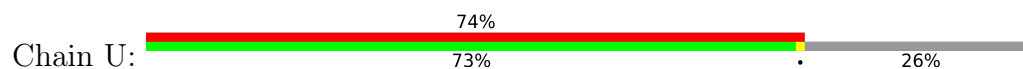


● Molecule 18: Pre-mRNA-splicing factor PRP9

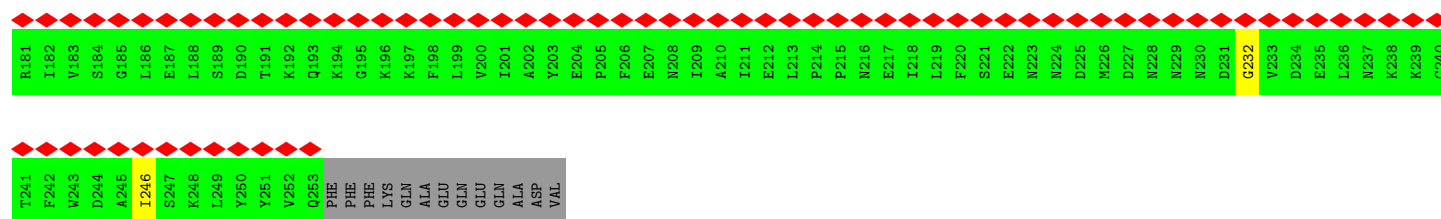


SER	GLN	LEU	THR	ILE	ALA	ALA	VAL	PRO	PRO	LYS	ASN	PRO	SER	GLN	LEU	LYS	VAL	PRO	THR	E503	L504	E505	L506	E507	E508	E509	D510	E511	E512	G513	N514	V515	M516	S517	K518	K519	V520	Y521	D522	E523	L524	K525	K526	Q527	G528	LEU	VAL												
Y421	R422	C423	E424	I425	C426	S427	N428	K429	V430	Y431	N432	G433	R434	R435	T436	F437	E438	R439	H440	F441	N442	E443	E444	R445	H446	I447	Y448	H449	L450	R451	C452	L453	G454	I455	E456	P457	S458	S459	V460	F461	K462	G463	I464	T465	K466	I467	K468	E469	A470	Q471	E472	L473	W474	K475	N476	M477	Q478	GLY	GLN
Y361	E362	A363	P364	A365	Y366	D367	S368	T369	E370	K371	E372	G373	A374	E375	Q376	V377	D378	GLY	GLU	ARG	ASP	GLY	GLN	LEU	GLN	GLU	HIS	LEU	SER	GLY	LYS	PHE	ASP	MET	PRO	GLY	PRO	ASP	GLY	PRO	M407	P408	Y409	W410	L411	Y412	K413	L414	H415	G416	L417	D418	R419	E420					
G301	K302	I303	H304	K305	K306	N307	E308	S309	K310	R311	R312	N313	F314	V315	Y316	S317	E318	Y319	K320	L321	H322	R323	Y324	L325	K326	Y327	L328	N329	D330	E331	F332	S333	R334	T335	R336	S337	F338	V339	E340	R341	K342	L343	A344	F345	T346	A347	N348	E349	R350	M351	A352	S353	M354	D355	I356	L357	T358	Q359	K360
E241	T242	F243	F244	F245	K246	S247	Y248	A249	L250	L251	D252	A253	A254	A255	V256	E257	N258	L259	T260	K261	S262	D263	F264	E265	H266	S267	Y268	C269	R270	G271	S272	L273	R274	S275	E276	A277	K278	G279	L280	Y281	C282	P283	F284	C285	S286	R287	W288	F289	K290	T291	S292	S293	V294	F295	E296	S297	H298	L299	V300
E181	L182	E183	Q184	F185	H186	S187	L188	W189	L190	M191	V192	I193	K194	R195	G196	I197	C198	S199	L200	L201	S202	F203	L204	D205	L206	L207	E208	L209	F210	L211	D212	D213	E214	K215	Y216	L217	L218	T219	P220	P221	M222	D223	R224	K225	N226	D227	R228	Y229	M230	A231	F232	L233	K235	L236	S237	K238	Y239	V240	
K121	E122	L123	K124	M125	E126	D127	E128	M129	F130	E131	L132	D133	I134	M135	S136	I137	K138	D139	K140	Y141	A142	L143	F144	S145	S146	S147	S148	D149	P150	S151	R152	R153	T154	M155	I156	L157	S158	D159	R160	A161	R162	D163	L164	D165	L166	M167	E168	I169	F170	T171	R172	D173	E174	Q175	Y176	G177	E178	I179	M180
K61	F62	K63	K64	V65	K66	K67	K68	K69	K70	Q71	I72	I73	L74	Q75	Q76	H77	E78	I79	N80	I81	F82	L83	R84	D85	Y86	Q87	E88	R89	Q90	Q91	T92	F93	N94	K95	I96	I97	PRO	GLU	GLU	THR	GLN	ASP	LYS	ASP	LEU	PRO	ASN	F112	E113	R114	K115	L116	Q117	Q118	L119	E120			
M1	N2	L3	L4	E5	T6	R7	H8	S9	L10	L11	E12	E13	M14	E15	I16	I17	E18	M19	A20	I21	A22	E23	R24	I25	Q26	R27	N28	P29	E30	L31	Y32	Y33	H34	Y35	I36	Q37	E38	S39	S40	K41	V42	F43	P44	D45	T46	K47	L48	P49	R50	S51	S52	L53	T54	A55	E56	N57	K58	I59	V60

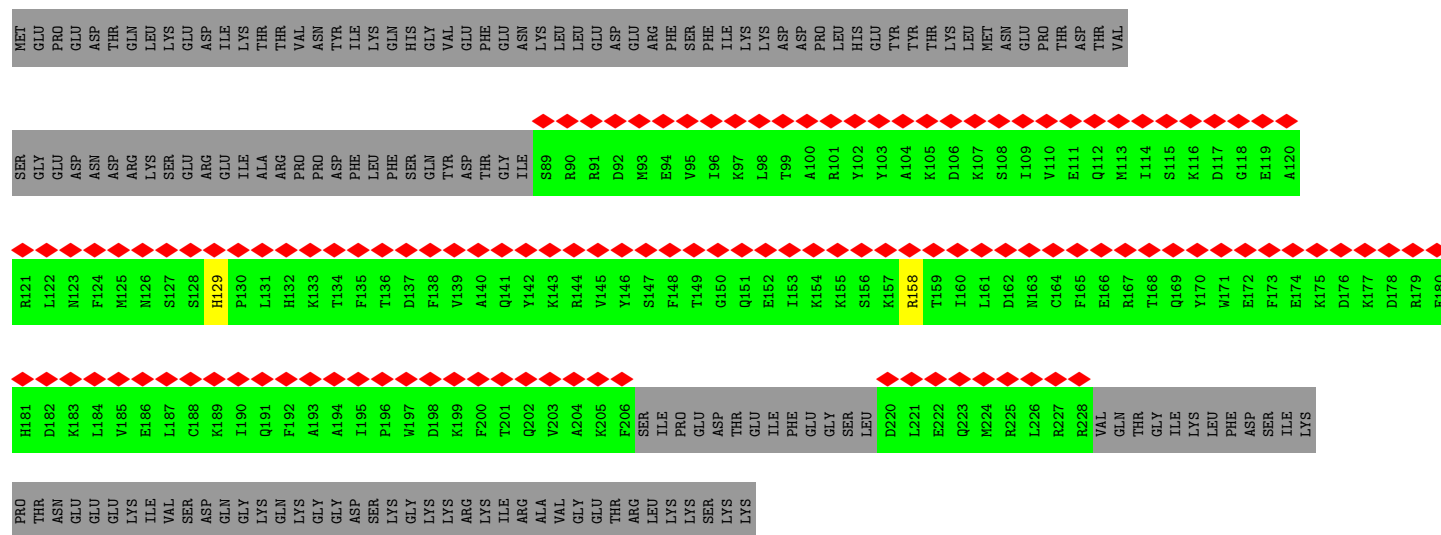
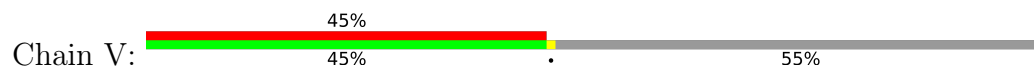
- Molecule 19: Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11



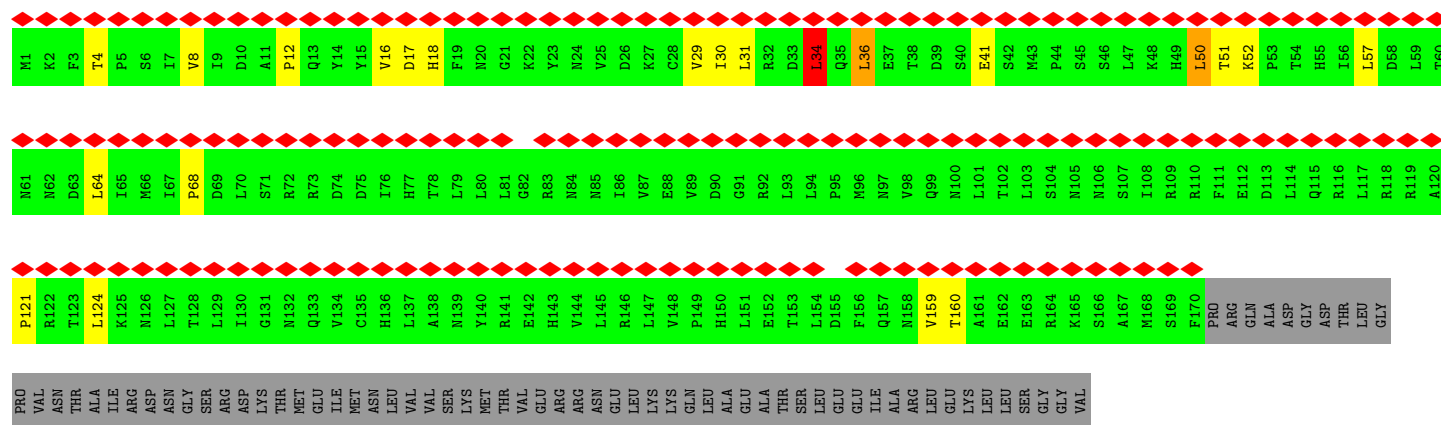
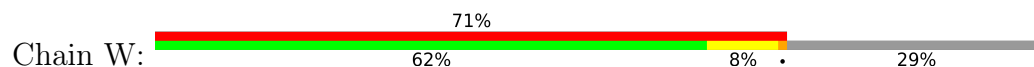
MET	ASN	TYR	LEU	GLU	GLY	VAL	GLY	SER	SER	LYS	LYS	GLY	GLY	ILE	ALA	SER	GLU	SER	GLN	PHE	ASN	LEU	GLN	ARG	ARG	LYS	GLU	VAL	GLU	SER	SER	LEU	L34	S35	K36	G37	E38	N39	V40	P41	Y42	T43	F44	Q45	D46	E47	LYS	ASP	ASP	Q51	V52	R53	S54	N55	P56	Y57	I58	Y59	K60
N61	H62	S63	G64	K65	L66	V67	C68	K69	L70	C71	H72	T73	M74	H75	M76	S77	W78	S79	S80	W81	E82	R83	H84	L85	G86	G87	K88	R89	H90	G91	L92	N93	V94	L95	R96	R97	G98	I99	S100	I101	E102	K103	S104	S105	LEU	GLY	ARG	GLU	GLY	GLN	THR	HIS	X115	X116	X117	X118	X119	X120	
X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	VAL	CYS	LYS	ILE	ALA	THR	VAL	LYS	ASN	PRO	LYS	ASN	G149	S150	V151	G152	L153	A154	I155	Q156	V157	N158	Y159	S160	S161	E162	V163	K164	E165	N166	S167	V168	D169	S170	D171	D172	K173	A174	K175	V176	P177	P178	L179	I180



• Molecule 20: Pre-mRNA-splicing factor PRP21

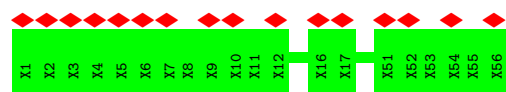


• Molecule 21: U2 small nuclear ribonucleoprotein A'

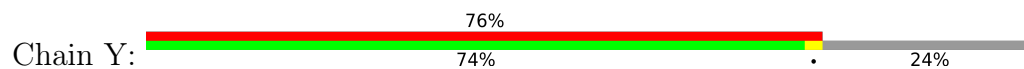


• Molecule 22: Unknown

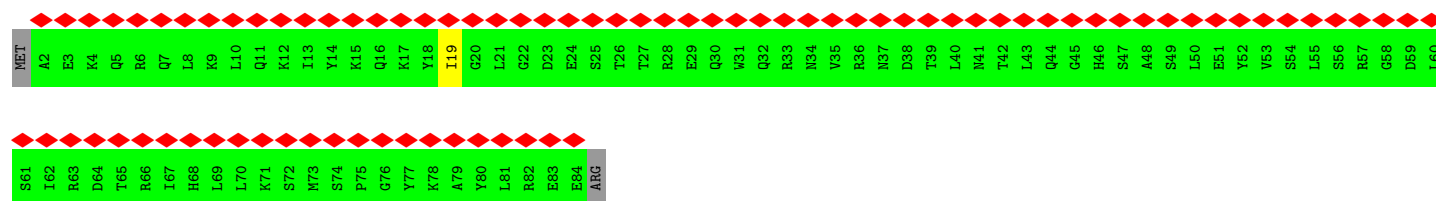




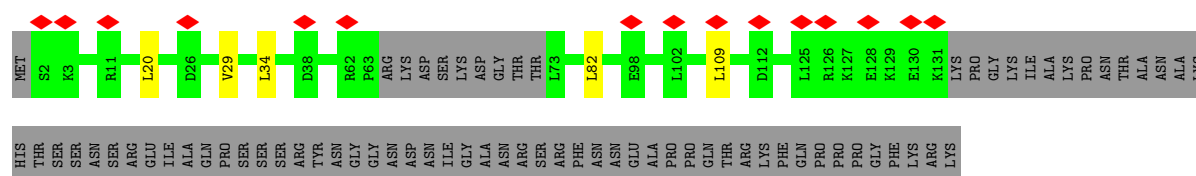
• Molecule 23: U2 small nuclear ribonucleoprotein B''



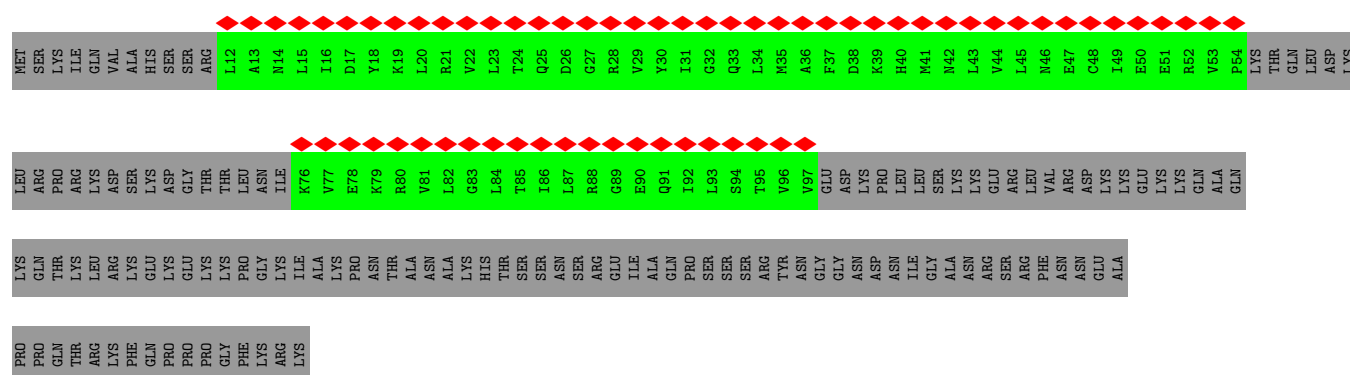
• Molecule 24: RDS3 complex subunit 10




• Molecule 25: Small nuclear ribonucleoprotein-associated protein B

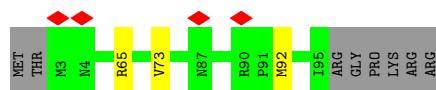


• Molecule 25: Small nuclear ribonucleoprotein-associated protein B




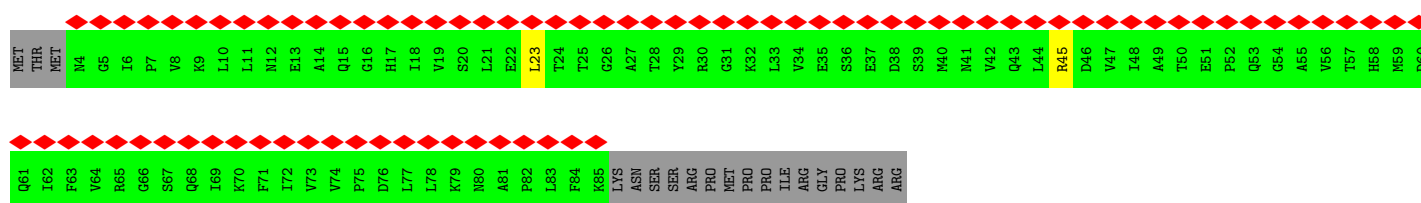
- Molecule 26: Small nuclear ribonucleoprotein Sm D3

Chain d:  89% 8%




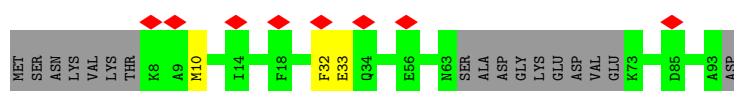
- Molecule 26: Small nuclear ribonucleoprotein Sm D3

Chain v:  81% 79% 19%




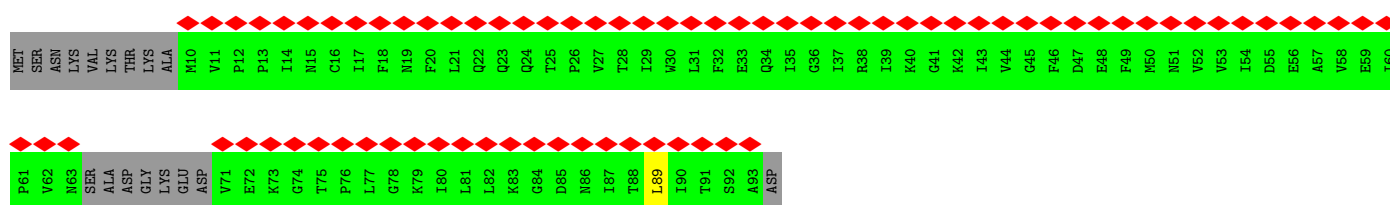
- Molecule 27: Small nuclear ribonucleoprotein E

Chain e:  9% 79% 18%




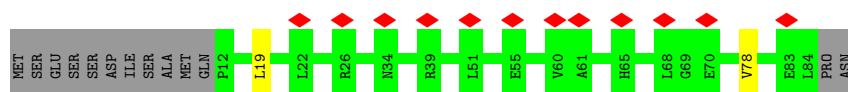
- Molecule 27: Small nuclear ribonucleoprotein E

Chain w:  82% 81% 18%




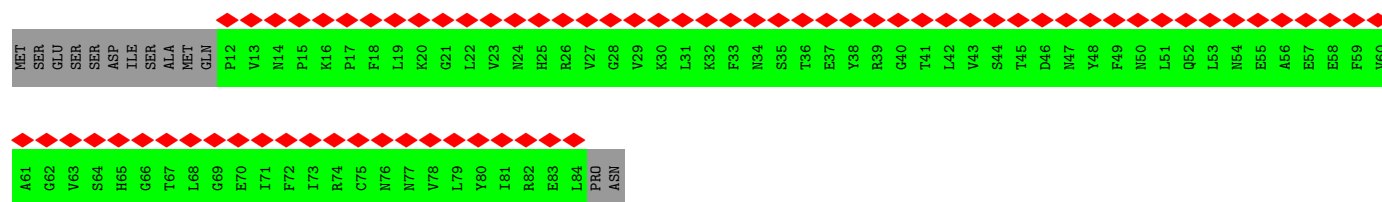
- Molecule 28: Small nuclear ribonucleoprotein F

Chain f:  14% 83% 15%

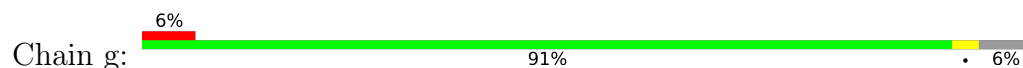


- Molecule 28: Small nuclear ribonucleoprotein F

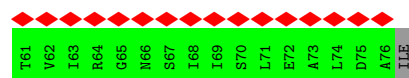
Chain x:  85% 85% 15%



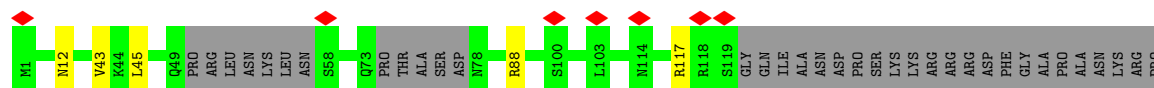
• Molecule 29: Small nuclear ribonucleoprotein G



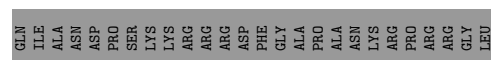
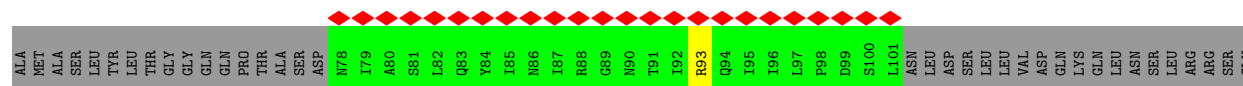
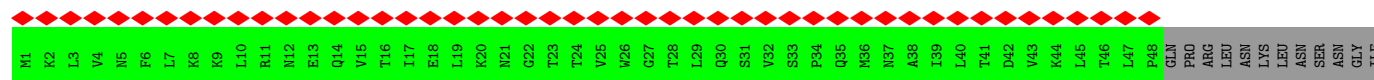
• Molecule 29: Small nuclear ribonucleoprotein G



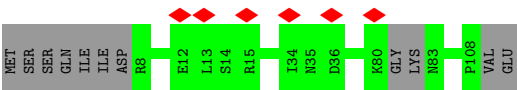
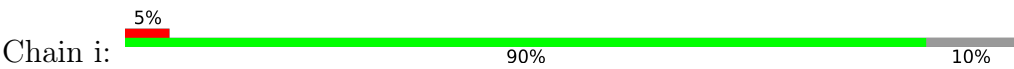
• Molecule 30: Small nuclear ribonucleoprotein Sm D1



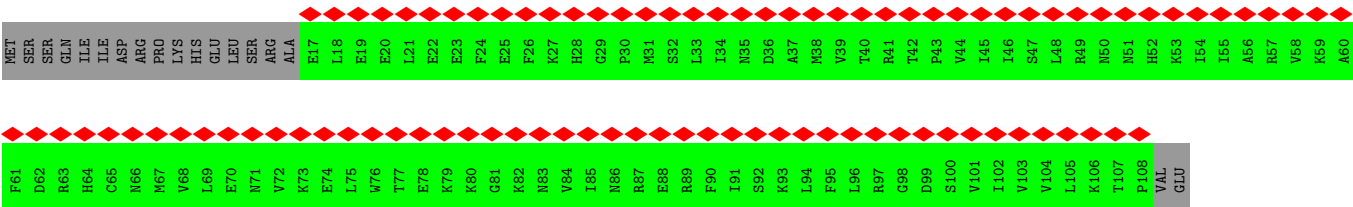
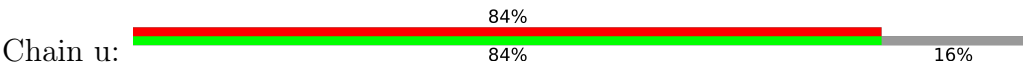
• Molecule 30: Small nuclear ribonucleoprotein Sm D1



• Molecule 31: Small nuclear ribonucleoprotein Sm D2



● Molecule 31: Small nuclear ribonucleoprotein Sm D2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153556	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0369	Depositor
Map size (Å)	632.8, 632.8, 632.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.76	0/6890	1.31	72/10700 (0.7%)
2	2	1.40	52/3302 (1.6%)	1.72	120/5123 (2.3%)
3	A	0.28	0/388	0.60	1/535 (0.2%)
4	B	0.45	0/1325	0.79	2/1784 (0.1%)
5	C	0.57	0/1348	0.76	2/1825 (0.1%)
6	D	0.51	0/3499	0.71	7/4772 (0.1%)
7	E	0.77	4/4688 (0.1%)	0.94	26/6331 (0.4%)
8	F	0.65	0/1361	0.89	3/1843 (0.2%)
9	G	0.58	0/1716	0.74	1/2314 (0.0%)
10	H	0.49	0/816	0.69	0/1094
11	I	0.48	0/878	0.93	0/1357
12	J	0.50	0/331	0.78	0/448
13	O	0.28	0/6745	0.45	0/9157
14	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
15	Q	0.27	0/1835	0.46	0/2480
16	R	0.26	0/1453	0.42	0/1954
17	S	0.29	0/827	0.46	0/1105
18	T	0.27	0/3992	0.41	0/5346
19	U	0.24	0/1403	0.40	0/1889
20	V	0.24	0/1105	0.36	0/1475
21	W	0.41	0/1406	0.69	4/1905 (0.2%)
23	Y	0.30	0/692	0.54	0/923
24	Z	0.28	0/694	0.47	0/929
25	b	0.65	1/978 (0.1%)	0.93	4/1306 (0.3%)
25	s	0.39	0/521	0.62	0/701
26	d	0.68	1/726 (0.1%)	0.83	1/984 (0.1%)
26	v	0.43	0/641	0.65	2/868 (0.2%)
27	e	0.58	0/610	0.79	0/826
27	w	0.40	0/612	0.61	1/830 (0.1%)
28	f	0.63	1/597 (0.2%)	0.89	2/807 (0.2%)
28	x	0.42	0/597	0.63	0/807
29	g	0.63	0/559	0.83	0/751

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	y	0.26	0/582	0.49	0/785
30	h	0.52	0/839	0.77	2/1132 (0.2%)
30	t	0.42	0/574	0.68	1/777 (0.1%)
31	i	0.57	0/818	0.75	0/1099
31	u	0.40	0/764	0.57	0/1026
All	All	0.57	60/65735 (0.1%)	0.84	252/91029 (0.3%)

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
2	2	0	1
4	B	0	3
5	C	0	3
6	D	0	5
7	E	0	12
8	F	0	8
9	G	0	1
10	H	0	1
14	P	0	2
18	T	0	1
21	W	0	1
27	e	0	1
29	g	0	1
30	h	0	1
All	All	0	41

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1149	G	O3'-P	24.38	1.90	1.61
2	2	143	G	O3'-P	18.83	1.83	1.61
2	2	1161	U	O3'-P	-15.58	1.42	1.61
2	2	143	G	C3'-O3'	15.30	1.63	1.42
2	2	1092	A	O3'-P	-14.80	1.43	1.61
2	2	1090	A	O3'-P	14.46	1.78	1.61
2	2	144	G	O3'-P	-14.32	1.44	1.61
2	2	1116	A	O3'-P	-11.61	1.47	1.61
2	2	1166	G	O3'-P	9.98	1.73	1.61
2	2	1149	G	C3'-O3'	9.95	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1163	C	O5'-C5'	9.12	1.59	1.44
2	2	1116	A	C3'-O3'	-8.88	1.29	1.42
2	2	1127	A	O3'-P	-8.75	1.50	1.61
2	2	1167	U	O3'-P	8.63	1.71	1.61
2	2	1164	C	O3'-P	-8.24	1.51	1.61
2	2	1090	A	C3'-O3'	7.79	1.53	1.42
7	E	157	ARG	CZ-NH1	-7.60	1.23	1.33
2	2	1162	U	P-O5'	7.57	1.67	1.59
2	2	1163	C	P-O5'	7.49	1.67	1.59
2	2	1117	G	P-O5'	7.26	1.67	1.59
2	2	144	G	P-O5'	7.09	1.66	1.59
2	2	1096	C	O3'-P	6.98	1.69	1.61
2	2	1154	U	C1'-N1	6.95	1.59	1.48
2	2	1128	C	C5'-C4'	-6.91	1.43	1.51
2	2	1140	U	C1'-N1	6.89	1.59	1.48
2	2	1165	C	O3'-P	6.54	1.69	1.61
2	2	1095	U	O3'-P	6.53	1.69	1.61
2	2	1169	C	C1'-N1	6.47	1.58	1.48
2	2	145	G	P-O5'	-6.46	1.53	1.59
2	2	1090	A	C4'-O4'	6.42	1.53	1.45
2	2	1150	U	O5'-C5'	6.38	1.54	1.44
2	2	1168	U	C5'-C4'	-6.26	1.43	1.51
2	2	1117	G	C5'-C4'	6.23	1.58	1.51
2	2	1162	U	O3'-P	6.15	1.68	1.61
2	2	1165	C	O5'-C5'	6.05	1.54	1.44
2	2	1162	U	C2-N3	6.03	1.42	1.37
14	P	188	SER	C-N	-6.00	1.22	1.34
2	2	1162	U	O5'-C5'	6.00	1.54	1.44
2	2	1151	U	O5'-C5'	-5.90	1.33	1.42
2	2	1163	C	O3'-P	5.83	1.68	1.61
25	b	29	VAL	CB-CG2	-5.79	1.40	1.52
2	2	68	U	C1'-N1	5.76	1.57	1.48
2	2	1097	G	O3'-P	5.70	1.68	1.61
2	2	1161	U	C3'-O3'	-5.69	1.34	1.42
2	2	1162	U	C3'-C2'	-5.66	1.46	1.52
2	2	118	U	C1'-N1	5.60	1.57	1.48
2	2	144	G	C3'-O3'	-5.46	1.34	1.42
2	2	121	C	C1'-N1	5.44	1.56	1.48
28	f	78	VAL	CB-CG1	-5.41	1.41	1.52
2	2	143	G	P-O5'	-5.40	1.54	1.59
2	2	111	C	C1'-N1	5.39	1.56	1.48
2	2	109	C	C1'-N1	5.31	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	73	VAL	CB-CG1	-5.28	1.41	1.52
7	E	109	TRP	CB-CG	-5.25	1.40	1.50
2	2	147	A	O3'-P	-5.25	1.54	1.61
2	2	1166	G	C5'-C4'	5.25	1.57	1.51
2	2	85	A	C1'-N9	-5.14	1.39	1.46
2	2	1090	A	O5'-C5'	5.12	1.52	1.44
7	E	60	TYR	CD1-CE1	-5.10	1.31	1.39
7	E	30	TRP	CB-CG	-5.06	1.41	1.50

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40
2	2	1162	U	C5'-C4'-O4'	14.81	126.87	109.10
2	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
2	2	1147	A	C5'-C4'-C3'	-14.18	93.31	116.00
2	2	1092	A	C2'-C3'-O3'	14.12	140.56	109.50
7	E	157	ARG	NE-CZ-NH1	-13.86	113.37	120.30
2	2	143	G	C4'-C3'-O3'	13.62	140.24	113.00
1	1	557	U	N1-C2-O2	13.50	132.25	122.80
2	2	1098	C	N1-C1'-C2'	-13.40	96.58	114.00
2	2	1151	U	C4'-C3'-O3'	-12.57	83.00	109.40
1	1	557	U	N3-C2-O2	-12.35	113.56	122.20
2	2	144	G	C2'-C3'-O3'	12.24	136.44	109.50
2	2	143	G	P-O3'-C3'	11.89	133.97	119.70
2	2	1149	G	P-O3'-C3'	11.89	133.96	119.70
2	2	144	G	C5'-C4'-O4'	-11.83	94.91	109.10
2	2	1151	U	P-O5'-C5'	11.70	139.62	120.90
2	2	1117	G	C5'-C4'-O4'	11.43	122.82	109.10
2	2	145	G	C5'-C4'-C3'	-11.23	98.04	116.00
2	2	1150	U	C5'-C4'-C3'	11.09	133.74	116.00
1	1	27	A	O4'-C1'-N9	11.07	117.06	108.20
2	2	1117	G	C5'-C4'-C3'	-10.88	98.59	116.00
2	2	1163	C	C5'-C4'-O4'	10.59	121.81	109.10
2	2	144	G	C5'-C4'-C3'	10.46	132.74	116.00
2	2	141	A	N9-C1'-C2'	-10.43	100.45	114.00
2	2	1126	G	N9-C1'-C2'	-10.06	100.92	114.00
2	2	1091	G	C5'-C4'-C3'	9.90	131.84	116.00
2	2	143	G	C5'-C4'-C3'	-9.88	100.19	116.00
2	2	1163	C	C5'-C4'-C3'	-9.73	100.43	116.00
2	2	1139	G	N9-C1'-C2'	-9.71	101.32	112.00
2	2	1147	A	P-O5'-C5'	9.59	136.24	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1090	A	P-O3'-C3'	9.54	131.15	119.70
7	E	113	LEU	CB-CG-CD2	-9.45	94.94	111.00
1	1	27	A	N9-C1'-C2'	9.42	126.24	114.00
2	2	1162	U	C5'-C4'-C3'	-9.19	101.29	116.00
2	2	1168	U	C4'-C3'-O3'	-9.00	90.51	109.40
2	2	1150	U	C4'-C3'-O3'	-8.98	90.55	109.40
2	2	142	C	N1-C1'-C2'	-8.84	102.28	112.00
1	1	117	U	O5'-P-OP1	-8.81	97.77	105.70
7	E	536	LEU	CA-CB-CG	8.72	135.35	115.30
2	2	1151	U	O4'-C1'-N1	8.67	115.14	108.20
2	2	1152	U	P-O5'-C5'	8.67	134.77	120.90
28	f	19	LEU	CB-CG-CD2	-8.66	96.27	111.00
2	2	1090	A	C4'-C3'-O3'	8.63	130.27	113.00
2	2	1092	A	P-O5'-C5'	8.53	134.55	120.90
2	2	1148	U	C4'-C3'-O3'	-8.53	91.48	109.40
7	E	415	LEU	CA-CB-CG	8.53	134.92	115.30
1	1	56	C	C5-C6-N1	8.40	125.20	121.00
1	1	557	U	C2-N1-C1'	8.39	127.76	117.70
7	E	334	LEU	CB-CG-CD2	-8.35	96.80	111.00
2	2	145	G	P-O5'-C5'	8.32	134.21	120.90
2	2	148	G	C5'-C4'-C3'	-8.26	102.78	116.00
2	2	1165	C	C5'-C4'-C3'	-8.25	102.79	116.00
7	E	449	SER	N-CA-CB	-8.22	98.17	110.50
1	1	56	C	C2-N1-C1'	8.20	127.82	118.80
2	2	1150	U	C2'-C3'-O3'	8.12	127.37	109.50
6	D	500	LEU	CA-CB-CG	8.12	133.98	115.30
2	2	1151	U	C5'-C4'-O4'	8.11	118.84	109.10
6	D	619	LEU	CB-CG-CD2	-8.09	97.25	111.00
7	E	16	LEU	CB-CG-CD2	-8.08	97.27	111.00
2	2	1090	A	C5'-C4'-O4'	8.06	118.77	109.10
2	2	144	G	O3'-P-O5'	-8.02	88.75	104.00
2	2	1149	G	O3'-P-O5'	8.00	119.21	104.00
2	2	1150	U	P-O5'-C5'	7.98	133.66	120.90
1	1	115	C	C2-N1-C1'	7.96	127.56	118.80
2	2	1168	U	P-O5'-C5'	-7.90	108.25	120.90
2	2	1167	U	C2'-C3'-O3'	7.88	126.83	109.50
1	1	115	C	N1-C2-O2	7.85	123.61	118.90
2	2	1092	A	C4'-C3'-O3'	-7.83	92.95	109.40
2	2	1165	C	C5'-C4'-O4'	7.79	118.45	109.10
7	E	63	MET	CB-CG-SD	-7.76	89.11	112.40
2	2	1107	C	N1-C1'-C2'	-7.75	103.47	112.00
2	2	1161	U	C5'-C4'-C3'	-7.75	103.60	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1147	A	C4'-C3'-O3'	7.75	128.49	113.00
2	2	1093	C	C5'-C4'-C3'	-7.70	103.69	116.00
2	2	1169	C	P-O5'-C5'	-7.63	108.69	120.90
2	2	1097	G	C3'-C2'-O2'	7.62	135.40	113.30
2	2	1165	C	C4'-C3'-O3'	7.54	128.08	113.00
8	F	309	ASP	CB-CG-OD2	7.38	124.94	118.30
2	2	1128	C	C5'-C4'-O4'	7.28	117.84	109.10
2	2	1168	U	C2'-C3'-O3'	7.28	125.51	109.50
2	2	1089	G	C4'-C3'-O3'	7.24	127.48	113.00
1	1	127	C	C6-N1-C2	-7.24	117.40	120.30
2	2	1115	G	O5'-P-OP1	-7.21	99.21	105.70
2	2	1159	U	O5'-P-OP1	-7.21	99.21	105.70
2	2	1149	G	C4'-C3'-O3'	7.21	127.42	113.00
21	W	50	LEU	CA-CB-CG	7.19	131.83	115.30
2	2	139	G	O5'-P-OP2	-7.18	99.24	105.70
1	1	56	C	N1-C2-O2	7.17	123.20	118.90
2	2	139	G	O5'-P-OP1	-7.15	99.26	105.70
2	2	1089	G	O5'-P-OP2	-7.12	99.29	105.70
2	2	1159	U	O5'-P-OP2	-7.11	99.30	105.70
25	b	20	LEU	CB-CG-CD1	-7.11	98.92	111.00
7	E	351	LEU	CA-CB-CG	7.08	131.58	115.30
2	2	1089	G	O5'-P-OP1	-7.08	99.33	105.70
1	1	557	U	C6-N1-C1'	-7.07	111.30	121.20
2	2	1115	G	C4'-C3'-O3'	7.04	127.08	113.00
2	2	1115	G	O5'-P-OP2	-7.04	99.37	105.70
1	1	285	C	C5-C6-N1	6.94	124.47	121.00
25	b	34	LEU	CA-CB-CG	6.93	131.23	115.30
4	B	19	ARG	NE-CZ-NH2	-6.92	116.84	120.30
5	C	39	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	1	11	U	N3-C2-O2	-6.86	117.40	122.20
2	2	1090	A	C5'-C4'-C3'	-6.69	105.30	116.00
2	2	1096	C	C1'-C2'-O2'	-6.69	90.54	110.60
1	1	27	A	N1-C6-N6	-6.67	114.60	118.60
1	1	555	U	N3-C2-O2	-6.66	117.54	122.20
8	F	380	LEU	CB-CG-CD1	-6.65	99.69	111.00
2	2	1129	U	C5'-C4'-O4'	6.62	117.04	109.10
1	1	135	U	P-O3'-C3'	6.59	127.61	119.70
2	2	148	G	C5'-C4'-O4'	6.58	116.99	109.10
1	1	11	U	N1-C2-O2	6.51	127.36	122.80
30	t	93	ARG	CG-CD-NE	-6.48	98.18	111.80
2	2	140	G	N9-C1'-C2'	-6.46	104.90	112.00
1	1	115	C	C6-N1-C2	-6.45	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	167	G	OP1-P-O3'	6.44	119.37	105.20
7	E	64	LEU	CB-CG-CD1	6.44	121.94	111.00
6	D	595	LEU	CA-CB-CG	6.41	130.04	115.30
2	2	1166	G	O5'-C5'-C4'	6.36	123.78	111.70
1	1	168	C	C5-C6-N1	6.34	124.17	121.00
1	1	285	C	C6-N1-C2	-6.33	117.77	120.30
2	2	1166	G	C5'-C4'-C3'	6.33	126.12	116.00
2	2	145	G	O4'-C1'-N9	6.32	113.26	108.20
9	G	98	LEU	CA-CB-CG	6.32	129.83	115.30
1	1	27	A	OP2-P-O3'	6.28	119.02	105.20
26	v	45	ARG	NE-CZ-NH1	-6.27	117.16	120.30
7	E	108	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	1	115	C	N3-C2-O2	-6.24	117.53	121.90
2	2	145	G	O5'-C5'-C4'	-6.23	99.86	111.70
2	2	1092	A	N9-C1'-C2'	6.22	122.08	114.00
1	1	259	U	C2-N1-C1'	6.18	125.12	117.70
7	E	34	LEU	CA-CB-CG	6.17	129.50	115.30
1	1	67	A	P-O3'-C3'	6.16	127.09	119.70
1	1	548	U	N3-C2-O2	-6.16	117.89	122.20
2	2	1096	C	C4'-C3'-O3'	6.14	125.27	113.00
2	2	1152	U	C5'-C4'-C3'	-6.14	106.18	116.00
27	w	89	LEU	CA-CB-CG	6.09	129.31	115.30
1	1	555	U	N1-C2-O2	6.09	127.06	122.80
7	E	157	ARG	NH1-CZ-NH2	6.07	126.08	119.40
1	1	136	C	P-O3'-C3'	6.05	126.95	119.70
7	E	34	LEU	CB-CG-CD2	-6.04	100.73	111.00
2	2	143	G	O4'-C1'-N9	6.04	113.03	108.20
2	2	1167	U	P-O3'-C3'	-6.02	112.47	119.70
5	C	117	LYS	CB-CG-CD	-6.02	95.95	111.60
2	2	1151	U	O3'-P-O5'	-6.01	92.57	104.00
2	2	143	G	O3'-P-O5'	5.99	115.38	104.00
2	2	144	G	P-O3'-C3'	-5.99	112.52	119.70
7	E	301	ARG	CG-CD-NE	-5.93	99.35	111.80
1	1	548	U	C2-N1-C1'	5.91	124.79	117.70
7	E	126	LEU	CA-CB-CG	5.90	128.86	115.30
2	2	1167	U	C5'-C4'-O4'	-5.90	102.03	109.10
2	2	1162	U	C4'-C3'-O3'	5.89	124.78	113.00
2	2	1091	G	O5'-C5'-C4'	5.88	122.88	111.70
1	1	154	G	C5-C6-O6	-5.87	125.08	128.60
2	2	1108	A	C3'-C2'-C1'	5.86	106.19	101.50
26	d	92	MET	CA-CB-CG	5.85	123.25	113.30
21	W	36	LEU	CA-CB-CG	5.82	128.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1150	U	N1-C1'-C2'	5.80	121.54	114.00
2	2	1115	G	P-O3'-C3'	5.79	126.65	119.70
1	1	50	C	C6-N1-C2	-5.77	117.99	120.30
2	2	1148	U	C5'-C4'-O4'	5.77	116.02	109.10
25	b	109	LEU	CA-CB-CG	5.77	128.56	115.30
1	1	115	C	C5-C6-N1	5.75	123.88	121.00
2	2	1162	U	C2'-C3'-O3'	-5.74	96.86	109.50
8	F	442	GLN	CA-CB-CG	5.74	126.03	113.40
1	1	548	U	N1-C2-O2	5.73	126.81	122.80
7	E	196	LEU	CA-CB-CG	5.73	128.47	115.30
1	1	134	G	P-O3'-C3'	5.70	126.53	119.70
2	2	141	A	C4'-C3'-O3'	5.68	124.37	113.00
7	E	16	LEU	CA-CB-CG	5.67	128.34	115.30
1	1	39	U	P-O3'-C3'	5.66	126.49	119.70
1	1	11	U	C2-N1-C1'	5.64	124.47	117.70
1	1	56	C	C6-N1-C2	-5.64	118.04	120.30
1	1	21	G	P-O3'-C3'	5.64	126.46	119.70
21	W	57	LEU	CA-CB-CG	5.63	128.25	115.30
1	1	168	C	C2-N1-C1'	5.62	124.99	118.80
1	1	253	C	C6-N1-C2	-5.62	118.05	120.30
1	1	280	G	N1-C6-O6	-5.60	116.54	119.90
2	2	1167	U	C5'-C4'-C3'	5.59	124.94	116.00
4	B	178	ASP	CB-CG-OD1	5.58	123.32	118.30
25	b	82	LEU	CB-CG-CD1	-5.56	101.54	111.00
2	2	1097	G	C2'-C3'-O3'	-5.56	97.26	109.50
1	1	56	C	C6-N1-C1'	-5.55	114.14	120.80
1	1	153	C	C6-N1-C2	-5.55	118.08	120.30
30	h	45	LEU	CA-CB-CG	5.54	128.03	115.30
2	2	1162	U	P-O3'-C3'	5.53	126.33	119.70
1	1	135	U	OP2-P-O3'	5.53	117.36	105.20
1	1	259	U	N3-C2-O2	-5.52	118.33	122.20
1	1	119	G	C4-N9-C1'	5.52	133.68	126.50
1	1	561	U	C2-N1-C1'	5.50	124.30	117.70
1	1	26	G	N3-C4-N9	5.50	129.30	126.00
2	2	145	G	C3'-C2'-O2'	-5.49	97.37	113.30
2	2	1091	G	C4'-C3'-O3'	-5.49	97.88	109.40
2	2	145	G	C5'-C4'-O4'	5.49	115.68	109.10
7	E	392	LEU	CA-CB-CG	5.48	127.90	115.30
2	2	1151	U	N1-C1'-C2'	5.47	121.11	114.00
2	2	1105	C	C4'-C3'-O3'	-5.45	97.95	109.40
2	2	1168	U	C4'-C3'-C2'	-5.45	97.15	102.60
2	2	1162	U	C4'-C3'-C2'	5.44	108.04	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	34	LEU	CB-CG-CD1	5.43	120.22	111.00
1	1	284	C	O4'-C1'-N1	5.41	112.53	108.20
1	1	155	G	N1-C6-O6	5.41	123.14	119.90
26	v	23	LEU	CA-CB-CG	5.40	127.71	115.30
1	1	168	C	C6-N1-C2	-5.36	118.15	120.30
2	2	1089	G	P-O3'-C3'	5.36	126.14	119.70
1	1	154	G	N1-C6-O6	5.36	123.11	119.90
1	1	561	U	N3-C2-O2	-5.34	118.46	122.20
2	2	144	G	C1'-C2'-O2'	-5.33	94.61	110.60
2	2	1168	U	O3'-P-O5'	-5.33	93.88	104.00
2	2	1150	U	P-O3'-C3'	-5.32	113.32	119.70
3	A	29	PRO	N-CA-CB	5.31	109.67	103.30
1	1	77	U	C5-C6-N1	5.30	125.35	122.70
1	1	164	U	C5-C6-N1	5.29	125.34	122.70
1	1	259	U	N1-C2-O2	5.29	126.50	122.80
1	1	11	U	C6-N1-C2	-5.26	117.84	121.00
1	1	11	U	C5-C6-N1	5.25	125.32	122.70
1	1	72	G	C6-N1-C2	-5.24	121.96	125.10
1	1	160	C	C6-N1-C2	-5.23	118.21	120.30
7	E	376	SER	C-N-CA	5.23	134.78	121.70
2	2	1152	U	O4'-C4'-C3'	5.23	110.28	106.10
7	E	448	TYR	C-N-CA	5.20	134.69	121.70
1	1	561	U	N1-C2-O2	5.19	126.43	122.80
1	1	117	U	C5-C6-N1	5.17	125.29	122.70
2	2	66	A	C4'-C3'-O3'	5.17	123.33	113.00
6	D	430	LEU	CB-CG-CD1	-5.16	102.24	111.00
1	1	81	C	C6-N1-C2	-5.15	118.24	120.30
1	1	39	U	C3'-C2'-C1'	5.15	105.62	101.50
7	E	64	LEU	CA-CB-CG	5.15	127.15	115.30
28	f	78	VAL	CG1-CB-CG2	-5.15	102.66	110.90
2	2	1163	C	C4'-C3'-O3'	5.14	123.29	113.00
6	D	346	LEU	CA-CB-CG	5.14	127.12	115.30
1	1	115	C	C6-N1-C1'	-5.14	114.64	120.80
7	E	348	ILE	CG1-CB-CG2	-5.12	100.12	111.40
6	D	430	LEU	CA-CB-CG	5.12	127.07	115.30
2	2	145	G	C4'-C3'-O3'	5.12	123.23	113.00
2	2	1148	U	P-O5'-C5'	5.12	129.09	120.90
14	P	962	LEU	CA-CB-CG	5.11	127.06	115.30
30	h	88	ARG	NE-CZ-NH1	-5.10	117.75	120.30
21	W	34	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	1	134	G	C4-N9-C1'	5.09	133.11	126.50
7	E	367	LEU	CB-CG-CD1	-5.08	102.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	25	A	O4'-C1'-N9	5.06	112.25	108.20
1	1	168	C	C2-N3-C4	5.06	122.43	119.90
2	2	1169	C	O5'-C5'-C4'	-5.05	102.11	111.70
2	2	1147	A	O5'-C5'-C4'	5.03	121.26	111.70
2	2	146	A	C5'-C4'-C3'	-5.03	107.95	116.00
2	2	1161	U	C5'-C4'-O4'	5.03	115.14	109.10
1	1	253	C	N1-C2-O2	5.02	121.92	118.90
2	2	145	G	P-O3'-C3'	5.02	125.73	119.70
7	E	303	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	1	130	C	N1-C2-O2	5.01	121.91	118.90
2	2	146	A	C5'-C4'-O4'	5.00	115.10	109.10
6	D	619	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	141	A	Sidechain
4	B	166	LYS	Peptide
4	B	170	VAL	Peptide
4	B	43	GLY	Peptide
5	C	103	ASP	Peptide
5	C	122	ALA	Peptide
5	C	154	ARG	Peptide
6	D	364	ASN	Peptide
6	D	424	LEU	Peptide
6	D	531	ASP	Peptide
6	D	533	ASN	Peptide
6	D	573	HIS	Peptide
7	E	262	ASN	Peptide
7	E	265	THR	Peptide
7	E	306	LEU	Peptide
7	E	376	SER	Peptide
7	E	377	ASP	Peptide
7	E	403	TYR	Peptide
7	E	410	SER	Peptide
7	E	447	PHE	Peptide
7	E	448	TYR	Peptide
7	E	451	ASP	Peptide
7	E	506	TRP	Peptide
7	E	511	LYS	Peptide
8	F	304	LEU	Peptide

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Mol	Chain	Res	Type	Group
8	F	309	ASP	Peptide
8	F	323	LEU	Peptide
8	F	324	VAL	Peptide
8	F	325	THR	Peptide
8	F	384	ARG	Peptide
8	F	385	SER	Peptide
8	F	413	PRO	Peptide
9	G	227	CYS	Peptide
10	H	69	PRO	Peptide
14	P	1013	ASP	Peptide
14	P	1014	LYS	Peptide
18	T	458	SER	Peptide
21	W	16	VAL	Peptide
27	e	32	PHE	Peptide
29	g	17	LEU	Peptide
30	h	43	VAL	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	
3	A	72/298 (24%)	59 (82%)	12 (17%)	1 (1%)	9	40
4	B	158/300 (53%)	135 (85%)	22 (14%)	1 (1%)	22	58
5	C	171/231 (74%)	152 (89%)	18 (10%)	1 (1%)	22	58
6	D	475/629 (76%)	435 (92%)	37 (8%)	3 (1%)	22	58
7	E	539/544 (99%)	482 (89%)	44 (8%)	13 (2%)	5	31
8	F	165/523 (32%)	142 (86%)	17 (10%)	6 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	204/492 (42%)	186 (91%)	18 (9%)	0	100	100
10	H	94/261 (36%)	89 (95%)	5 (5%)	0	100	100
12	J	40/620 (6%)	34 (85%)	6 (15%)	0	100	100
13	O	829/971 (85%)	788 (95%)	41 (5%)	0	100	100
14	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	22	58
15	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	25	61
16	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
17	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
18	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
19	U	168/266 (63%)	143 (85%)	24 (14%)	1 (1%)	22	58
20	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
21	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	16
23	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	11	43
24	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	11	43
25	b	117/196 (60%)	108 (92%)	9 (8%)	0	100	100
25	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
26	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
26	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
27	e	73/94 (78%)	68 (93%)	4 (6%)	1 (1%)	9	40
27	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
28	f	71/86 (83%)	66 (93%)	5 (7%)	0	100	100
28	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
29	g	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	8	40
29	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	2	22
30	h	101/146 (69%)	97 (96%)	4 (4%)	0	100	100
30	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
31	i	95/110 (86%)	90 (95%)	5 (5%)	0	100	100
31	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
All	All	6605/10115 (65%)	6038 (91%)	515 (8%)	52 (1%)	19	53

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	426	ASN
6	D	608	LEU
7	E	448	TYR
8	F	325	THR
8	F	385	SER
8	F	386	ALA
8	F	387	LYS
14	P	1299	ILE
15	Q	368	ILE
21	W	34	LEU
21	W	52	LYS
27	e	33	GLU
29	y	50	ASP
3	A	29	PRO
6	D	574	ILE
7	E	411	GLN
7	E	412	SER
7	E	449	SER
7	E	510	ASP
8	F	326	GLU
8	F	412	GLN
14	P	363	VAL
14	P	413	ILE
21	W	17	ASP
21	W	18	HIS
21	W	51	THR
21	W	68	PRO
21	W	121	PRO
21	W	124	LEU
23	Y	71	GLN
4	B	44	VAL
5	C	122	ALA
7	E	377	ASP
7	E	512	LYS
7	E	513	PHE
7	E	530	PRO
21	W	29	VAL
29	g	21	GLY
7	E	447	PHE
14	P	107	ALA
21	W	12	PRO
24	Z	19	ILE
7	E	267	PRO

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Mol	Chain	Res	Type
19	U	232	GLY
29	y	30	ARG
29	y	60	GLN
7	E	266	SER
14	P	364	THR
14	P	486	PRO
21	W	159	VAL
7	E	509	ILE
14	P	1031	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	136/236 (58%)	135 (99%)	1 (1%)	81	86
5	C	127/214 (59%)	124 (98%)	3 (2%)	44	63
6	D	266/603 (44%)	266 (100%)	0	100	100
7	E	515/519 (99%)	512 (99%)	3 (1%)	84	88
8	F	148/451 (33%)	144 (97%)	4 (3%)	40	60
9	G	175/448 (39%)	174 (99%)	1 (1%)	84	88
10	H	84/183 (46%)	83 (99%)	1 (1%)	67	78
12	J	34/568 (6%)	33 (97%)	1 (3%)	37	58
13	O	739/867 (85%)	738 (100%)	1 (0%)	92	94
14	P	1093/1244 (88%)	1093 (100%)	0	100	100
15	Q	192/391 (49%)	192 (100%)	0	100	100
16	R	154/189 (82%)	154 (100%)	0	100	100
17	S	93/97 (96%)	93 (100%)	0	100	100
18	T	429/492 (87%)	424 (99%)	5 (1%)	67	78
19	U	158/216 (73%)	157 (99%)	1 (1%)	84	88
20	V	118/259 (46%)	116 (98%)	2 (2%)	56	72
21	W	161/219 (74%)	151 (94%)	10 (6%)	15	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Y	76/100 (76%)	75 (99%)	1 (1%)	65	77
24	Z	75/77 (97%)	75 (100%)	0	100	100
25	b	108/176 (61%)	108 (100%)	0	100	100
25	s	58/176 (33%)	58 (100%)	0	100	100
26	d	81/89 (91%)	80 (99%)	1 (1%)	67	78
26	v	71/89 (80%)	71 (100%)	0	100	100
27	e	68/83 (82%)	67 (98%)	1 (2%)	60	75
27	w	69/83 (83%)	69 (100%)	0	100	100
28	f	65/77 (84%)	65 (100%)	0	100	100
28	x	65/77 (84%)	65 (100%)	0	100	100
29	g	62/66 (94%)	62 (100%)	0	100	100
29	y	64/66 (97%)	64 (100%)	0	100	100
30	h	96/129 (74%)	94 (98%)	2 (2%)	48	66
30	t	67/129 (52%)	67 (100%)	0	100	100
31	i	90/103 (87%)	90 (100%)	0	100	100
31	u	85/103 (82%)	85 (100%)	0	100	100
All	All	5822/8819 (66%)	5784 (99%)	38 (1%)	80	86

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	38	ASN
5	C	40	ASN
5	C	43	ARG
5	C	47	ASN
7	E	25	LYS
7	E	344	LYS
7	E	417	ASN
8	F	325	THR
8	F	410	LEU
8	F	411	GLN
8	F	445	ASN
9	G	217	ASN
10	H	216	ARG
12	J	2	ARG
13	O	321	CYS

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Mol	Chain	Res	Type
18	T	27	ARG
18	T	35	TYR
18	T	81	ILE
18	T	298	HIS
18	T	317	SER
19	U	246	ILE
20	V	129	HIS
20	V	158	ARG
21	W	4	THR
21	W	8	VAL
21	W	30	ILE
21	W	31	LEU
21	W	34	LEU
21	W	36	LEU
21	W	41	GLU
21	W	50	LEU
21	W	64	LEU
21	W	160	THR
23	Y	37	GLU
26	d	65	ARG
27	e	10	MET
30	h	12	ASN
30	h	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	38	ASN
5	C	40	ASN
5	C	94	GLN
6	D	343	ASN
6	D	349	ASN
6	D	447	ASN
6	D	488	ASN
6	D	519	HIS
6	D	582	GLN
6	D	585	ASN
6	D	604	ASN
6	D	612	ASN
7	E	19	ASN
7	E	72	ASN
7	E	125	GLN

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Mol	Chain	Res	Type
7	E	177	HIS
7	E	245	GLN
7	E	298	ASN
7	E	300	GLN
7	E	366	ASN
7	E	381	ASN
7	E	393	GLN
7	E	417	ASN
7	E	442	ASN
8	F	354	GLN
8	F	445	ASN
9	G	202	GLN
9	G	217	ASN
9	G	240	ASN
10	H	72	HIS
10	H	76	HIS
13	O	376	HIS
13	O	539	HIS
13	O	695	ASN
13	O	769	ASN
13	O	853	HIS
13	O	882	ASN
13	O	887	ASN
13	O	894	HIS
13	O	908	GLN
14	P	209	GLN
14	P	248	ASN
14	P	375	ASN
14	P	382	GLN
14	P	385	HIS
14	P	436	ASN
14	P	481	GLN
14	P	504	HIS
14	P	546	ASN
14	P	590	HIS
14	P	609	HIS
14	P	754	HIS
14	P	920	GLN
14	P	944	ASN
14	P	945	HIS
14	P	950	GLN
14	P	1023	HIS

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Mol	Chain	Res	Type
14	P	1117	HIS
14	P	1154	HIS
14	P	1203	HIS
14	P	1359	ASN
15	Q	145	GLN
15	Q	288	HIS
16	R	31	GLN
16	R	47	GLN
16	R	50	GLN
16	R	170	ASN
18	T	34	HIS
18	T	91	GLN
18	T	167	ASN
18	T	202	GLN
18	T	415	HIS
18	T	440	HIS
21	W	55	HIS
21	W	85	ASN
21	W	99	GLN
21	W	133	GLN
21	W	157	GLN
21	W	158	ASN
23	Y	47	ASN
23	Y	90	ASN
24	Z	7	GLN
24	Z	37	ASN
24	Z	41	ASN
25	b	5	GLN
26	d	68	GLN
27	e	86	ASN
30	h	12	ASN
30	h	78	ASN
31	i	35	ASN
31	i	64	HIS
31	i	86	ASN
30	t	30	GLN
31	u	51	ASN
31	u	52	HIS
26	v	4	ASN
28	x	77	ASN
29	y	20	ASN
29	y	54	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	281/407 (69%)	66 (23%)	12 (4%)
11	I	35/38 (92%)	8 (22%)	2 (5%)
2	2	136/143 (95%)	46 (33%)	25 (18%)
All	All	452/588 (76%)	120 (26%)	39 (8%)

All (120) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	C
1	1	11	U
1	1	12	A
1	1	17	A
1	1	21	G
1	1	22	A
1	1	25	A
1	1	26	G
1	1	27	A
1	1	30	A
1	1	33	A
1	1	35	G
1	1	40	A
1	1	41	C
1	1	53	G
1	1	55	G
1	1	56	C
1	1	57	U
1	1	61	A
1	1	68	G
1	1	69	A
1	1	74	C
1	1	77	U
1	1	79	A
1	1	80	G
1	1	86	A
1	1	87	U
1	1	117	U
1	1	118	U
1	1	119	G
1	1	124	A
1	1	133	G
1	1	134	G

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Mol	Chain	Res	Type
1	1	135	U
1	1	136	C
1	1	137	A
1	1	140	C
1	1	141	A
1	1	142	C
1	1	143	A
1	1	144	C
1	1	154	G
1	1	155	G
1	1	167	G
1	1	168	C
1	1	172	C
1	1	187	G
1	1	254	U
1	1	256	U
1	1	257	G
1	1	258	U
1	1	259	U
1	1	540	G
1	1	541	G
1	1	551	U
1	1	554	U
1	1	555	U
1	1	556	U
1	1	557	U
1	1	558	U
1	1	559	G
1	1	560	A
1	1	561	U
1	1	562	U
1	1	563	U
1	1	564	A
2	2	33	U
2	2	41	C
2	2	46	C
2	2	47	U
2	2	66	A
2	2	67	A
2	2	68	U
2	2	83	U
2	2	111	C

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Mol	Chain	Res	Type
2	2	112	A
2	2	113	U
2	2	117	U
2	2	140	G
2	2	141	A
2	2	142	C
2	2	1094	G
2	2	1095	U
2	2	1096	C
2	2	1097	G
2	2	1098	C
2	2	1100	A
2	2	1101	C
2	2	1102	C
2	2	1103	C
2	2	1104	U
2	2	1105	C
2	2	1106	G
2	2	1107	C
2	2	1108	A
2	2	1119	C
2	2	1120	G
2	2	1121	U
2	2	1122	U
2	2	1123	C
2	2	1124	U
2	2	1125	U
2	2	1126	G
2	2	1130	U
2	2	1139	G
2	2	1141	C
2	2	1142	G
2	2	1143	C
2	2	1144	U
2	2	1145	U
2	2	1146	G
2	2	1149	G
11	I	58	U
11	I	62	A
11	I	70	A
11	I	71	C
11	I	72	A

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Mol	Chain	Res	Type
11	I	74	A
11	I	78	A
11	I	79	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	16	U
1	1	21	G
1	1	39	U
1	1	54	C
1	1	67	A
1	1	76	U
1	1	86	A
1	1	134	G
1	1	135	U
1	1	136	C
1	1	553	A
1	1	560	A
2	2	32	G
2	2	46	C
2	2	66	A
2	2	67	A
2	2	110	A
2	2	1095	U
2	2	1096	C
2	2	1097	G
2	2	1100	A
2	2	1101	C
2	2	1102	C
2	2	1105	C
2	2	1107	C
2	2	1119	C
2	2	1120	G
2	2	1121	U
2	2	1122	U
2	2	1123	C
2	2	1124	U
2	2	1125	U
2	2	1138	G
2	2	1141	C
2	2	1142	G

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Mol	Chain	Res	Type
2	2	1144	U
2	2	1145	U
11	I	77	C
11	I	78	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	5	1	18,21,22	1.47	2 (11%)	22,30,33	1.25	2 (9%)
2	PSU	2	35	11,2	18,21,22	1.06	1 (5%)	22,30,33	1.72	5 (22%)
2	PSU	2	42	11,2	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
2	PSU	2	44	11,2	18,21,22	1.03	1 (5%)	22,30,33	1.66	4 (18%)
1	PSU	1	6	11,1	18,21,22	1.35	1 (5%)	22,30,33	1.21	2 (9%)

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
1	PSU	1	5	1	-	0/7/25/26	0/2/2/2
2	PSU	2	35	11,2	-	0/7/25/26	0/2/2/2
2	PSU	2	42	11,2	-	0/7/25/26	0/2/2/2
2	PSU	2	44	11,2	-	0/7/25/26	0/2/2/2
1	PSU	1	6	11,1	-	0/7/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	5	PSU	C2-N1	4.33	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	6	PSU	C2-N1	3.91	1.42	1.36
2	2	42	PSU	C6-C5	3.50	1.39	1.35
2	2	35	PSU	C6-C5	3.33	1.39	1.35
2	2	44	PSU	C6-C5	3.25	1.39	1.35
1	1	5	PSU	C4-C5	-2.02	1.38	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	42	PSU	C4-N3-C2	-4.58	119.74	126.34
2	2	35	PSU	C4-N3-C2	-4.47	119.90	126.34
2	2	42	PSU	N1-C2-N3	4.38	120.09	115.13
2	2	35	PSU	N1-C2-N3	4.36	120.07	115.13
2	2	44	PSU	N1-C2-N3	4.32	120.02	115.13
2	2	44	PSU	C4-N3-C2	-4.09	120.45	126.34
1	1	6	PSU	C6-N1-C2	-3.62	118.98	122.68
1	1	5	PSU	O2-C2-N1	3.53	126.68	122.79
1	1	5	PSU	C6-N1-C2	-2.99	119.62	122.68
2	2	44	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	44	PSU	O2-C2-N1	-2.46	120.09	122.79
2	2	35	PSU	O2-C2-N1	-2.35	120.20	122.79
2	2	35	PSU	C6-N1-C2	-2.21	120.42	122.68
2	2	42	PSU	O2-C2-N1	-2.18	120.40	122.79
1	1	6	PSU	C5-C6-N1	2.06	125.19	122.11
2	2	42	PSU	C6-N1-C2	-2.05	120.59	122.68
2	2	35	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	10
1	1	4
11	I	2
10	H	2
22	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	10:A	O3'	51:C	P	64.91
1	1	440:N	O3'	516:U	P	49.12
1	1	325:A	O3'	378:N	P	48.87
1	2	122:A	O3'	139:G	P	46.36
1	1	532:U	O3'	538:C	P	25.27
1	2	86:U	O3'	108:A	P	24.04
1	2	1130:U	O3'	1138:G	P	22.40
1	2	150:G	O3'	1089:G	P	18.75
1	2	73:U	O3'	79:A	P	17.45
1	1	394:N	O3'	424:N	P	17.14
1	I	53:U	O3'	57:C	P	15.85
1	2	1154:U	O3'	1159:U	P	14.23
1	X	44:UNK	C	50:UNK	N	11.40
1	2	1108:A	O3'	1115:G	P	10.88
1	H	138:UNK	C	175:UNK	N	9.48
1	H	120:UNK	C	126:UNK	N	8.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1149:G	O3'	1150:U	P	1.90
1	2	143:G	O3'	144:G	P	1.83
1	2	1090:A	O3'	1091:G	P	1.78

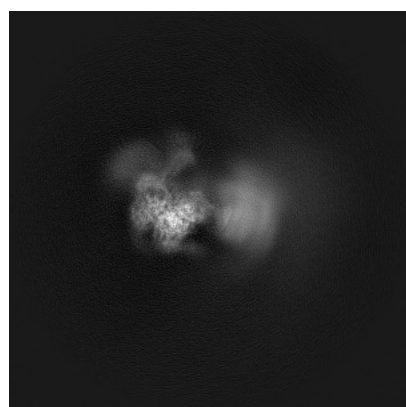
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4364. These allow visual inspection of the internal detail of the map and identification of artifacts.

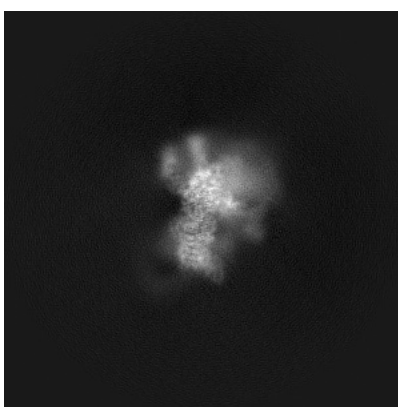
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

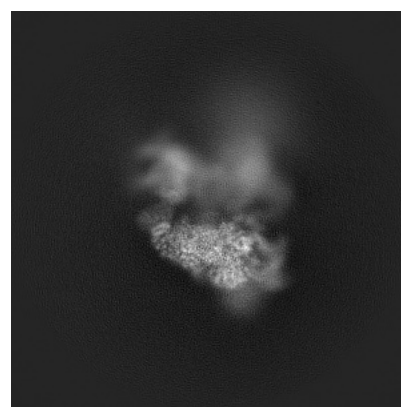
6.1.1 Primary map



X



Y

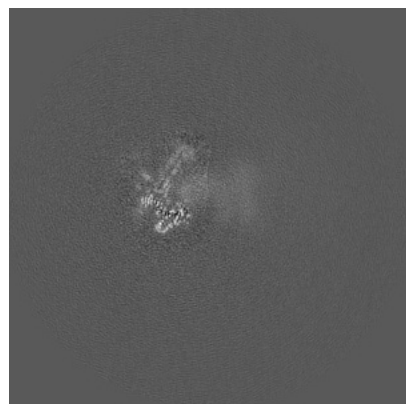


Z

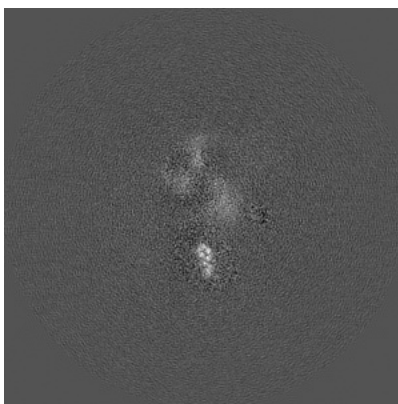
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

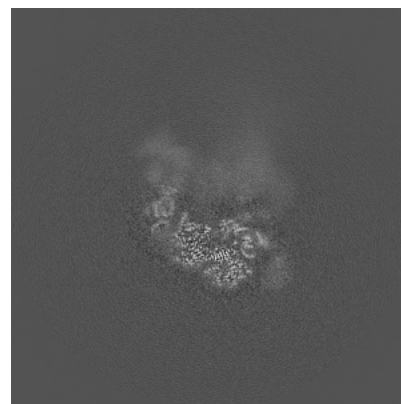
6.2.1 Primary map



X Index: 280



Y Index: 280

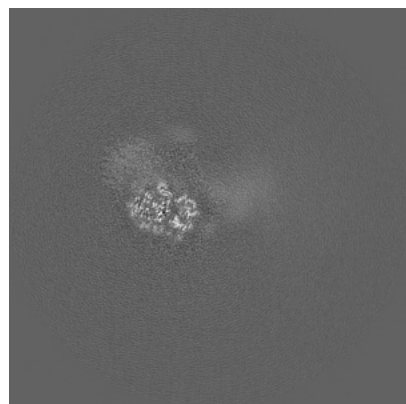


Z Index: 280

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

6.3 Largest variance slices [i](#)

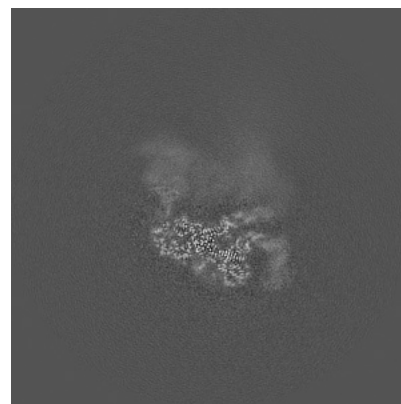
6.3.1 Primary map



X Index: 303



Y Index: 225

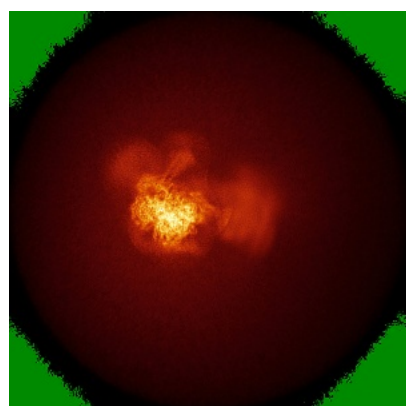


Z Index: 271

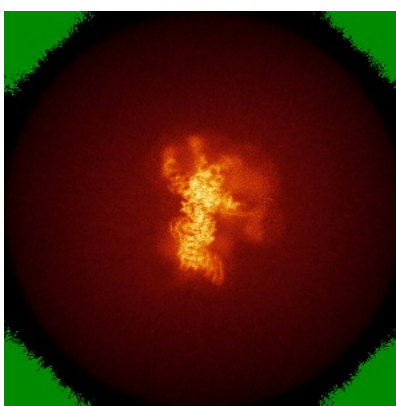
The images above show the largest variance slices of the map in three orthogonal directions.

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

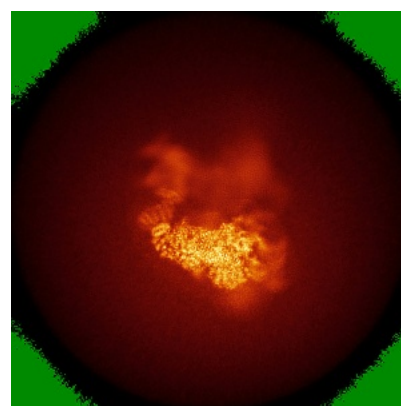
6.4.1 Primary map



X



Y

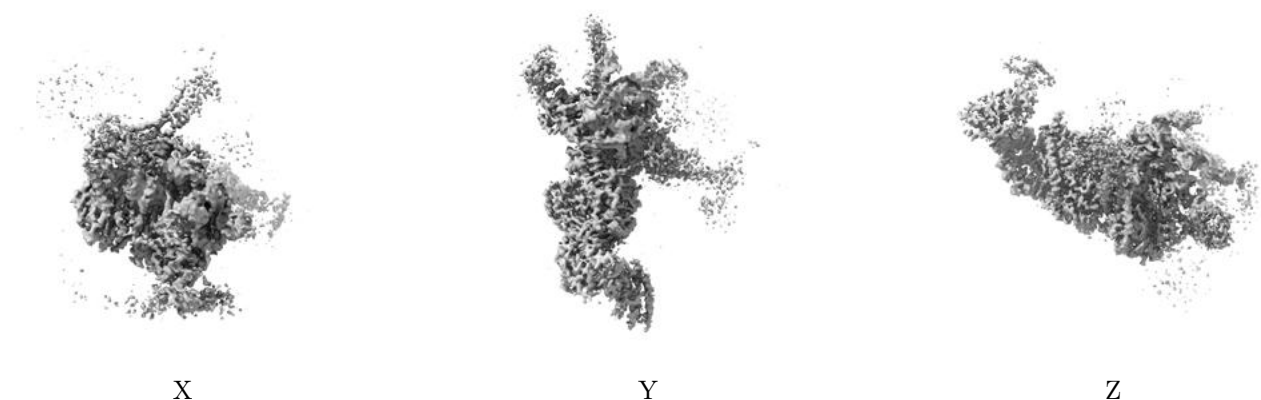


Z

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 0.0369. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

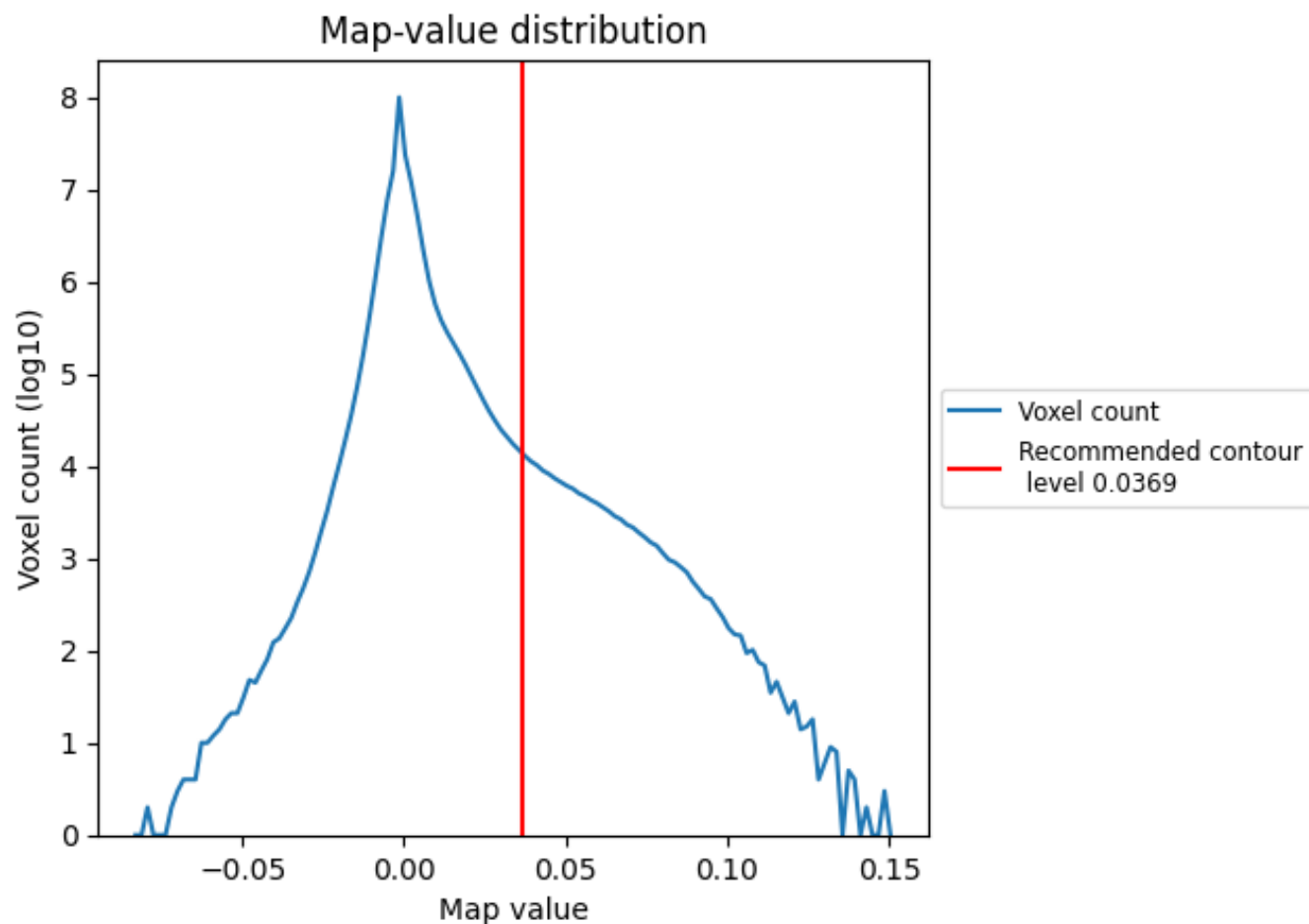
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

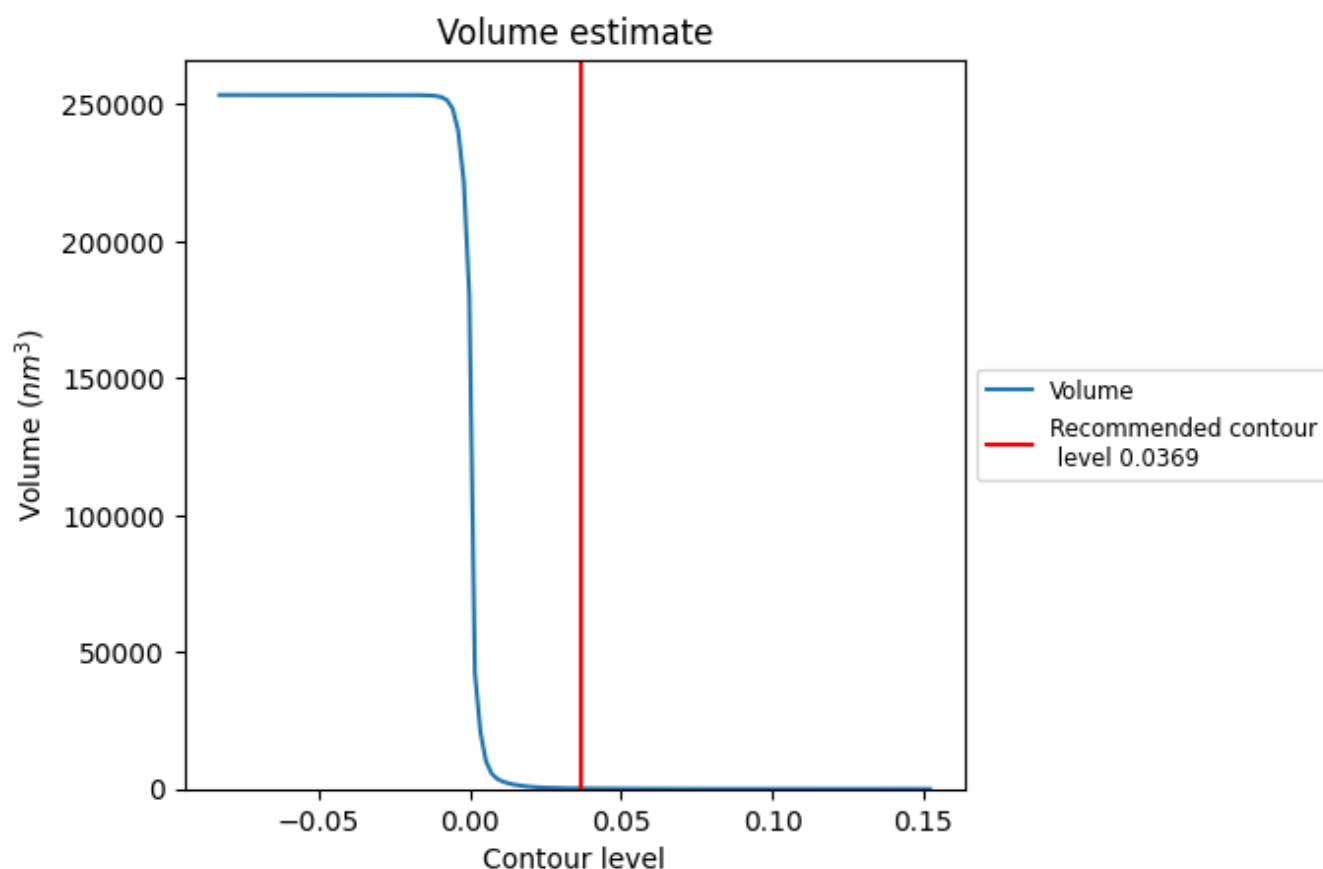
This section contains the results of statistical analysis of the map.

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.

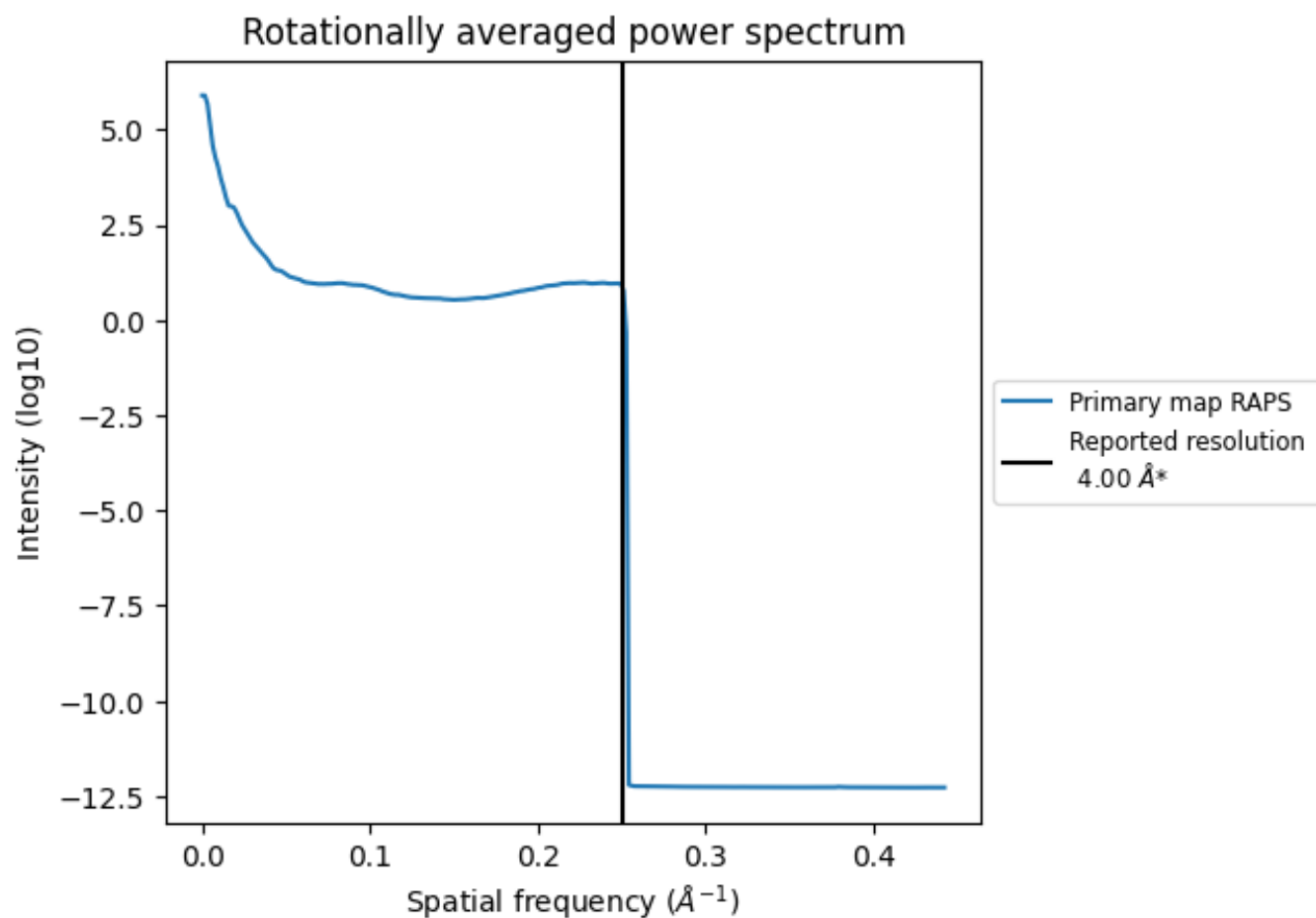
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm^3 ; this corresponds to an approximate mass of 171 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

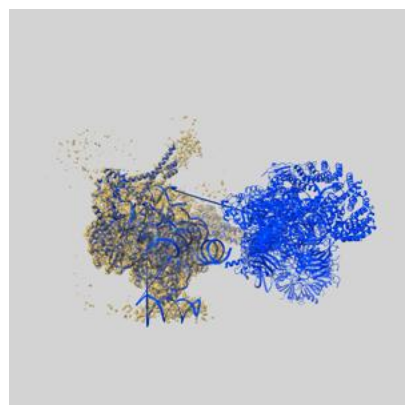
8 Fourier-Shell correlation ⓘ

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

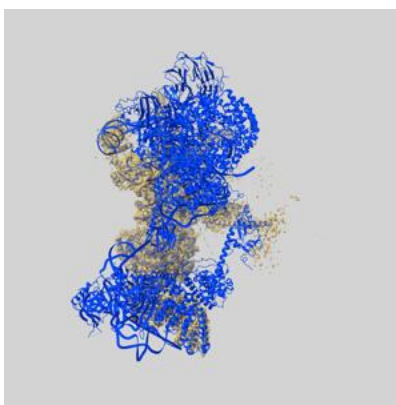
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4364 and PDB model 6G90. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

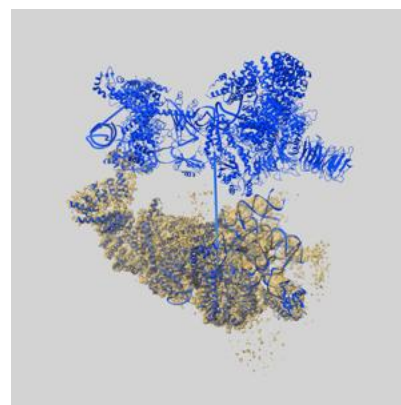
9.1 Map-model overlay [i](#)



X



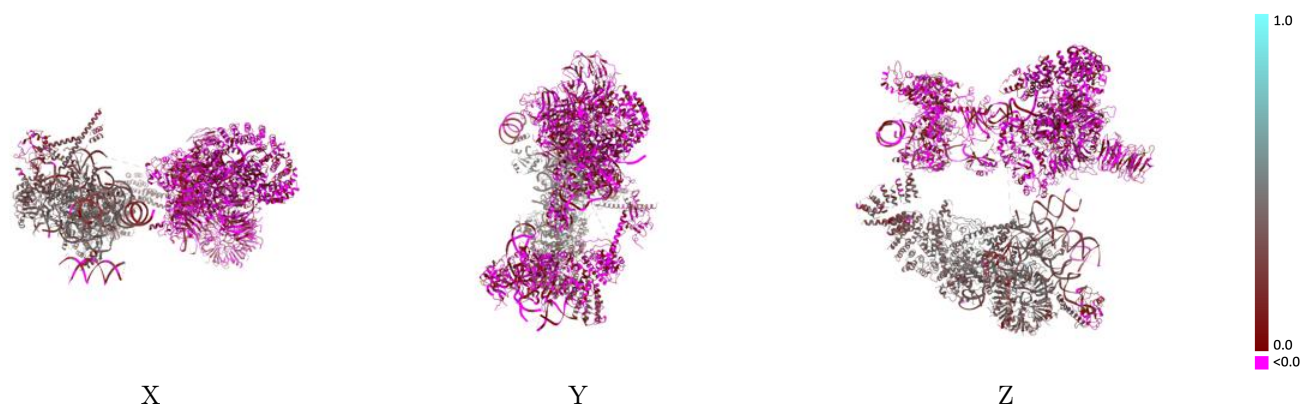
Y



Z

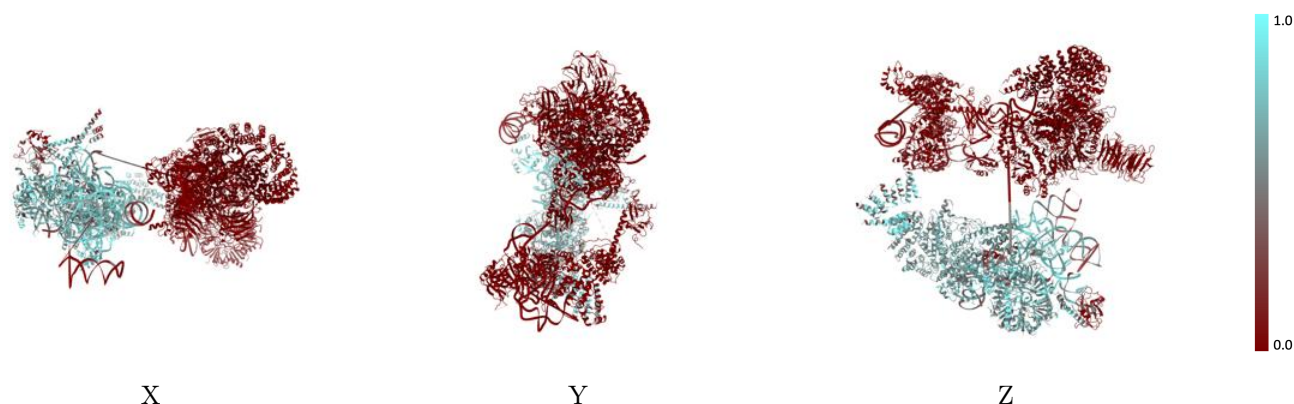
The images above show the 3D surface view of the map at the recommended contour level 0.0369 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



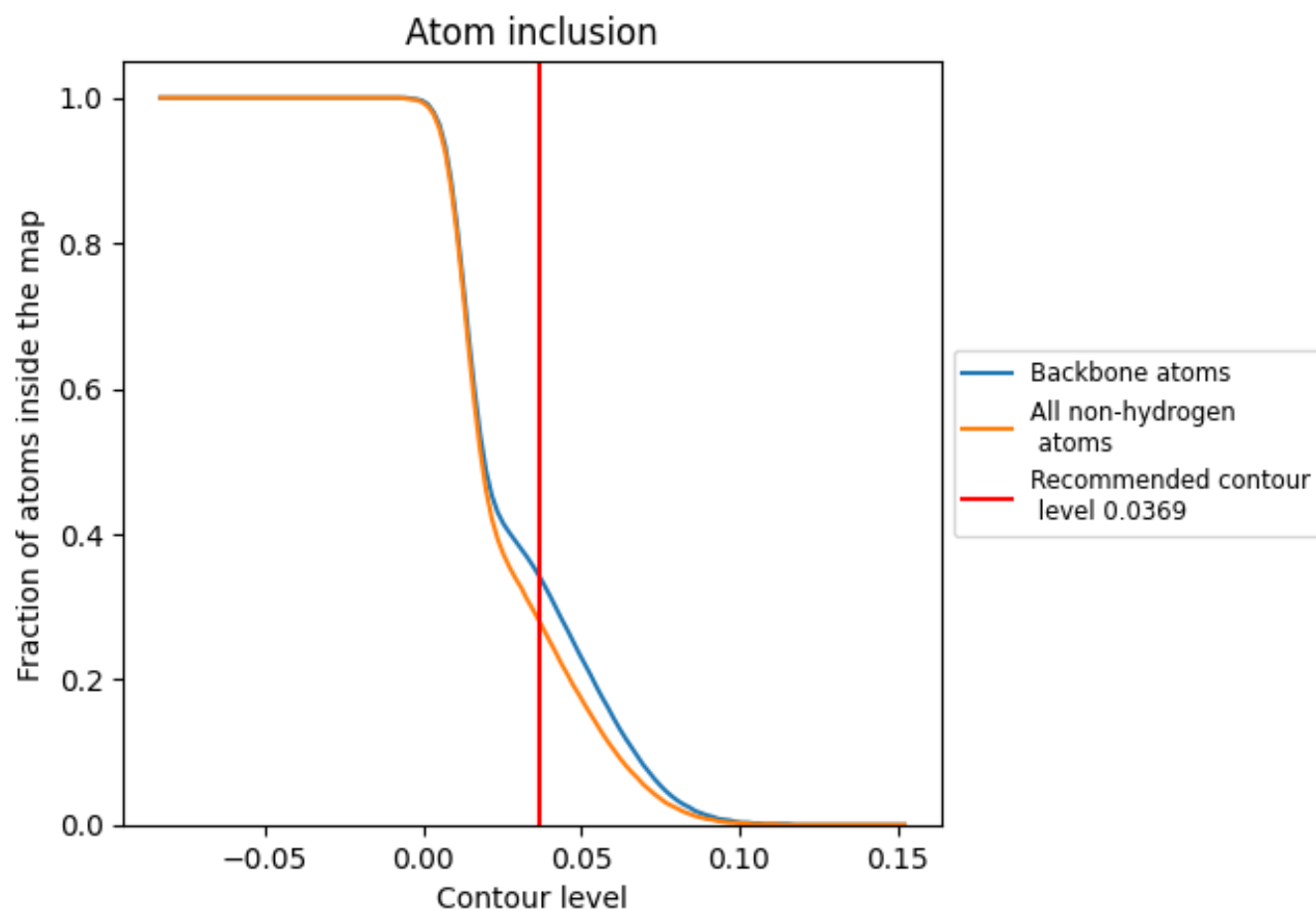
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0369).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 28% 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 (0.0369) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2790	 0.1520
1	 0.6780	 0.2970
2	 0.0000	 0.0010
A	 0.7990	 0.3950
B	 0.3390	 0.1890
C	 0.6650	 0.4050
D	 0.6580	 0.3440
E	 0.6800	 0.3970
F	 0.6370	 0.3920
G	 0.6570	 0.3800
H	 0.5710	 0.3040
I	 0.2190	 0.0990
J	 0.7040	 0.4150
O	 0.0000	 -0.0020
P	 0.0000	 0.0010
Q	 0.0000	 -0.0020
R	 0.0000	 0.0120
S	 0.0000	 0.0090
T	 0.0000	 0.0070
U	 0.0000	 0.0040
V	 0.0000	 -0.0060
W	 0.0310	 0.0250
X	 0.6120	 0.3000
Y	 0.0210	 0.0230
Z	 0.0000	 0.0080
b	 0.6260	 0.4070
d	 0.6770	 0.4380
e	 0.6250	 0.3770
f	 0.6290	 0.3320
g	 0.6440	 0.4250
h	 0.6390	 0.3970
i	 0.6240	 0.3460
s	 0.0000	 -0.0080
t	 0.0000	 -0.0400
u	 0.0000	 0.0300



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Chain	Atom inclusion	Q-score
v	 0.0000	 0.0160
w	 0.0000	 -0.0150
x	 0.0000	 0.0370
y	 0.0000	 0.0090