Full wwPDB EM Validation Report ⓘ

Aug 12, 2024 – 06:15 pm BST

PDB ID	:	8RO1
EMDB ID	:	EMD-19398
Title	:	Structure of the C. elegans Intron Lariat Spliceosome double-primed for disassembly (ILS")
Authors	:	Vorlaender, M.K.; Rothe, P.; Plaschka, C.
Deposited on	:	2024-01-11
Resolution	:	3.00 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:

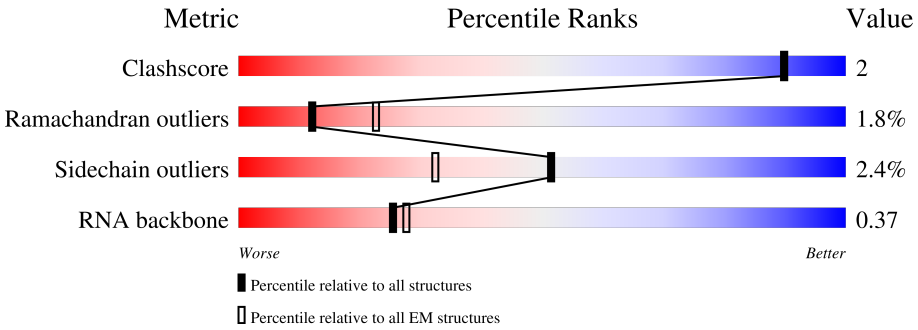
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
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 <=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	2	228	5% 21% 10% 67%
2	5	112	46% 36% 15%
3	6	101	38% 46% 14%
4	A	2329	74% 9% 15%
5	C	974	82% 9% 8%
6	D	267	21% 70% 26%
7	DX	739	8% 85% 7% 8%

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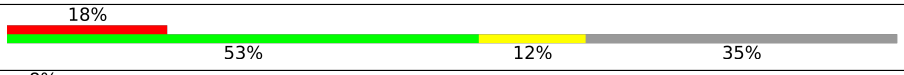
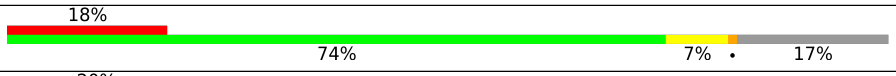
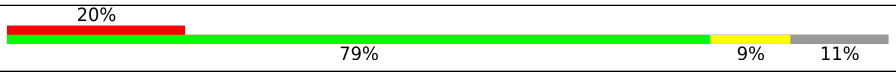
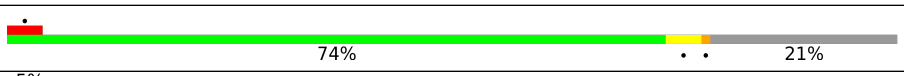
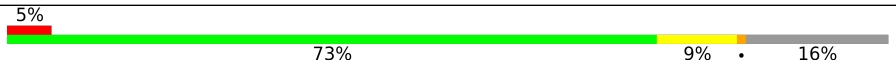
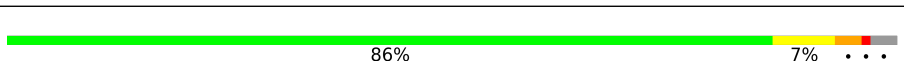
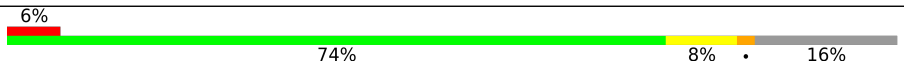
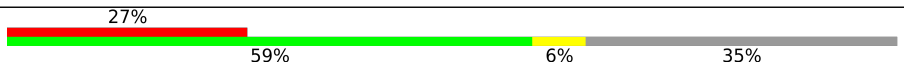
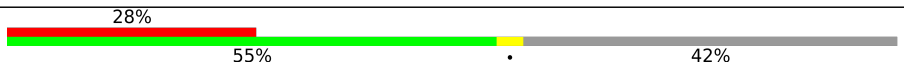
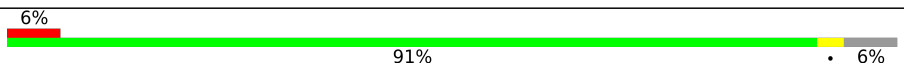
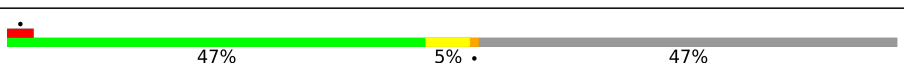
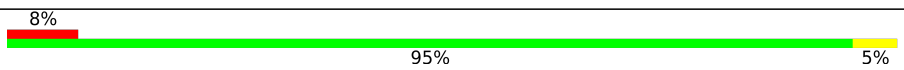
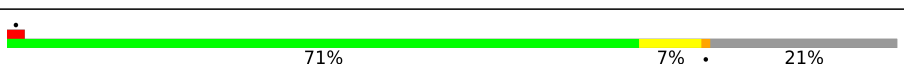
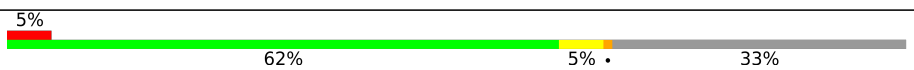
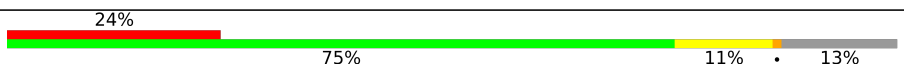
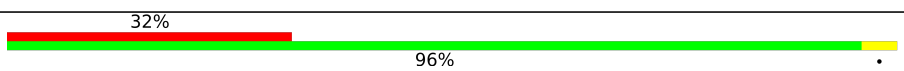
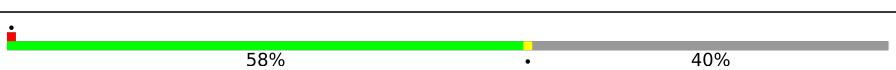
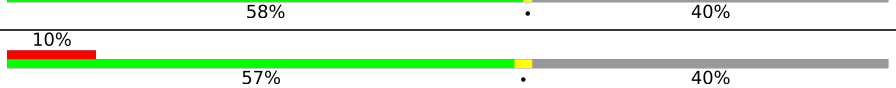
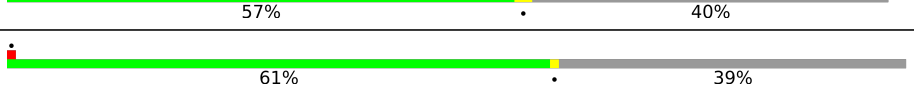
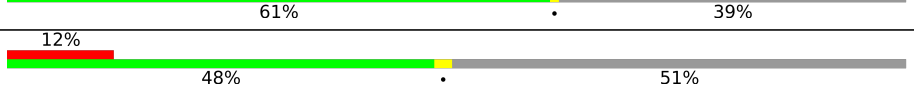
Mol	Chain	Length	Quality of chain
8	E	331	
9	I	855	
10	IN	51	
11	J	744	
12	K	238	
13	L	755	
14	L1	533	
15	L2	460	
16	M	234	
17	N	147	
18	O	408	
19	P	230	
20	PX	809	
21	Q	1467	
22	R	535	
23	S	169	
24	T	494	
25	TF	830	
26	W	567	
27	X	500	
28	Z	69	
29	a	136	
29	h	136	
30	b	160	
30	i	160	

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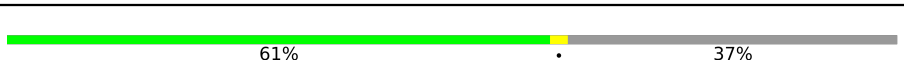
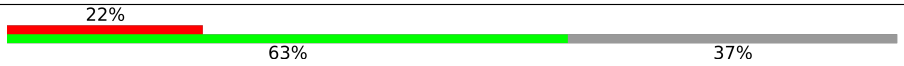
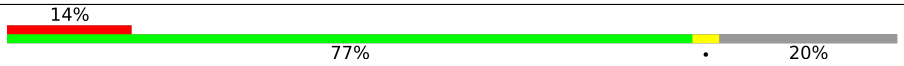
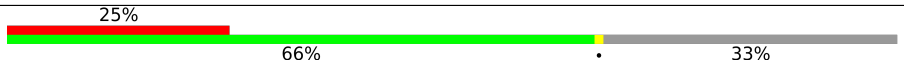
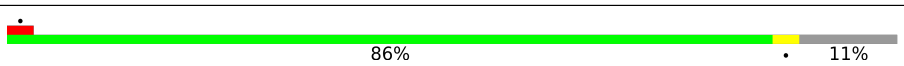
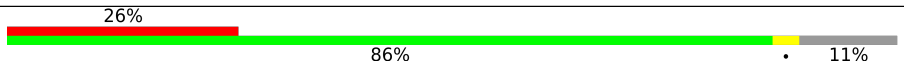
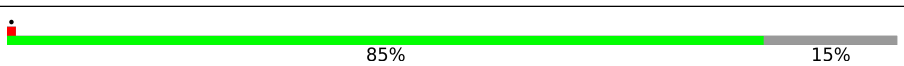
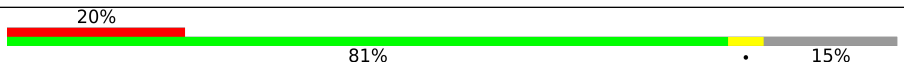
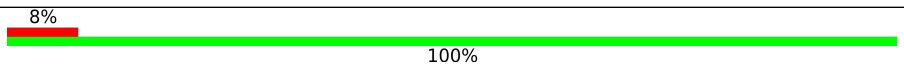
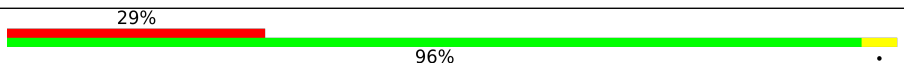
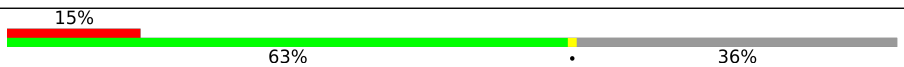
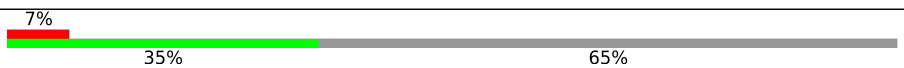
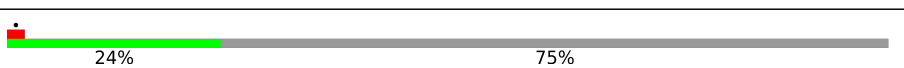
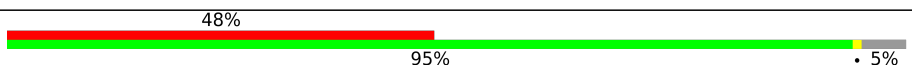
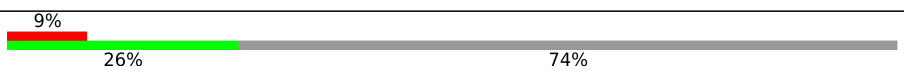
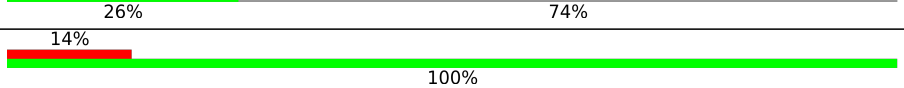
Mol	Chain	Length	Quality of chain
31	c	127	
31	j	127	
32	d	118	
32	k	118	
33	e	90	
33	l	90	
34	f	85	
34	m	85	
35	g	77	
35	n	77	
36	o	253	
37	p	217	
38	q	492	
38	r	492	
38	s	492	
38	t	492	
39	y	79	

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 120201 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	76	1268	554	140	498	76	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	111	2350	1052	405	782	111	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	101	2153	965	391	696	101	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1982	16424	10576	2868	2904	76	0	0

- Molecule 5 is a protein called Tr-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	898	7153	4558	1211	1338	46	0	0

- Molecule 6 is a protein called Protein isy-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	198	1629	1016	293	316	4	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DX	682	Total	C	N	O	S	0	0
			5465	3464	941	1026	34		

- Molecule 8 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	312	Total	C	N	O	S	0	0
			2445	1528	429	468	20		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	747	Total	C	N	O	S	0	0
			6169	3916	1081	1128	44		

- Molecule 10 is a RNA chain called Intron lariat RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	IN	33	Total	C	N	O	P	0	0
			425	179	12	201	33		

- Molecule 11 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	574	Total	C	N	O	S	0	0
			4895	3122	855	898	20		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	203	Total	C	N	O	S	0	0
			1666	1041	298	310	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	623	Total	C	N	O	S	0	0
			5030	3115	928	962	25		

- Molecule 14 is a protein called CWF19-like protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L1	472	Total	C	N	O	S	0	0
			3683	2345	616	701	21		

- Molecule 15 is a protein called CWF19-like protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L2	362	Total	C	N	O	S	0	0
			2974	1846	543	568	17		

- Molecule 16 is a protein called Pre-mRNA-splicing factor syf-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	196	Total	C	N	O	S	0	0
			1654	1021	308	319	6		

- Molecule 17 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	142	Total	C	N	O	S	0	0
			1163	731	212	208	12		

- Molecule 18 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	342	Total	C	N	O	S	0	0
			2721	1703	493	506	19		

- Molecule 19 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	150	Total	C	N	O	S	0	0
			1207	729	232	240	6		

- Molecule 20 is a protein called GCF C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	PX	472	Total	C	N	O	S	0	0
			3838	2396	695	720	27		

- Molecule 21 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	1378	Total	C	N	O	S	0	0
			11293	7218	1964	2064	47		

- Molecule 22 is a protein called Uncharacterized protein T27F2.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	282	Total	C	N	O	S	0	0
			2209	1379	404	416	10		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	169	Total	C	N	O	S	0	0
			1303	818	233	245	7		

- Molecule 24 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	389	Total	C	N	O	S	0	0
			3082	1946	557	560	19		

- Molecule 25 is a protein called Septin and tuftelin-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	TF	559	Total	C	N	O	S	0	0
			4542	2908	769	838	27		

- Molecule 26 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	496	Total	C	N	O	S	0	0
			4072	2584	726	747	15		

- Molecule 27 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	80	Total	C	N	O	S	0	0
			661	407	123	126	5		

- Molecule 28 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	69	Total	C	N	O	S	0	0
			569	356	104	107	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	81	Total	C	N	O	S	0	0
			635	396	113	120	6		
29	h	81	Total	C	N	O	S	0	0
			635	396	113	120	6		

- Molecule 30 is a protein called Probable small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	98	Total	C	N	O	S	0	0
			755	475	141	131	8		
30	i	79	Total	C	N	O	S	0	0
			639	405	117	111	6		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	80	Total	C	N	O	S	0	0
			622	396	109	113	4		
31	j	80	Total	C	N	O	S	0	0
			622	396	109	113	4		

- Molecule 32 is a protein called Probable small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	94	Total	C	N	O	S	0	0
			749	469	135	140	5		
32	k	79	Total	C	N	O	S	0	0
			632	398	118	111	5		

- Molecule 33 is a protein called Probable small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	80	Total	C	N	O	S	0	0
			665	424	118	121	2		
33	l	80	Total	C	N	O	S	0	0
			665	424	118	121	2		

- Molecule 34 is a protein called Probable small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			558	359	93	102	4		
34	m	72	Total	C	N	O	S	0	0
			558	359	93	102	4		

- Molecule 35 is a protein called Probable small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	77	Total	C	N	O	S	0	0
			608	379	107	115	7		
35	n	77	Total	C	N	O	S	0	0
			608	379	107	115	7		

- Molecule 36 is a protein called Probable U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	162	Total	C	N	O	S	0	0
			1335	849	236	243	7		

- Molecule 37 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	76	Total	C	N	O	S	0	0
			626	402	114	106	4		

- Molecule 38 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	121	Total	C	N	O	S	0	0
			941	585	165	186	5		
38	r	131	Total	C	N	O	S	0	0
			1004	621	179	199	5		
38	s	469	Total	C	N	O	S	0	0
			3571	2239	620	703	9		
38	t	128	Total	C	N	O	S	0	0
			993	620	173	195	5		

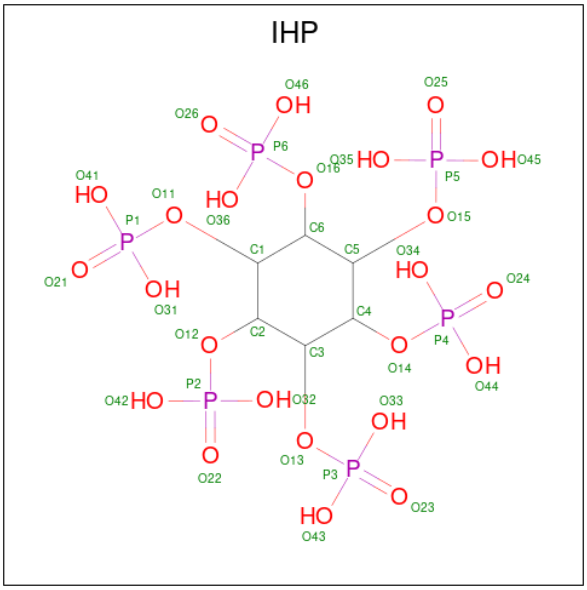
- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	79	Total	C	N	O	S	0	0
			619	396	100	118	5		

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

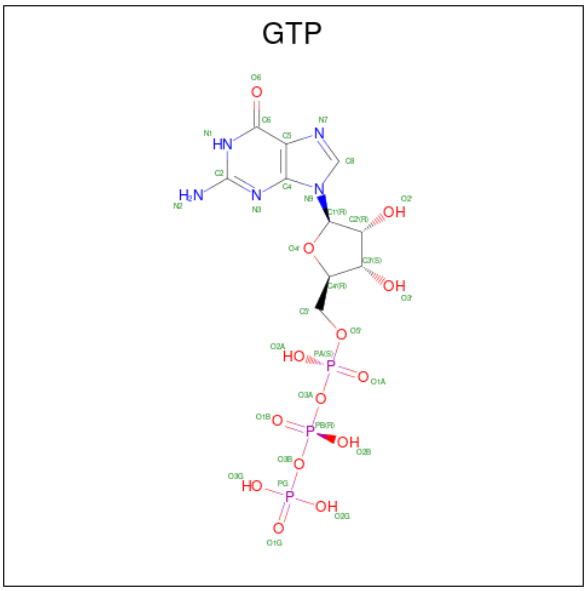
Mol	Chain	Residues	Atoms		AltConf
40	6	6	Total	Mg	0
			6	6	
40	C	1	Total	Mg	0
			1	1	

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 43 is ZINC ION (three-letter code: ZN) (formula: Zn).

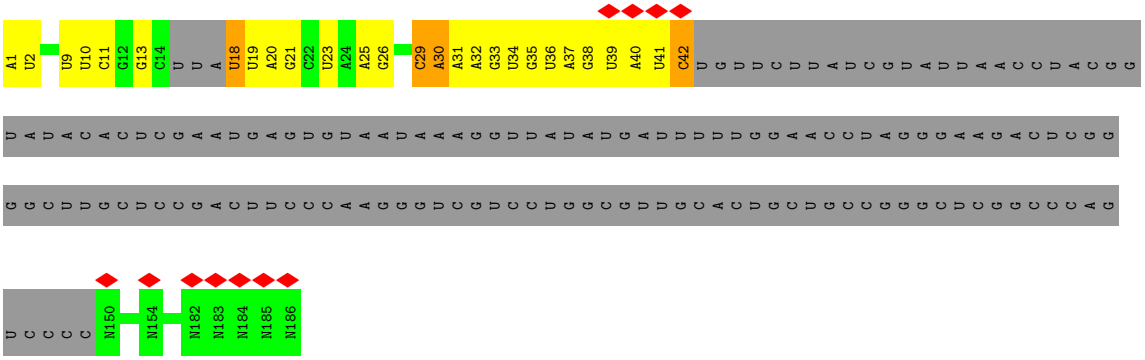
Mol	Chain	Residues	Atoms		AltConf
43	L2	1	Total	Zn	0
			1	1	
43	N	3	Total	Zn	0
			3	3	
43	O	3	Total	Zn	0
			3	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

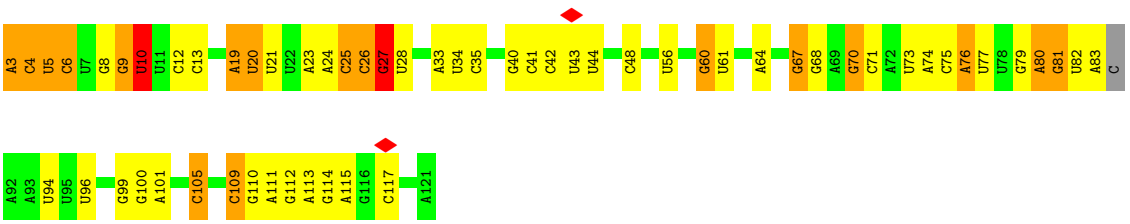
• Molecule 1: U2 snRNA

Chain 2:



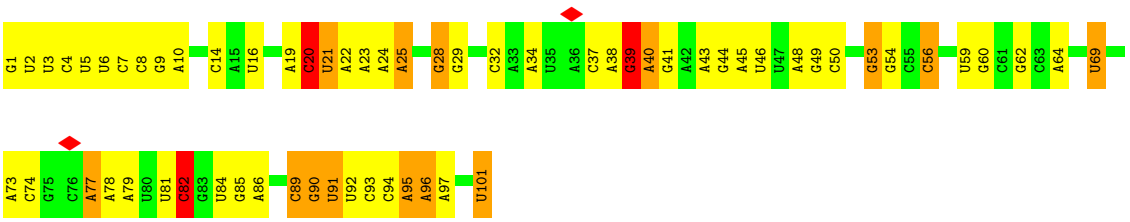
• Molecule 2: U5 snRNA

Chain 5:



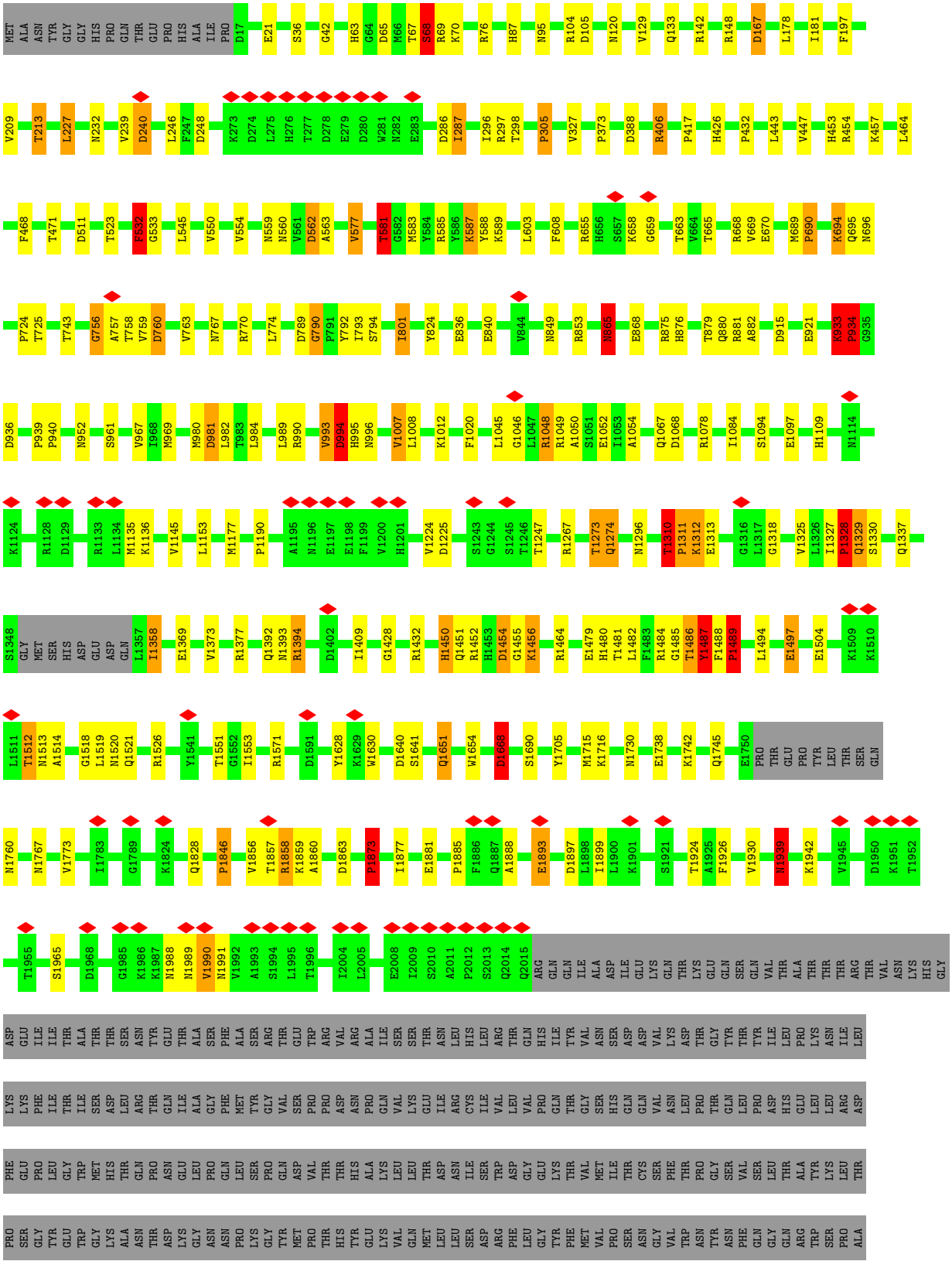
• Molecule 3: U6 snRNA

Chain 6:



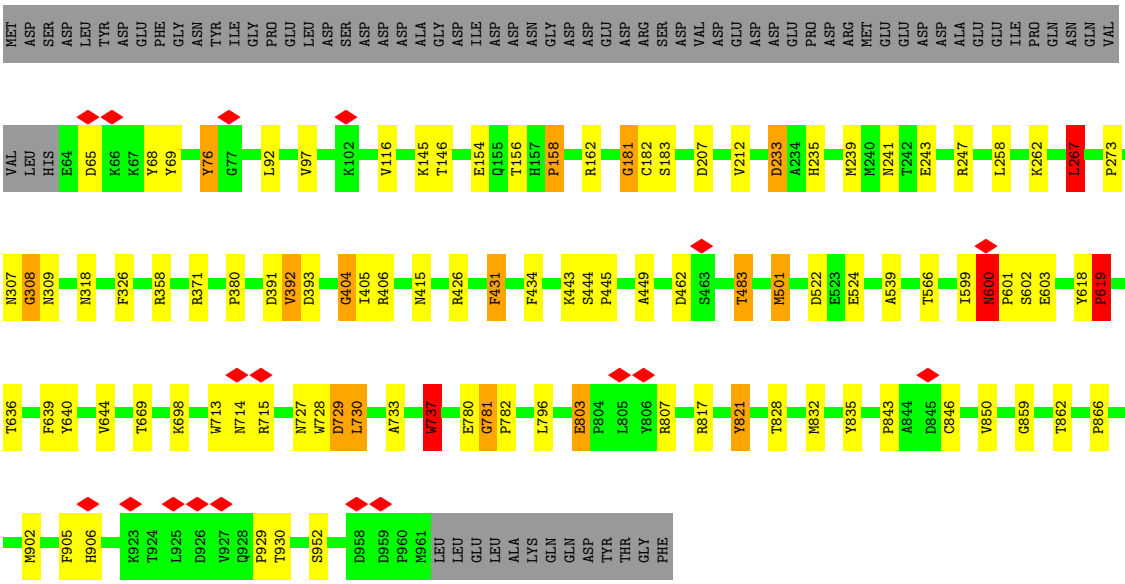
• Molecule 4: Pre-mRNA-splicing factor 8 homolog

Chain A:



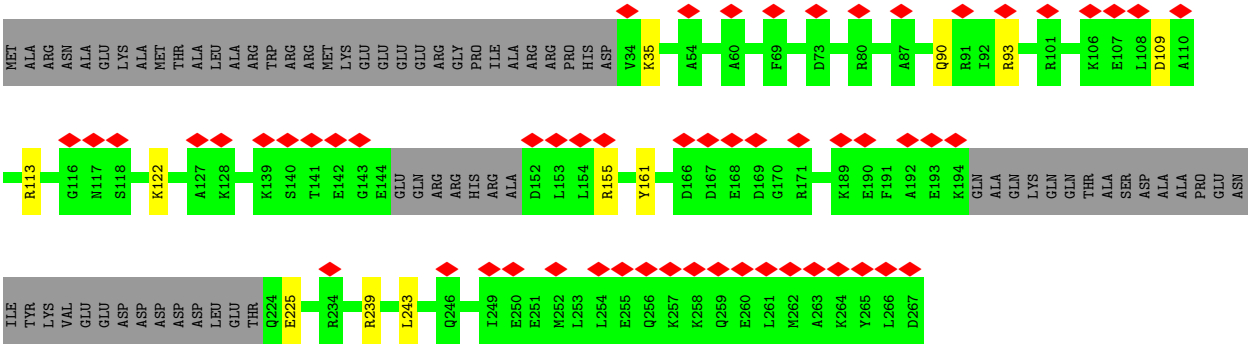
• Molecule 5: Tr-type G domain-containing protein

Chain C:



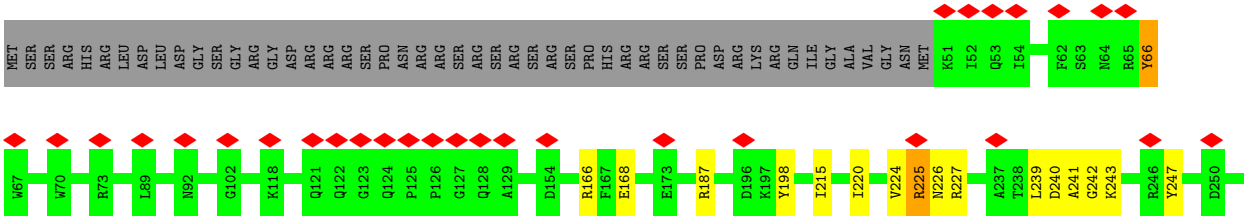
• Molecule 6: Protein isy-1

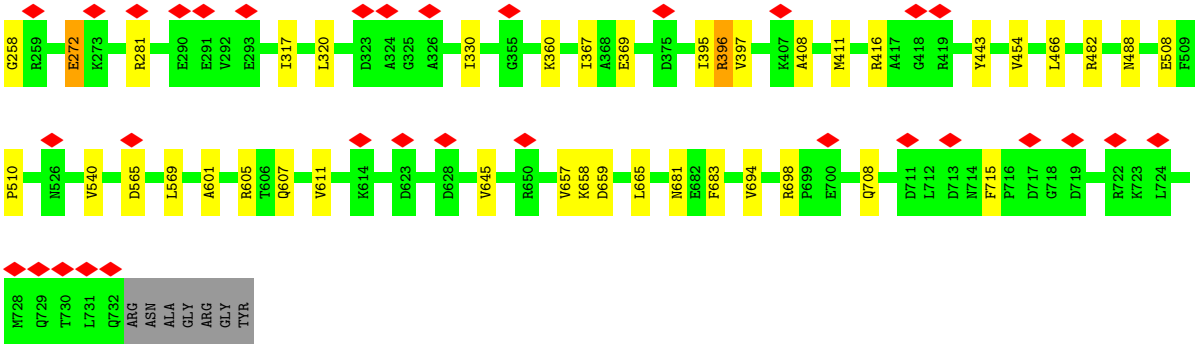
Chain D:



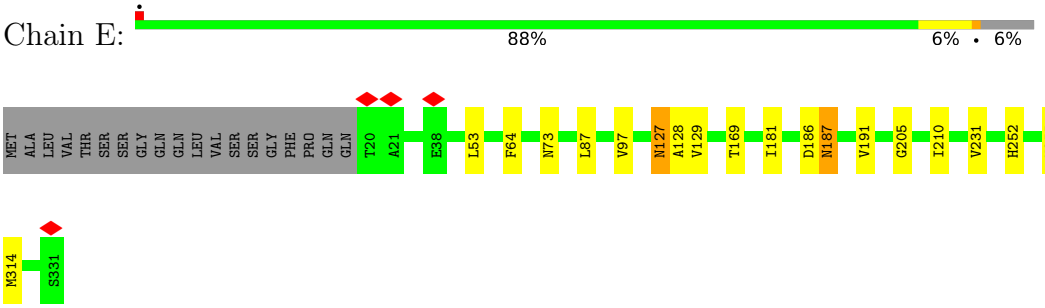
• Molecule 7: Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15

Chain DX:

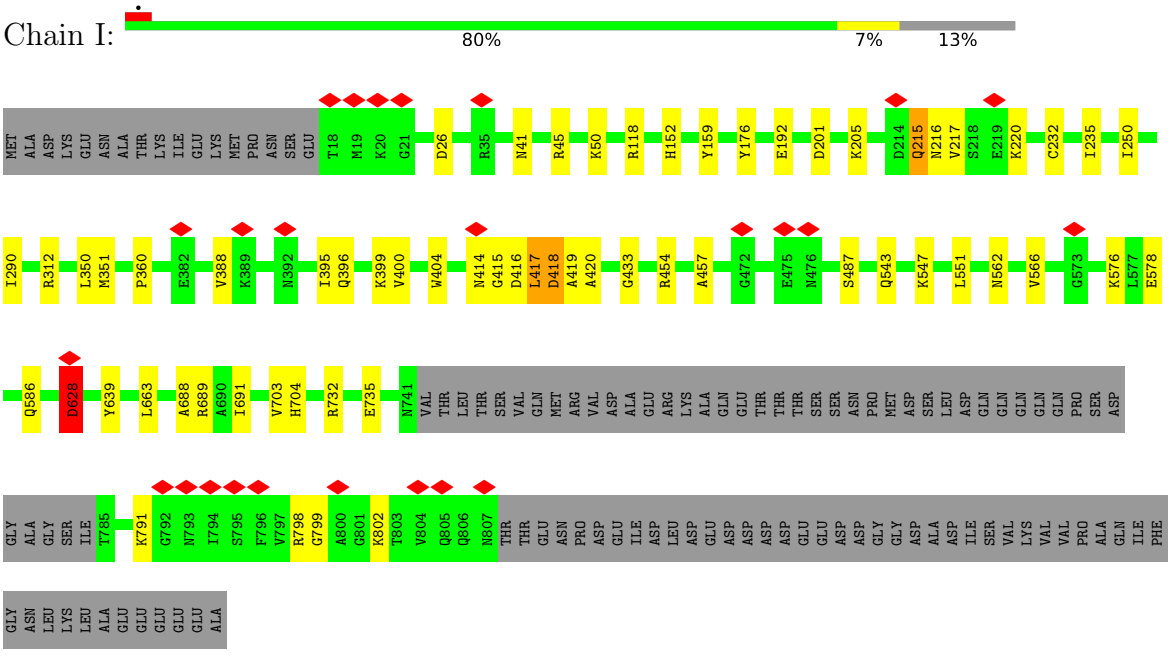




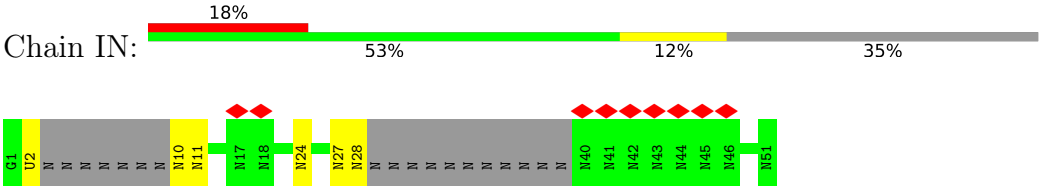
• Molecule 8: WD_REPEATS_REGION domain-containing protein



• Molecule 9: Pre-mRNA-splicing factor SYF1

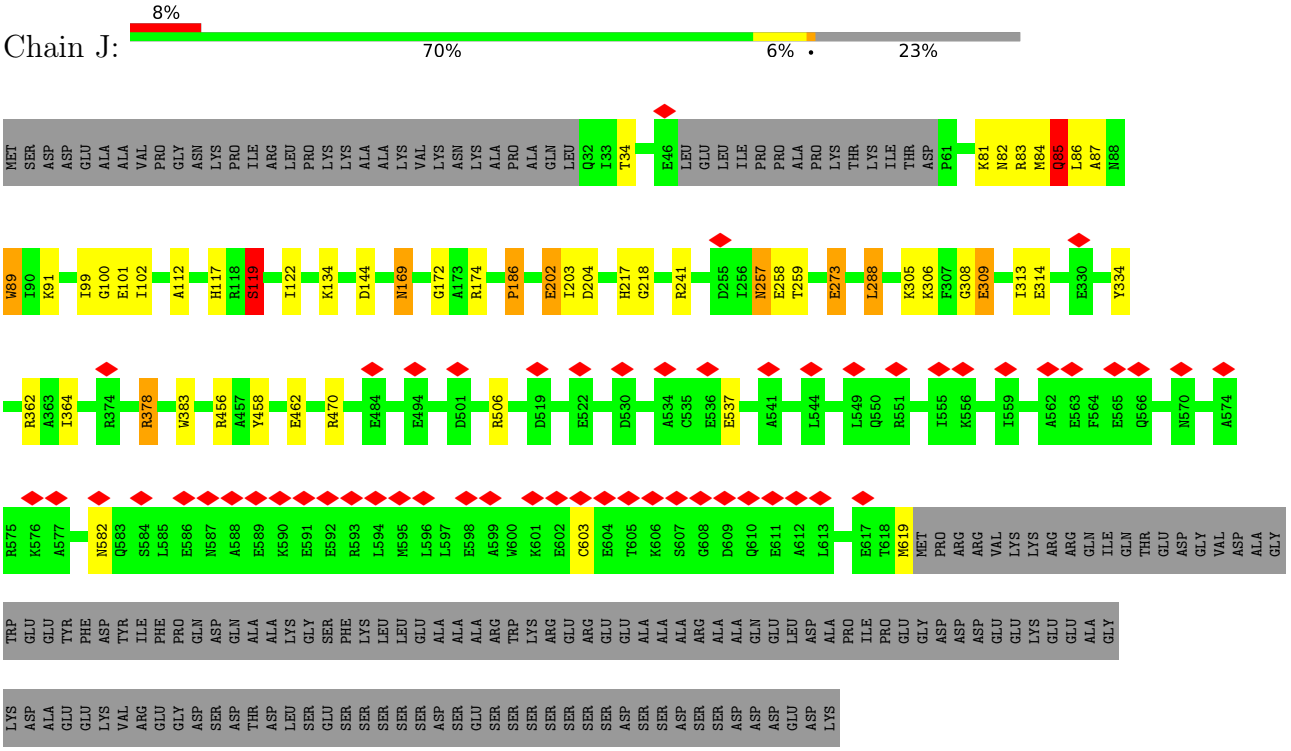


• Molecule 10: Intron lariat RNA



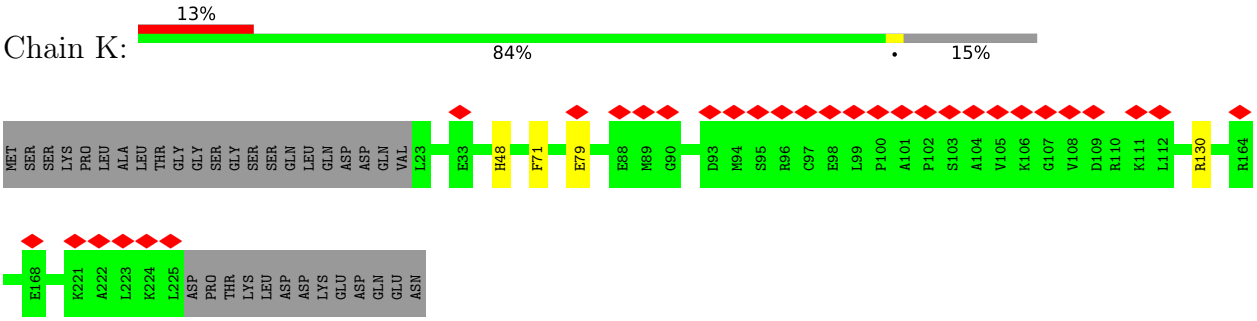
• Molecule 11: TPR_REGION domain-containing protein

Chain J:



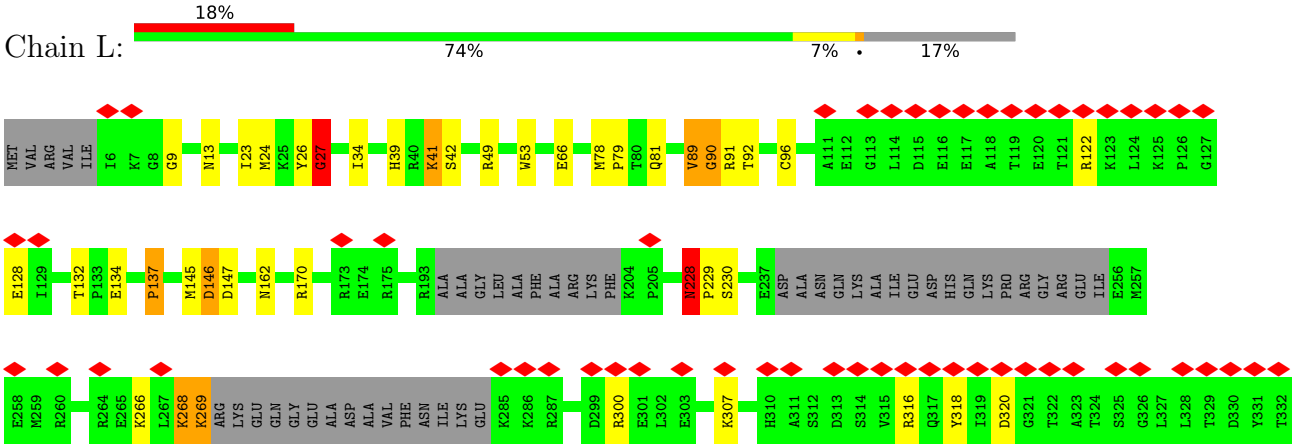
• Molecule 12: Pre-mRNA-splicing factor SPF27

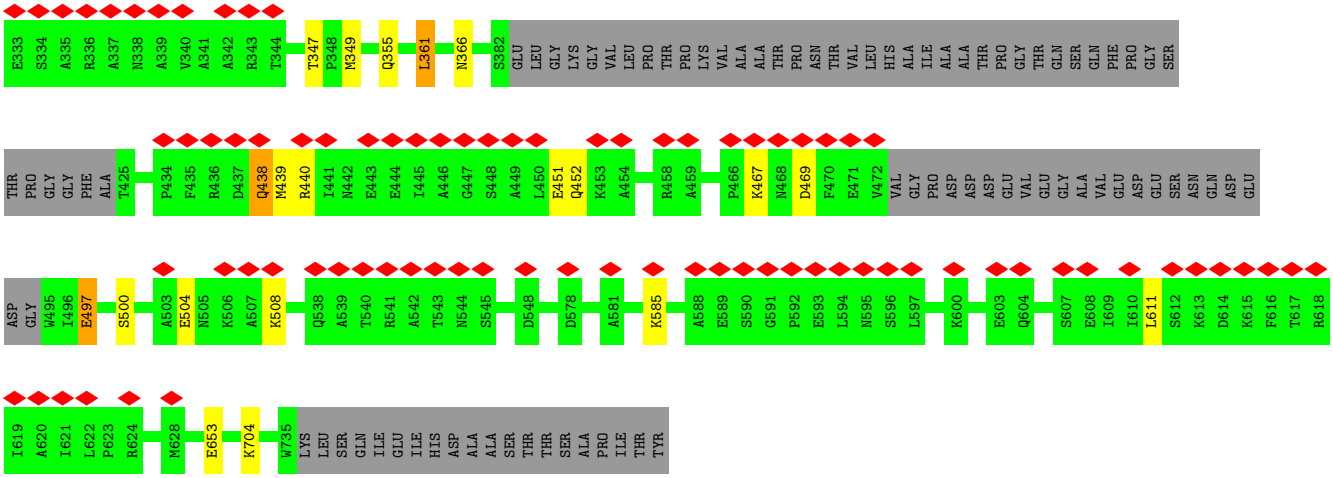
Chain K:



• Molecule 13: Cell division cycle 5-like protein

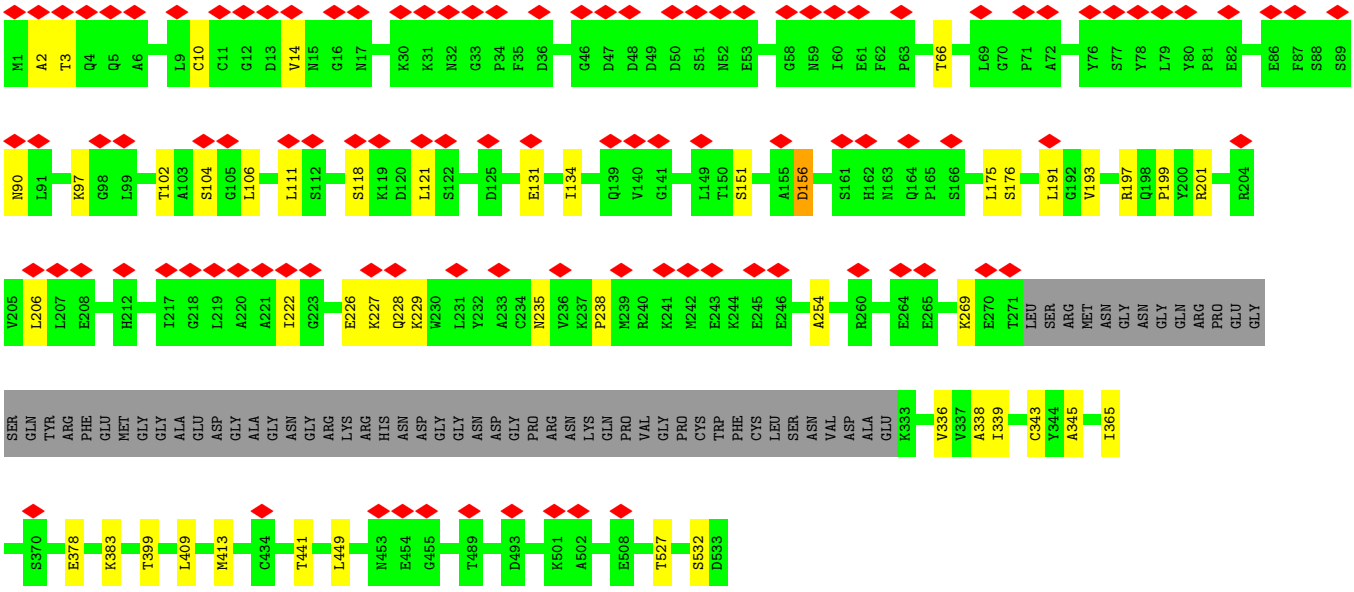
Chain L:





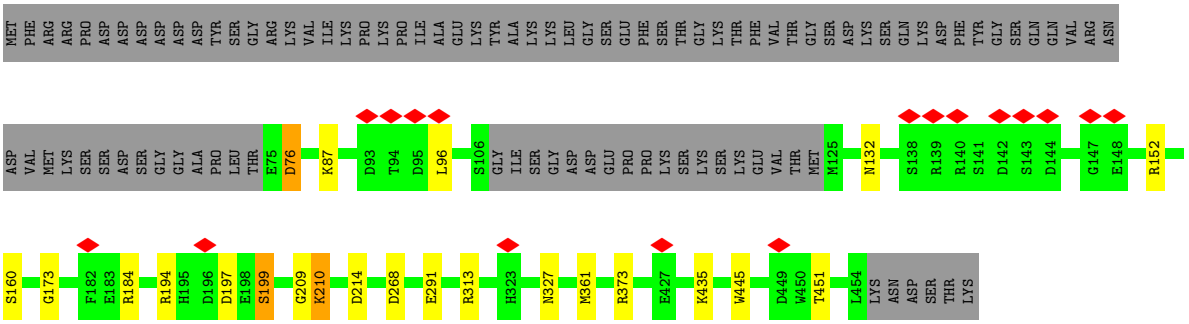
• Molecule 14: CWF19-like protein 1 homolog

Chain L1:



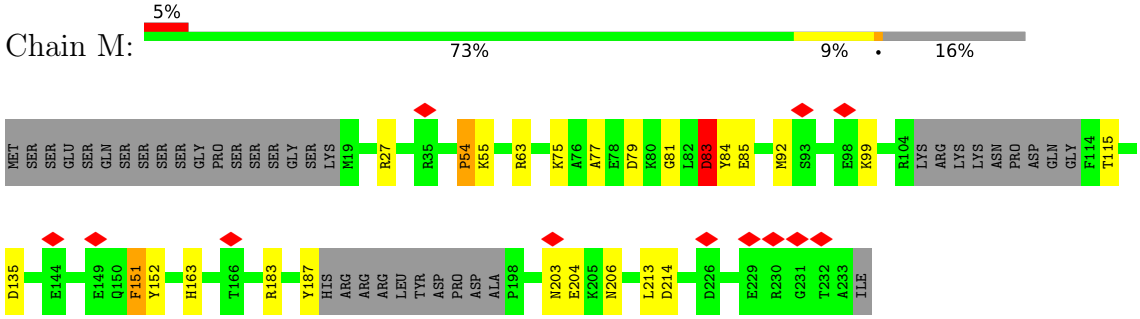
• Molecule 15: CWF19-like protein 2 homolog

Chain L2:



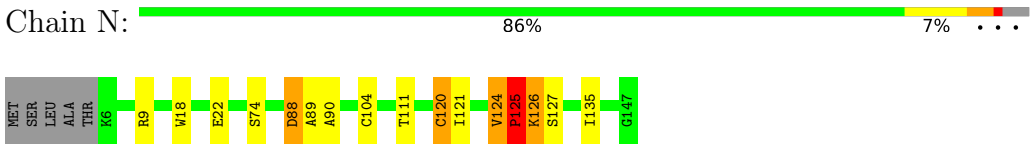
• Molecule 16: Pre-mRNA-splicing factor syf-2

Chain M:



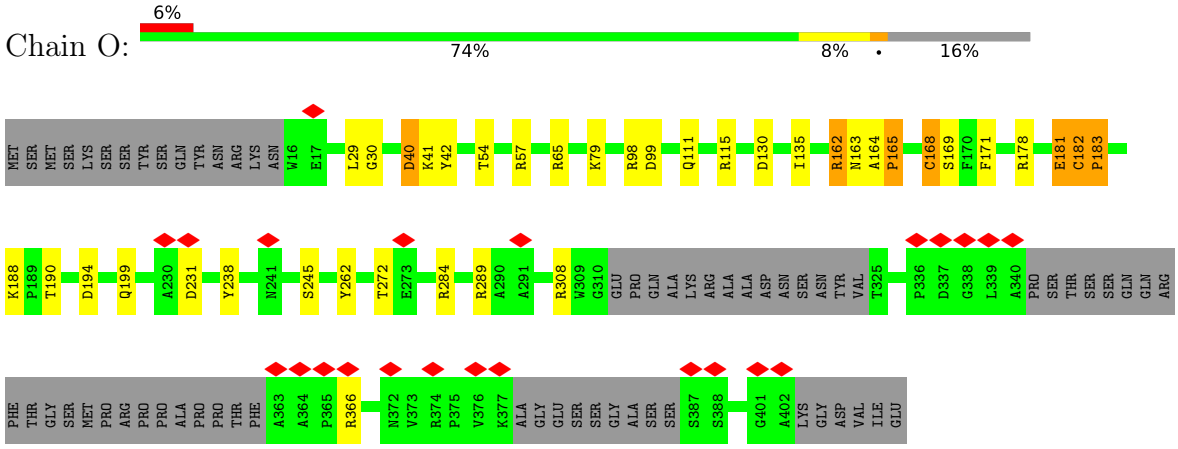
• Molecule 17: Protein BUD31 homolog

Chain N:



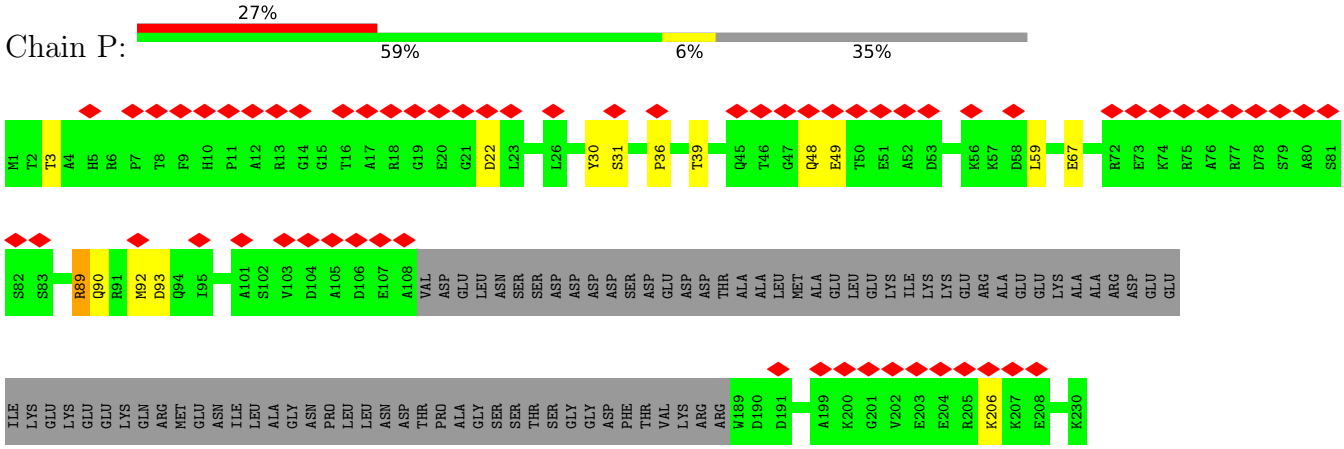
• Molecule 18: Pre-mRNA-splicing factor RBM22

Chain O:



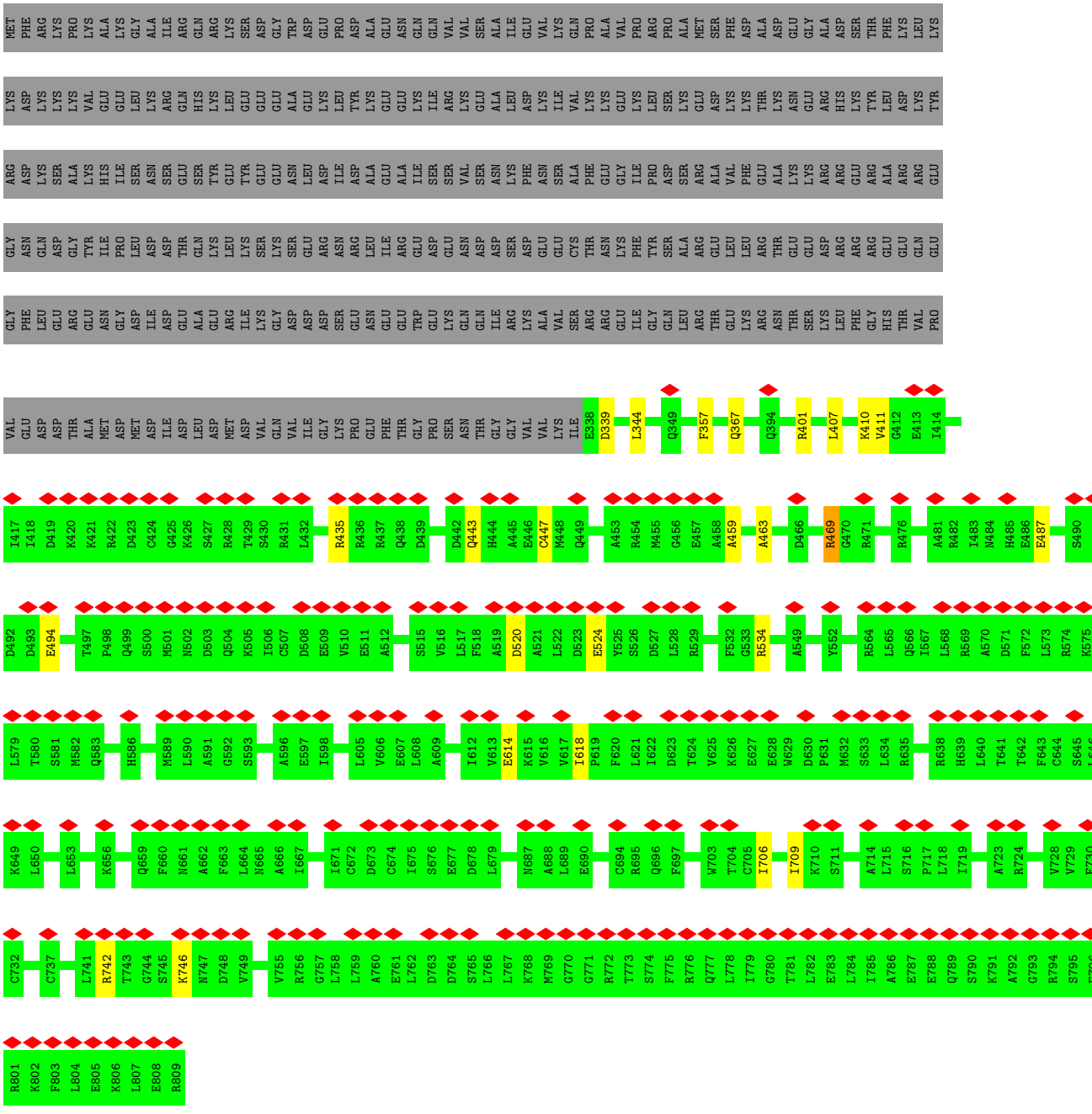
• Molecule 19: Spliceosome-associated protein CWC15 homolog

Chain P:



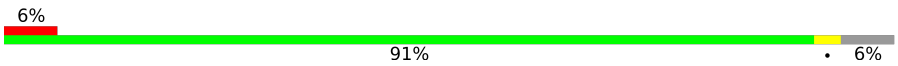
• Molecule 20: GCF C-terminal domain-containing protein

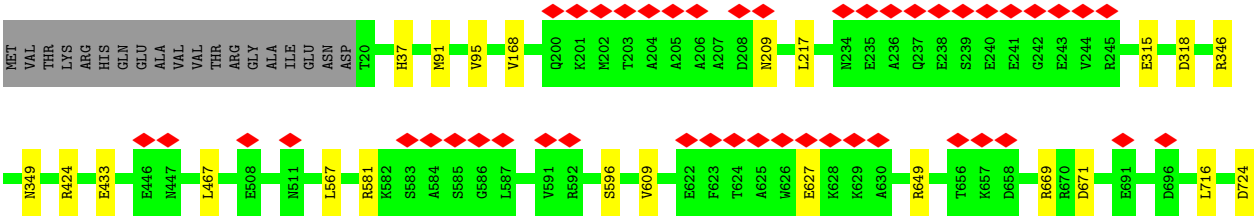
Chain PX:

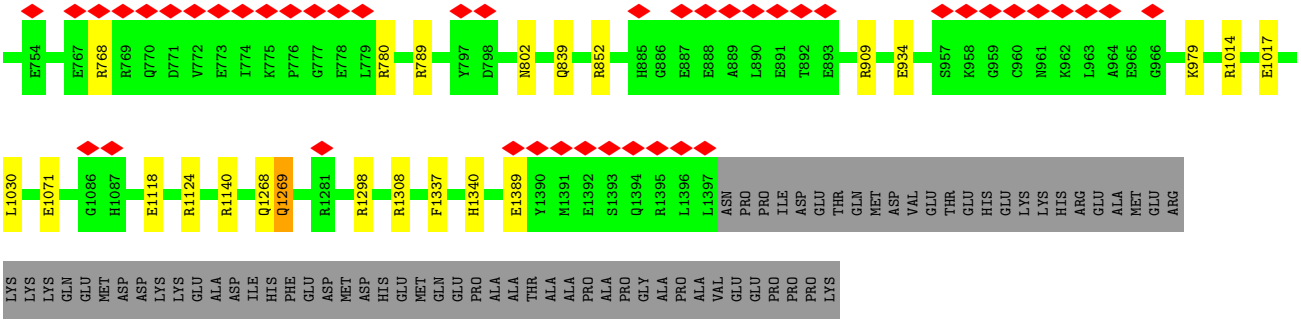


• Molecule 21: Intron-binding protein aquarius

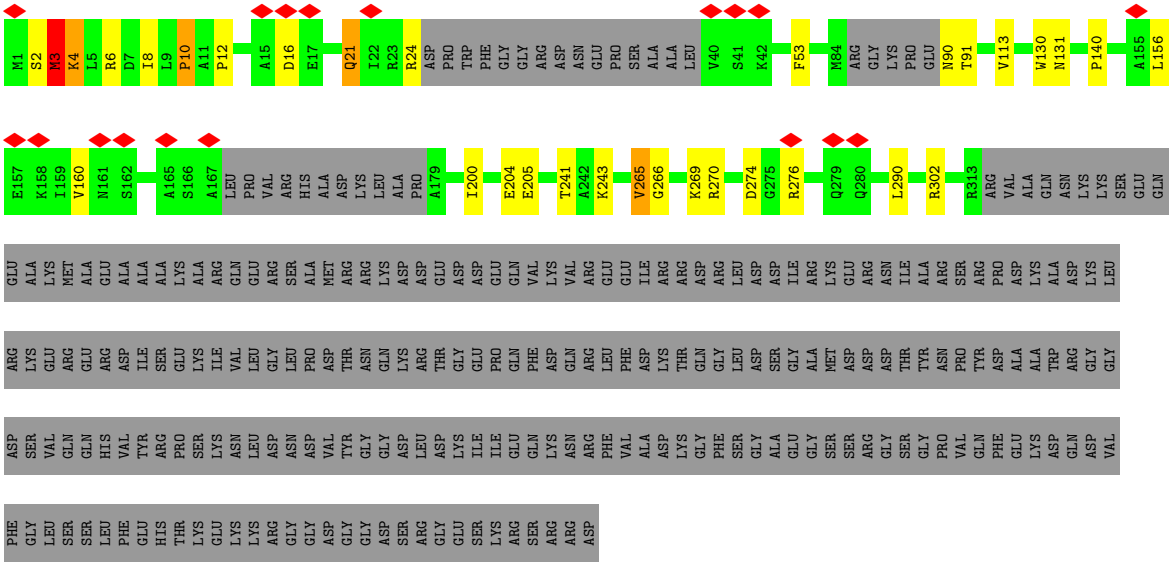
Chain Q:



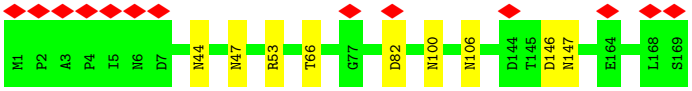




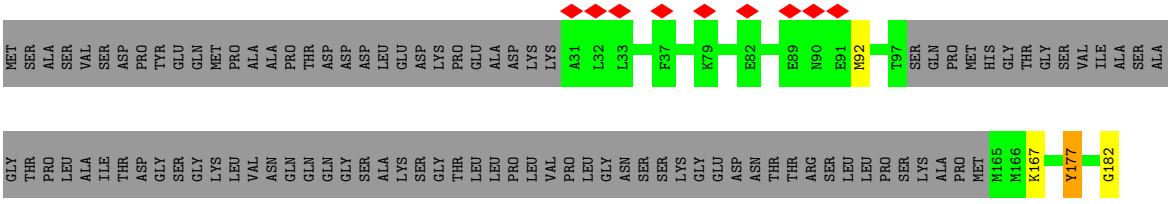
• Molecule 22: Uncharacterized protein T27F2.1

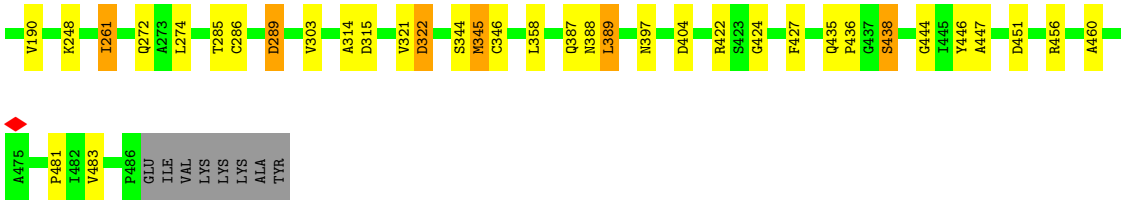


• Molecule 23: Peptidyl-prolyl cis-trans isomerase



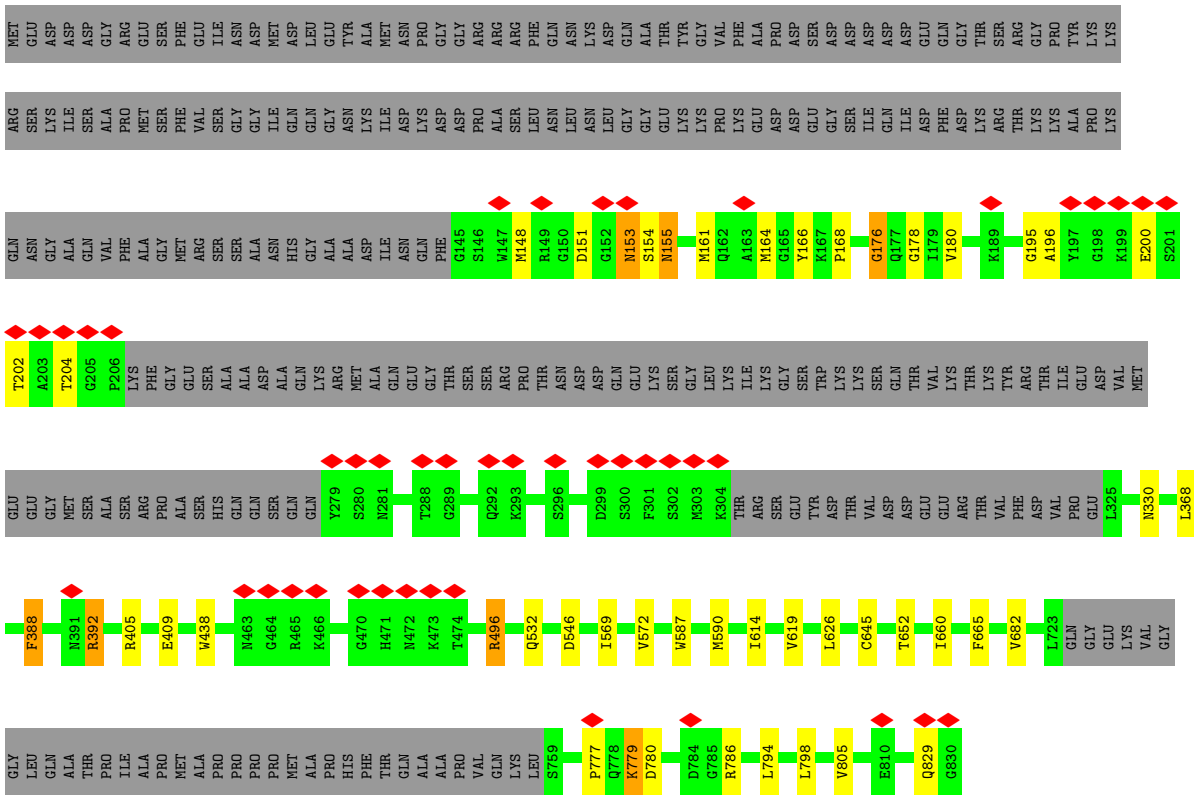
• Molecule 24: WD_REPEATS_REGION domain-containing protein





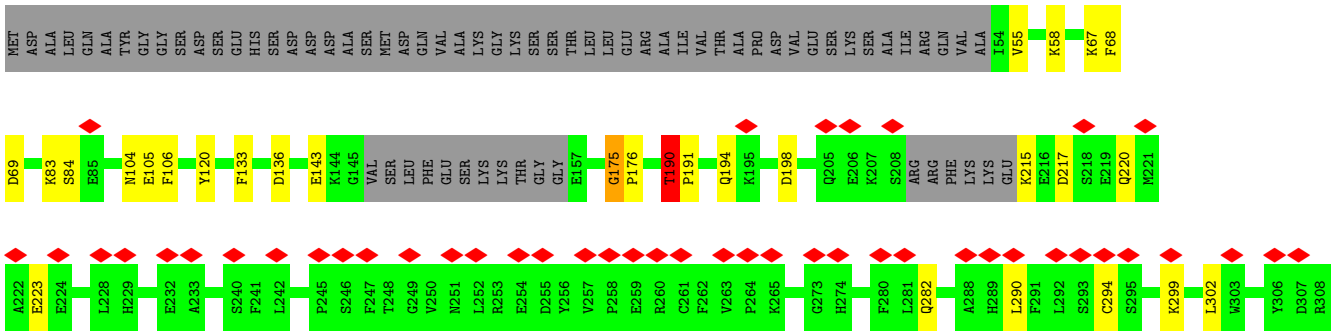
• Molecule 25: Septin and tuftelin-interacting protein 1 homolog

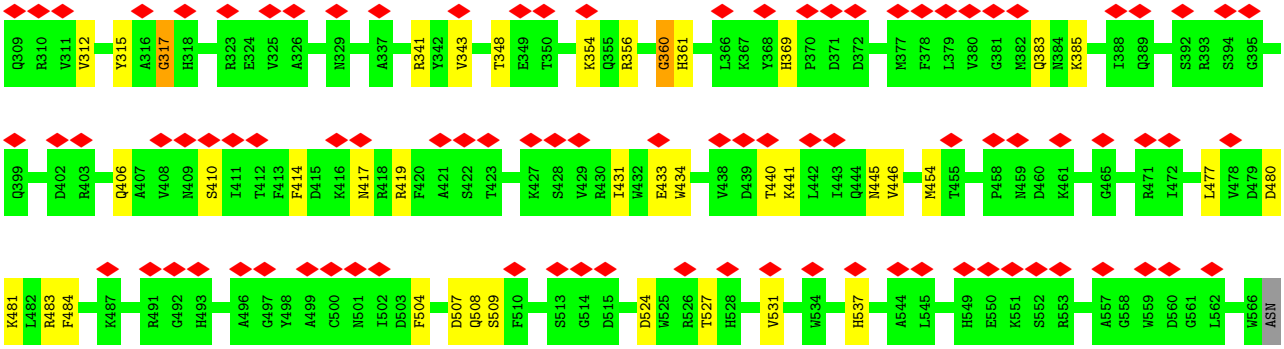
Chain TF:



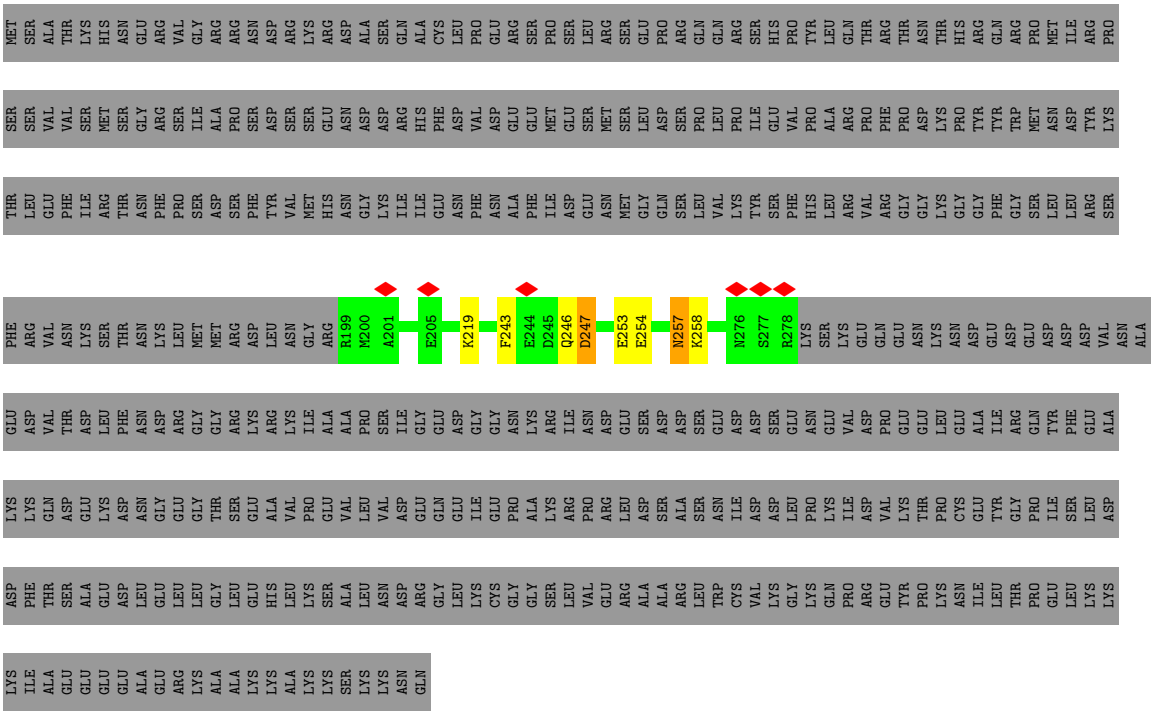
• Molecule 26: WD_REPEATS_REGION domain-containing protein

Chain W:

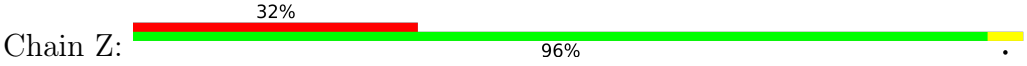


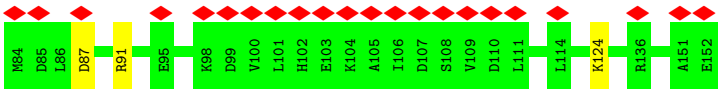


• Molecule 27: Replication stress response regulator SDE2

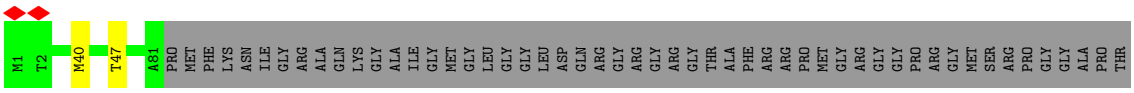


• Molecule 28: Coiled-coil domain-containing protein 12



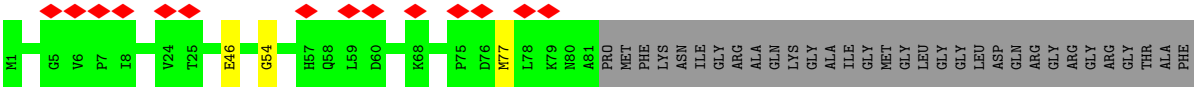


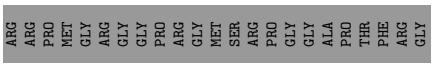
• Molecule 29: Small nuclear ribonucleoprotein Sm D3



• Molecule 29: Small nuclear ribonucleoprotein Sm D3

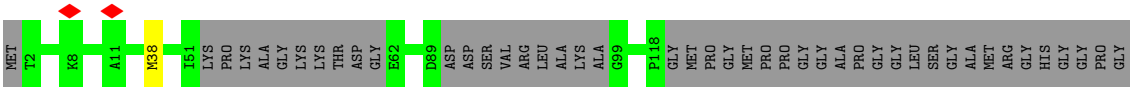
Chain h:

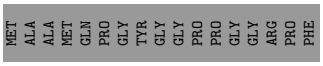




• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B

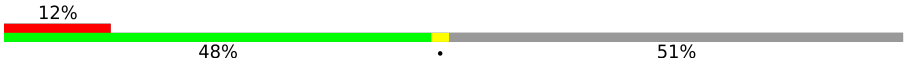
Chain b:

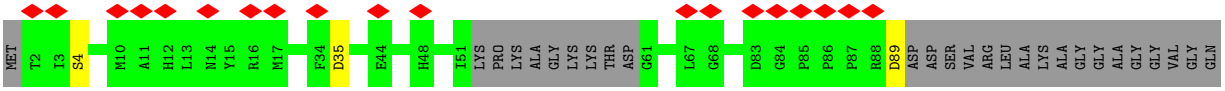


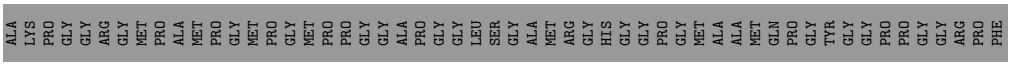


• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B

Chain i:





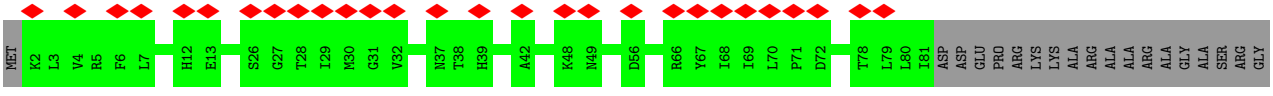


• Molecule 31: Small nuclear ribonucleoprotein Sm D1

Chain c:

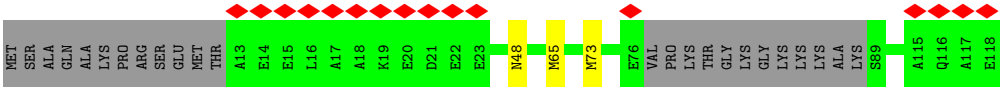
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

Chain j:



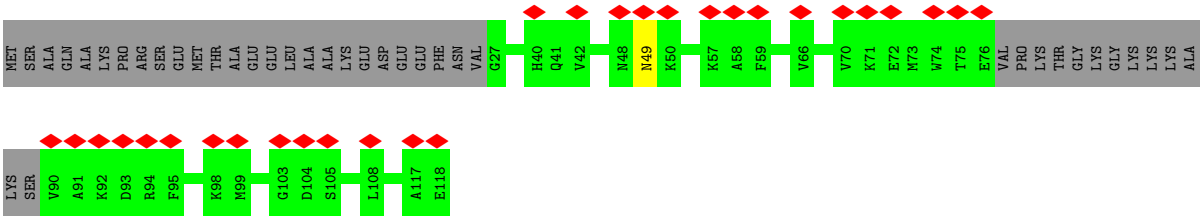
• Molecule 32: Probable small nuclear ribonucleoprotein Sm D2

Chain d:



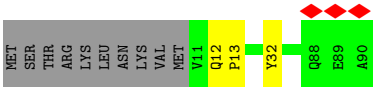
• Molecule 32: Probable small nuclear ribonucleoprotein Sm D2

Chain k:



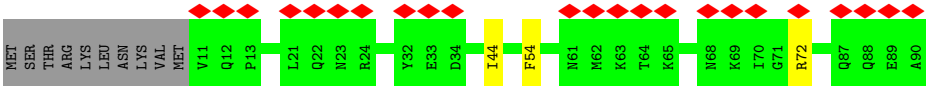
• Molecule 33: Probable small nuclear ribonucleoprotein E

Chain e:



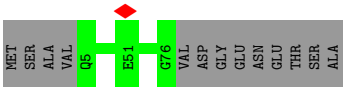
• Molecule 33: Probable small nuclear ribonucleoprotein E

Chain l:



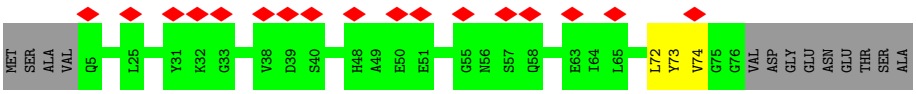
• Molecule 34: Probable small nuclear ribonucleoprotein F

Chain f:



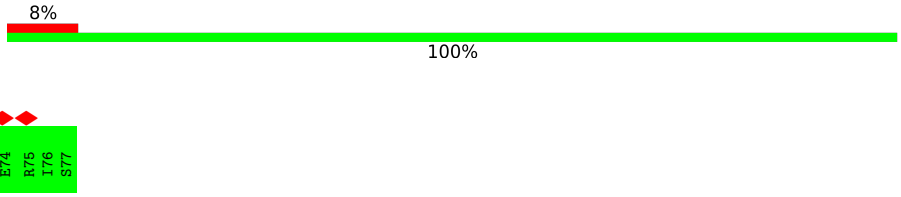
• Molecule 34: Probable small nuclear ribonucleoprotein F

Chain m:



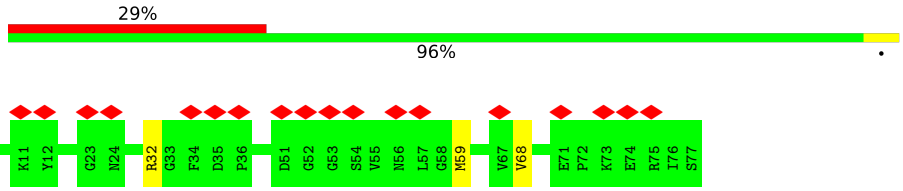
• Molecule 35: Probable small nuclear ribonucleoprotein G

Chain g:



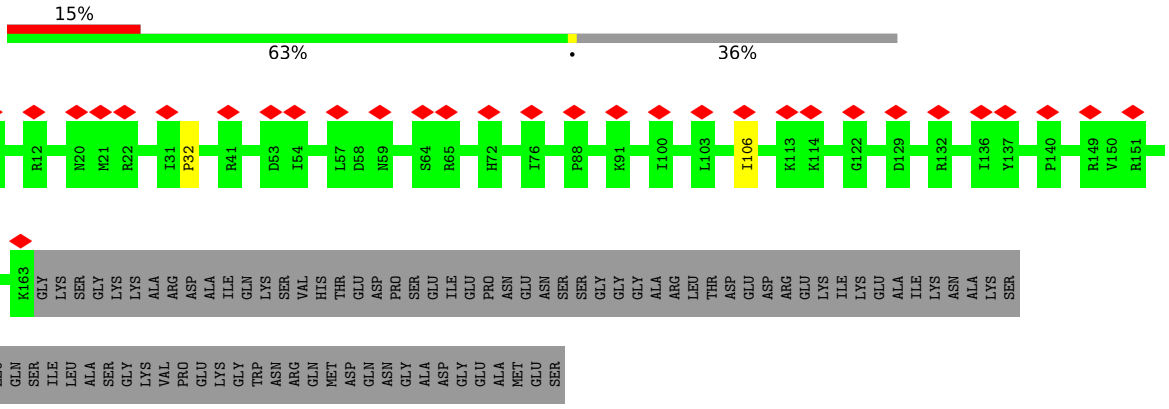
• Molecule 35: Probable small nuclear ribonucleoprotein G

Chain n:



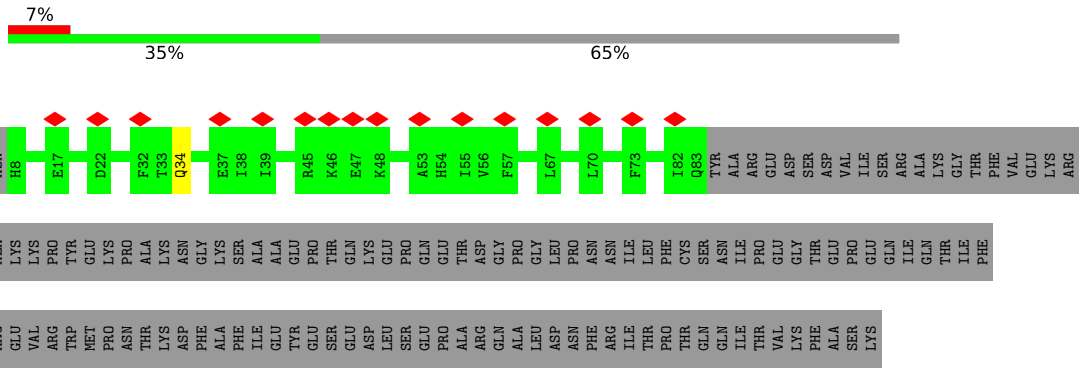
• Molecule 36: Probable U2 small nuclear ribonucleoprotein A'

Chain o:



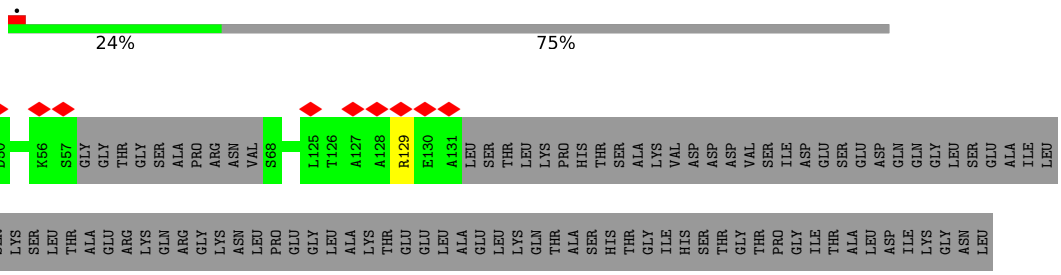
• Molecule 37: RRM domain-containing protein

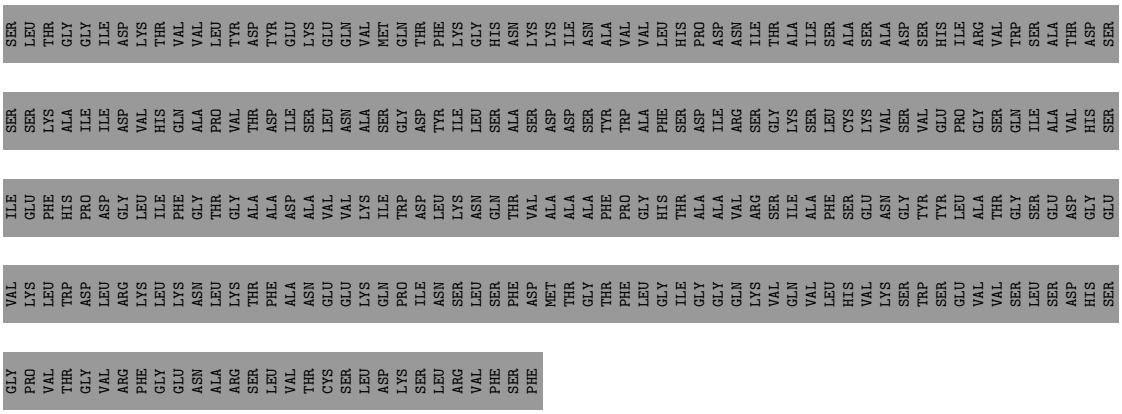
Chain p:



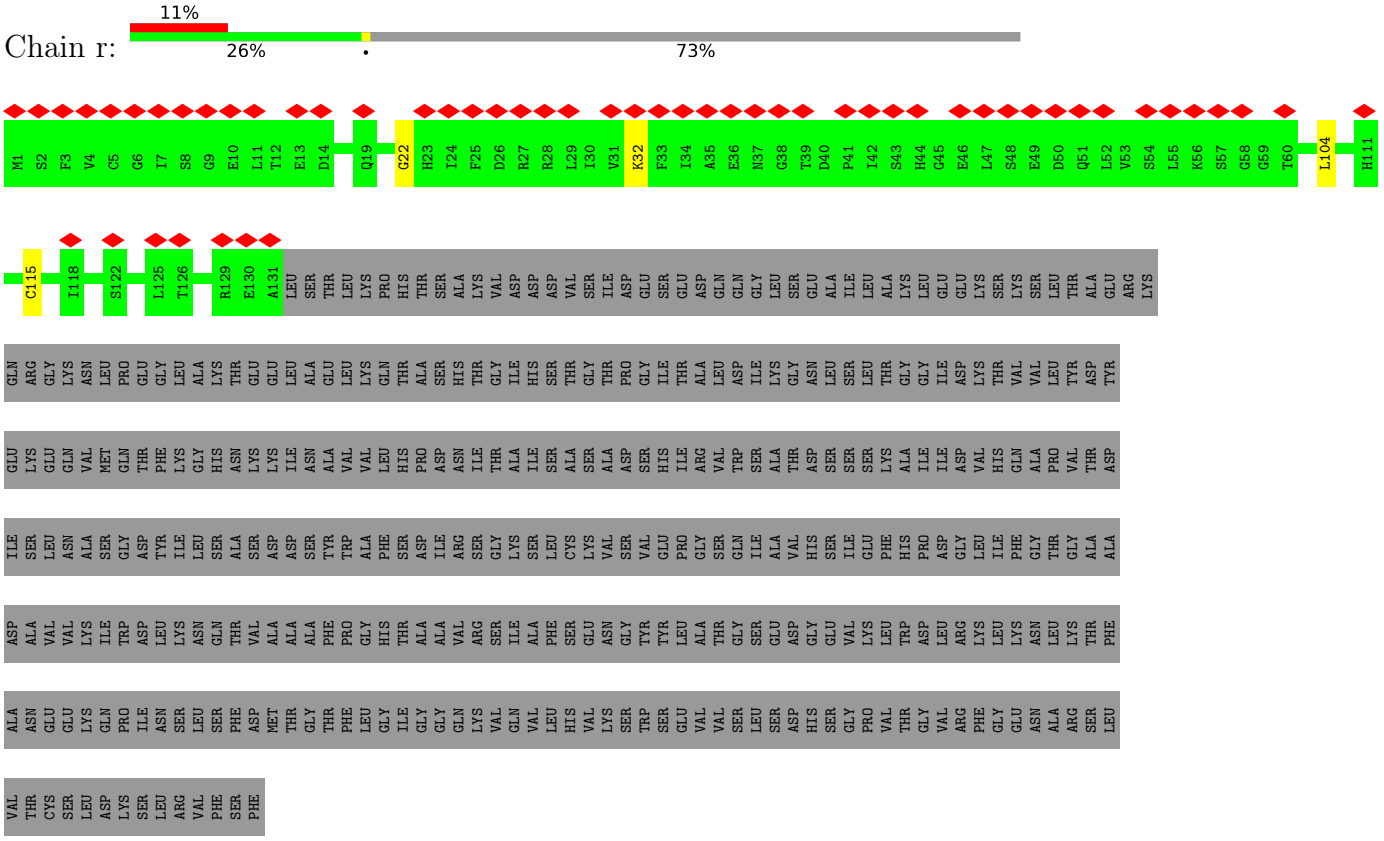
• Molecule 38: Pre-mRNA-processing factor 19

Chain q:

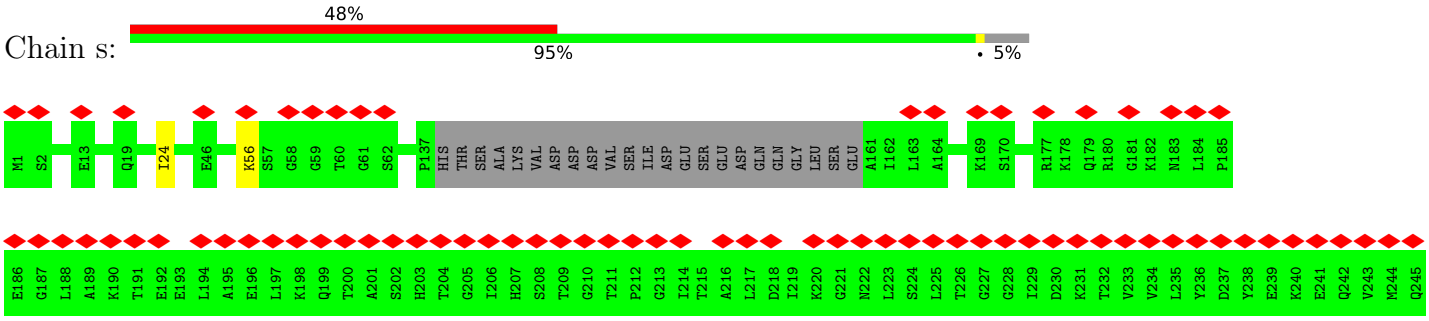


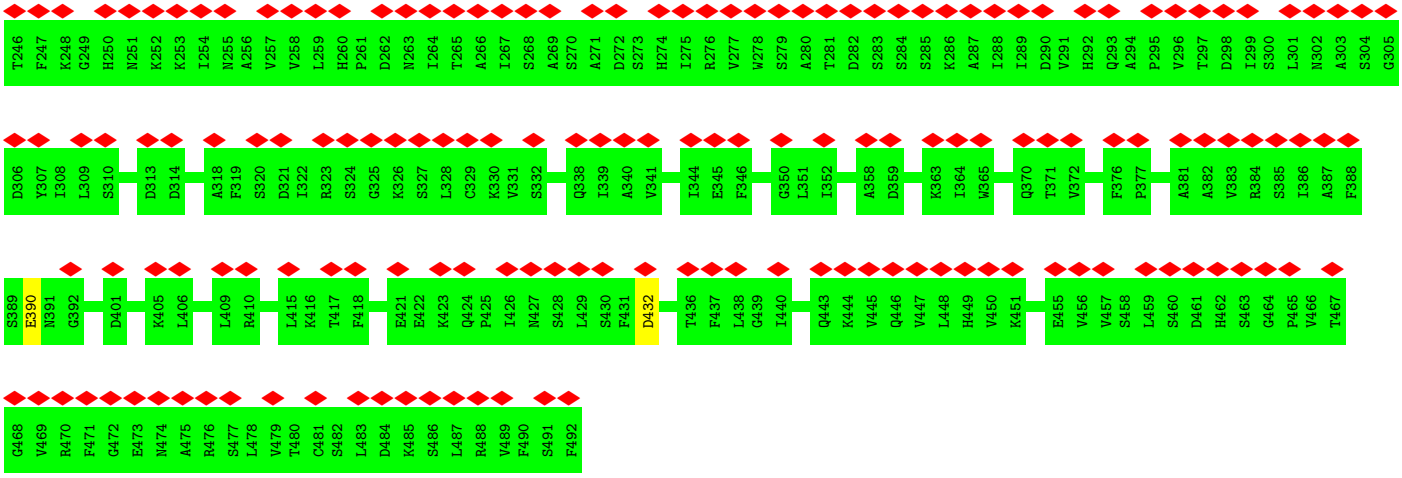


• Molecule 38: Pre-mRNA-processing factor 19



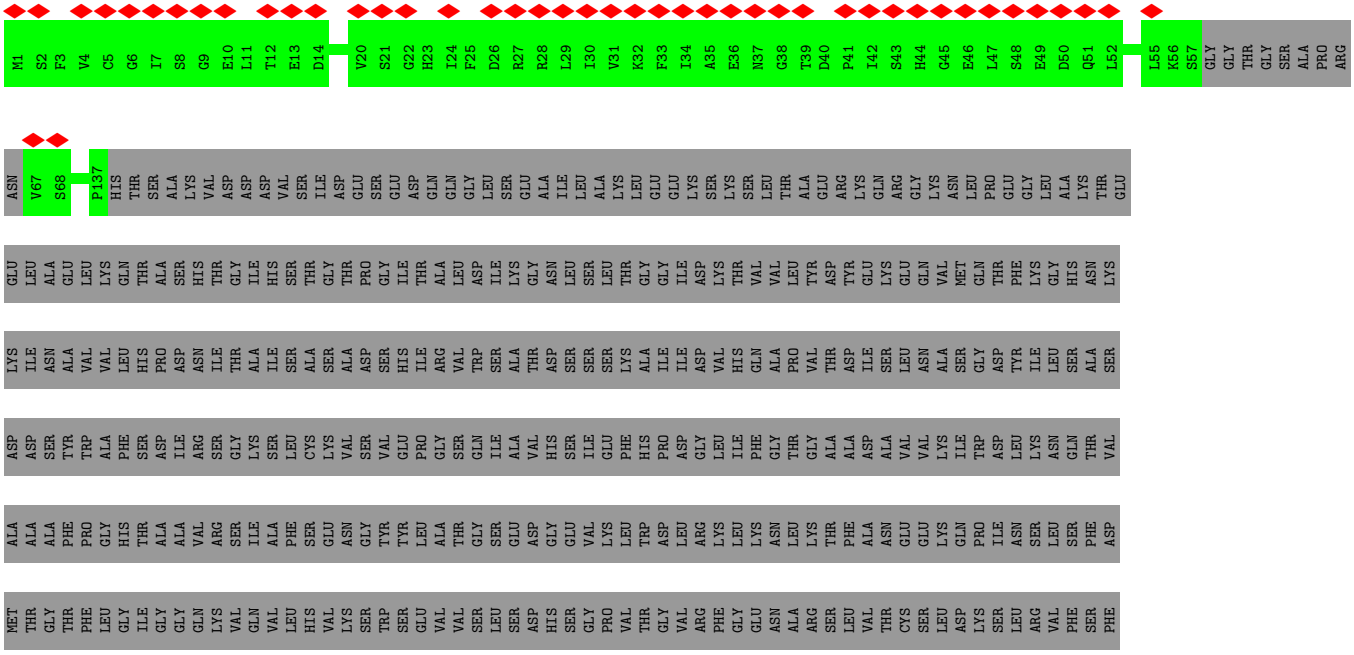
• Molecule 38: Pre-mRNA-processing factor 19





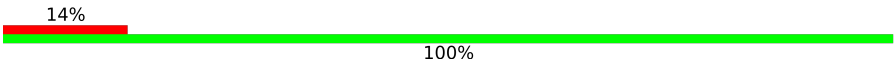
• Molecule 38: Pre-mRNA-processing factor 19

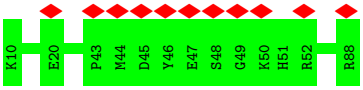
Chain t:



• Molecule 39: Peptidyl-prolyl cis-trans isomerase E

Chain y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247908	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.125	Depositor
Minimum map value	0.000	Depositor
Average map value	0.070	Depositor
Map value standard deviation	0.281	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	258.9587, 300.6003, 307.1068	wwPDB
Map dimensions	199, 231, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3013, 1.3013, 1.3013	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: ZN, IHP, MG, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.69	0/918	1.35	3/1424 (0.2%)
2	5	1.08	4/2623 (0.2%)	1.51	35/4079 (0.9%)
3	6	0.84	0/2410	1.39	25/3752 (0.7%)
4	A	0.51	0/16860	0.82	19/22857 (0.1%)
5	C	0.55	1/7310 (0.0%)	0.85	13/9907 (0.1%)
6	D	0.33	0/1649	0.68	0/2202
7	DX	0.53	0/5577	0.76	2/7566 (0.0%)
8	E	0.47	0/2502	0.78	1/3385 (0.0%)
9	I	0.49	0/6307	0.74	3/8518 (0.0%)
10	IN	0.39	0/71	1.37	0/106
11	J	0.50	0/5008	0.80	5/6737 (0.1%)
12	K	0.34	0/1689	0.62	0/2261
13	L	0.37	1/5101 (0.0%)	0.76	4/6840 (0.1%)
14	L1	0.37	0/3765	0.65	0/5090
15	L2	0.39	0/3024	0.73	0/4039
16	M	0.43	0/1680	0.82	1/2241 (0.0%)
17	N	0.67	1/1190 (0.1%)	0.79	0/1597
18	O	0.53	0/2783	0.84	6/3768 (0.2%)
19	P	0.38	0/1223	0.81	0/1626
20	PX	0.34	0/3893	0.69	0/5223
21	Q	0.43	0/11555	0.66	1/15627 (0.0%)
22	R	0.45	0/2254	0.84	2/3042 (0.1%)
23	S	0.34	0/1332	0.71	1/1801 (0.1%)
24	T	0.54	1/3161 (0.0%)	0.85	2/4283 (0.0%)
25	TF	0.41	0/4656	0.72	1/6312 (0.0%)
26	W	0.40	0/4180	0.79	2/5639 (0.0%)
27	X	0.31	0/666	0.69	1/879 (0.1%)
28	Z	0.27	0/573	0.69	0/766
29	a	0.42	0/643	0.78	1/865 (0.1%)
29	h	0.33	0/643	0.73	0/865
30	b	0.43	0/767	0.78	0/1022
30	i	0.31	0/649	0.71	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.42	1/628 (0.2%)	0.78	1/849 (0.1%)
31	j	0.34	0/628	0.68	0/849
32	d	0.39	0/757	0.70	0/1014
32	k	0.35	0/639	0.78	0/855
33	e	0.42	0/676	0.73	0/910
33	l	0.34	0/676	0.72	0/910
34	f	0.47	0/569	0.67	0/770
34	m	0.39	0/569	0.73	0/770
35	g	0.36	0/616	0.76	0/821
35	n	0.33	0/616	0.71	0/821
36	o	0.34	0/1358	0.67	0/1837
37	p	0.32	0/638	0.67	0/850
38	q	0.34	0/953	0.63	0/1284
38	r	0.33	0/1018	0.68	0/1374
38	s	0.34	0/3633	0.65	0/4914
38	t	0.32	0/1006	0.62	0/1357
39	y	0.38	0/631	0.66	0/846
All	All	0.48	9/122273 (0.0%)	0.81	129/166216 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	29
5	C	0	16
7	DX	0	5
8	E	0	3
9	I	0	5
11	J	0	8
13	L	0	9
15	L2	0	2
16	M	0	3
18	O	0	6
19	P	0	1
20	PX	0	1
22	R	0	4
24	T	0	7
25	TF	0	2
26	W	0	3
All	All	0	104

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	96	CYS	CB-SG	-6.74	1.70	1.82
2	5	27	G	C8-N7	-6.08	1.27	1.30
2	5	99	G	N3-C4	-5.59	1.31	1.35
31	c	69	ILE	C-N	-5.52	1.21	1.34
24	T	286	CYS	CB-SG	-5.39	1.73	1.81
17	N	120	CYS	CB-SG	-5.38	1.73	1.81
5	C	821	TYR	CD1-CE1	-5.22	1.31	1.39
2	5	19	A	N9-C4	-5.12	1.34	1.37
2	5	27	G	N7-C5	-5.01	1.36	1.39

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	70	G	O5'-P-OP1	16.43	130.41	110.70
2	5	27	G	O4'-C1'-N9	-11.37	99.11	108.20
9	I	628	ASP	CB-CG-OD1	10.90	128.11	118.30
13	L	27	GLY	N-CA-C	10.79	140.09	113.10
24	T	289	ASP	CB-CG-OD1	10.31	127.58	118.30
2	5	21	U	O4'-C1'-N1	10.23	116.39	108.20
5	C	781	GLY	N-CA-C	9.45	136.73	113.10
11	J	378	ARG	NE-CZ-NH2	8.86	124.73	120.30
4	A	1310	THR	C-N-CD	-8.70	101.46	120.60
5	C	267	LEU	CA-CB-CG	8.59	135.06	115.30
4	A	994	ASP	CB-CG-OD1	8.44	125.89	118.30
2	5	13	C	C6-N1-C2	-8.41	116.94	120.30
2	5	5	U	C5-C4-O4	-8.38	120.87	125.90
18	O	182	CYS	C-N-CD	-8.26	102.43	120.60
3	6	39	G	P-O3'-C3'	8.03	129.34	119.70
18	O	30	GLY	N-CA-C	8.03	133.17	113.10
2	5	10	U	C5-C4-O4	7.99	130.69	125.90
2	5	41	C	C6-N1-C2	-7.86	117.16	120.30
3	6	89	C	C6-N1-C2	-7.81	117.17	120.30
3	6	25	A	N1-C6-N6	7.70	123.22	118.60
2	5	13	C	C5-C6-N1	7.67	124.83	121.00
2	5	99	G	N3-C2-N2	-7.61	114.58	119.90
2	5	5	U	N3-C4-O4	7.60	124.72	119.40
5	C	599	ILE	C-N-CA	7.54	140.55	121.70
2	5	68	G	N3-C4-C5	-7.53	124.84	128.60
25	TF	587	TRP	C-N-CA	7.52	140.50	121.70
13	L	300	ARG	NE-CZ-NH2	7.49	124.04	120.30
4	A	790	GLY	N-CA-C	7.46	131.74	113.10
2	5	109	C	O4'-C1'-N1	7.28	114.03	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	6	3	U	C5-C6-N1	7.23	126.31	122.70
2	5	35	C	C6-N1-C2	-7.21	117.42	120.30
2	5	99	G	C8-N9-C4	-7.05	103.58	106.40
3	6	20	C	N1-C2-O2	6.97	123.08	118.90
9	I	418	ASP	CB-CG-OD1	6.94	124.54	118.30
11	J	362	ARG	NE-CZ-NH2	6.93	123.77	120.30
2	5	70	G	OP1-P-OP2	-6.78	109.43	119.60
2	5	10	U	N3-C4-O4	-6.62	114.77	119.40
22	R	266	GLY	N-CA-C	6.62	129.65	113.10
3	6	25	A	C5-N7-C8	-6.57	100.62	103.90
2	5	99	G	N9-C4-C5	6.56	108.02	105.40
3	6	25	A	C4-C5-N7	6.47	113.94	110.70
2	5	21	U	C6-N1-C2	-6.37	117.18	121.00
4	A	1311	PRO	N-CA-C	6.37	128.66	112.10
23	S	146	ASP	CB-CG-OD1	6.29	123.96	118.30
18	O	182	CYS	N-CA-C	6.27	127.92	111.00
26	W	175	GLY	C-N-CD	-6.27	106.81	120.60
26	W	190	THR	C-N-CD	-6.24	106.88	120.60
3	6	89	C	C2-N1-C1'	6.18	125.60	118.80
18	O	162	ARG	CD-NE-CZ	6.15	132.21	123.60
3	6	14	C	C6-N1-C2	-6.13	117.85	120.30
2	5	25	C	C6-N1-C2	-6.13	117.85	120.30
3	6	2	U	C5-C4-O4	-6.11	122.23	125.90
3	6	25	A	C5-C6-N6	-6.11	118.81	123.70
2	5	25	C	C2'-C3'-O3'	6.11	123.47	113.70
1	2	29	C	C6-N1-C2	-6.10	117.86	120.30
5	C	158	PRO	CA-N-CD	-6.10	102.96	111.50
4	A	756	GLY	N-CA-C	6.09	128.32	113.10
4	A	933	LYS	C-N-CD	-6.07	107.25	120.60
3	6	1	G	N3-C4-N9	6.05	129.63	126.00
4	A	511	ASP	CB-CG-OD1	6.04	123.73	118.30
27	X	247	ASP	CB-CG-OD1	6.04	123.73	118.30
5	C	737	TRP	CA-CB-CG	6.00	125.09	113.70
18	O	181	GLU	C-N-CA	5.98	136.66	121.70
4	A	981	ASP	CB-CG-OD1	5.90	123.61	118.30
3	6	25	A	N7-C8-N9	5.88	116.74	113.80
3	6	25	A	C6-C5-N7	-5.86	128.20	132.30
22	R	10	PRO	CA-N-CD	-5.86	103.30	111.50
13	L	361	LEU	CA-CB-CG	5.84	128.74	115.30
4	A	689	MET	C-N-CD	-5.84	107.76	120.60
2	5	105	C	O4'-C1'-N1	5.82	112.86	108.20
5	C	308	GLY	N-CA-C	5.81	127.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	532	PHE	CB-CG-CD1	5.80	124.86	120.80
3	6	1	G	N3-C4-C5	-5.78	125.71	128.60
16	M	151	PHE	CB-CG-CD1	5.77	124.84	120.80
9	I	417	LEU	CA-CB-CG	5.74	128.51	115.30
5	C	618	TYR	C-N-CD	-5.74	107.97	120.60
2	5	21	U	N3-C2-O2	-5.70	118.21	122.20
3	6	20	C	N3-C2-O2	-5.68	117.92	121.90
21	Q	671	ASP	CB-CG-OD1	5.67	123.40	118.30
2	5	68	G	N3-C4-N9	5.66	129.40	126.00
11	J	334	TYR	CB-CG-CD1	-5.64	117.62	121.00
7	DX	66	TYR	CB-CG-CD1	5.64	124.38	121.00
5	C	404	GLY	N-CA-C	5.62	127.14	113.10
5	C	233	ASP	CB-CG-OD1	5.61	123.35	118.30
3	6	89	C	N1-C2-O2	5.57	122.24	118.90
18	O	183	PRO	CA-N-CD	-5.56	103.71	111.50
3	6	89	C	N1-C1'-C2'	5.56	121.23	114.00
2	5	67	G	O4'-C1'-N9	5.55	112.64	108.20
2	5	34	U	C5-C6-N1	5.54	125.47	122.70
4	A	532	PHE	CB-CG-CD2	-5.51	116.94	120.80
24	T	427	PHE	CB-CG-CD1	5.47	124.63	120.80
4	A	227	LEU	CA-CB-CG	5.46	127.85	115.30
2	5	109	C	C6-N1-C2	-5.45	118.12	120.30
5	C	619	PRO	CA-N-CD	-5.45	103.88	111.50
2	5	80	A	O4'-C1'-N9	5.42	112.54	108.20
3	6	16	U	C5-C4-O4	5.39	129.13	125.90
3	6	89	C	N3-C2-O2	-5.39	118.13	121.90
3	6	89	C	C6-N1-C1'	-5.37	114.35	120.80
4	A	583	MET	CA-CB-CG	5.36	122.42	113.30
2	5	6	C	O4'-C1'-N1	5.34	112.47	108.20
5	C	76	TYR	CA-CB-CG	5.33	123.53	113.40
5	C	207	ASP	CB-CG-OD1	5.32	123.08	118.30
2	5	64	A	C8-N9-C4	-5.30	103.68	105.80
4	A	934	PRO	CA-N-CD	-5.28	104.11	111.50
4	A	1487	TYR	N-CA-C	5.27	125.24	111.00
1	2	42	C	C6-N1-C2	-5.23	118.21	120.30
8	E	87	LEU	CA-CB-CG	5.21	127.28	115.30
5	C	181	GLY	N-CA-C	5.18	126.06	113.10
3	6	82	C	C6-N1-C2	-5.17	118.23	120.30
1	2	23	U	C6-N1-C2	-5.17	117.90	121.00
11	J	378	ARG	NE-CZ-NH1	-5.17	117.72	120.30
7	DX	66	TYR	CA-CB-CG	5.17	123.21	113.40
2	5	68	G	O4'-C1'-N9	5.16	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	99	G	N3-C4-N9	-5.16	122.91	126.00
13	L	90	GLY	N-CA-C	5.15	125.98	113.10
2	5	71	C	C6-N1-C2	-5.13	118.25	120.30
3	6	28	G	P-O3'-C3'	5.12	125.84	119.70
29	a	40	MET	CA-CB-CG	5.10	121.96	113.30
2	5	68	G	C2-N3-C4	5.09	114.45	111.90
2	5	20	U	P-O3'-C3'	5.08	125.80	119.70
4	A	1489	PRO	N-CA-C	5.08	125.30	112.10
11	J	134	LYS	C-N-CA	5.08	134.39	121.70
2	5	33	A	N7-C8-N9	5.07	116.33	113.80
4	A	581	THR	N-CA-C	5.07	124.68	111.00
4	A	583	MET	CB-CA-C	-5.05	100.30	110.40
3	6	53	G	N3-C4-N9	-5.04	122.98	126.00
4	A	1873	PRO	N-CA-C	5.01	125.13	112.10
31	c	33	ASP	CB-CG-OD1	5.01	122.81	118.30
3	6	20	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1045	LEU	Peptide
4	A	1054	ALA	Peptide
4	A	1078	ARG	Peptide
4	A	1109	HIS	Peptide
4	A	1310	THR	Peptide
4	A	1328	PRO	Peptide
4	A	1409	ILE	Peptide
4	A	1428	GLY	Peptide
4	A	1454	ASP	Peptide
4	A	1486	THR	Peptide
4	A	1504	GLU	Peptide
4	A	1668	ASP	Peptide
4	A	167	ASP	Peptide
4	A	1939	ASN	Peptide
4	A	1991	ASN	Peptide
4	A	239	VAL	Peptide
4	A	406	ARG	Sidechain
4	A	532	PHE	Peptide
4	A	533	GLY	Peptide
4	A	581	THR	Peptide
4	A	63	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	A	68	SER	Peptide
4	A	76	ARG	Sidechain
4	A	760	ASP	Peptide
4	A	789	ASP	Peptide
4	A	865	ASN	Peptide
4	A	879	THR	Peptide
4	A	933	LYS	Peptide
4	A	990	ARG	Sidechain
5	C	307	ASN	Peptide
5	C	462	ASP	Peptide
5	C	483	THR	Peptide
5	C	501	MET	Peptide
5	C	600	ASN	Peptide
5	C	69	TYR	Peptide
5	C	713	TRP	Peptide
5	C	727	ASN	Peptide
5	C	729	ASP	Peptide
5	C	780	GLU	Peptide
5	C	781	GLY	Peptide
5	C	803	GLU	Peptide
5	C	862	THR	Peptide
5	C	905	PHE	Peptide
5	C	906	HIS	Peptide
5	C	952	SER	Peptide
7	DX	166	ARG	Sidechain
7	DX	225	ARG	Sidechain
7	DX	396	ARG	Sidechain
7	DX	482	ARG	Sidechain
7	DX	605	ARG	Sidechain
8	E	127	ASN	Peptide
8	E	169	THR	Peptide
8	E	292	VAL	Peptide
9	I	312	ARG	Sidechain
9	I	433	GLY	Peptide
9	I	628	ASP	Peptide
9	I	689	ARG	Sidechain
9	I	732	ARG	Sidechain
11	J	119	SER	Peptide
11	J	174	ARG	Sidechain
11	J	241	ARG	Sidechain
11	J	273	GLU	Peptide
11	J	288	LEU	Peptide

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Mol	Chain	Res	Type	Group
11	J	308	GLY	Peptide
11	J	378	ARG	Sidechain
11	J	85	GLN	Peptide
13	L	145	MET	Peptide
13	L	228	ASN	Peptide
13	L	26	TYR	Peptide
13	L	268	LYS	Peptide
13	L	27	GLY	Peptide
13	L	41	LYS	Peptide
13	L	497	GLU	Peptide
13	L	78	MET	Peptide
13	L	89	VAL	Peptide
15	L2	199	SER	Peptide
15	L2	313	ARG	Sidechain
16	M	115	THR	Peptide
16	M	135	ASP	Peptide
16	M	83	ASP	Peptide
18	O	163	ASN	Peptide
18	O	178	ARG	Peptide
18	O	181	GLU	Peptide
18	O	29	LEU	Peptide
18	O	41	LYS	Peptide
18	O	65	ARG	Sidechain
19	P	31	SER	Peptide
20	PX	469	ARG	Sidechain
22	R	265	VAL	Peptide
22	R	3	MET	Peptide
22	R	302	ARG	Sidechain
22	R	8	ILE	Peptide
24	T	177	TYR	Mainchain
24	T	261	ILE	Peptide
24	T	303	VAL	Peptide
24	T	314	ALA	Peptide
24	T	345	MET	Peptide
24	T	397	ASN	Peptide
24	T	438	SER	Peptide
25	TF	779	LYS	Peptide
25	TF	780	ASP	Peptide
26	W	175	GLY	Peptide
26	W	190	THR	Peptide
26	W	83	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1268	0	715	7	0
2	5	2350	0	1189	13	0
3	6	2153	0	1088	18	0
4	A	16424	0	16438	85	0
5	C	7153	0	7140	32	0
6	D	1629	0	1627	5	0
7	DX	5465	0	5468	22	0
8	E	2445	0	2362	5	0
9	I	6169	0	6076	22	0
10	IN	425	0	274	4	0
11	J	4895	0	4774	21	0
12	K	1666	0	1707	1	0
13	L	5030	0	5111	18	0
14	L1	3683	0	3664	17	0
15	L2	2974	0	2960	11	0
16	M	1654	0	1626	9	0
17	N	1163	0	1142	6	0
18	O	2721	0	2661	13	0
19	P	1207	0	1182	3	0
20	PX	3838	0	3891	12	0
21	Q	11293	0	11206	17	0
22	R	2209	0	2212	10	0
23	S	1303	0	1282	3	0
24	T	3082	0	3042	9	0
25	TF	4542	0	4481	18	0
26	W	4072	0	3967	19	0
27	X	661	0	679	2	0
28	Z	569	0	603	1	0
29	a	635	0	643	0	0
29	h	635	0	643	0	0
30	b	755	0	772	0	0
30	i	639	0	655	0	0
31	c	622	0	672	0	0
31	j	622	0	673	0	0
32	d	749	0	764	0	0
32	k	632	0	662	0	0
33	e	665	0	666	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	l	665	0	666	0	0
34	f	558	0	560	0	0
34	m	558	0	560	0	0
35	g	608	0	624	0	0
35	n	608	0	624	0	0
36	o	1335	0	1367	0	0
37	p	626	0	646	0	0
38	q	941	0	941	0	0
38	r	1004	0	1003	0	0
38	s	3571	0	3573	0	0
38	t	993	0	1004	0	0
39	y	619	0	598	0	0
40	6	6	0	0	0	0
40	C	1	0	0	0	0
41	A	36	0	6	0	0
41	J	36	0	6	2	0
42	C	32	0	12	6	0
43	L2	1	0	0	0	0
43	N	3	0	0	0	0
43	O	3	0	0	0	0
All	All	120201	0	116907	348	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:67:G:O2'	4:A:42:GLY:O	1.97	0.81
5:C:145:LYS:NZ	42:C:1101:GTP:O2G	2.14	0.80
1:2:20:A:OP1	3:6:77:A:N6	2.16	0.78
3:6:59:U:OP2	4:A:655:ARG:NH1	2.18	0.76
9:I:586:GLN:OE1	11:J:305:LYS:NZ	2.19	0.75
3:6:60:G:N7	4:A:655:ARG:NH2	2.35	0.74
22:R:2:SER:O	22:R:6:ARG:NH1	2.22	0.73
2:5:40:G:N2	2:5:48:C:O2	2.19	0.71
3:6:73:A:O4'	11:J:81:LYS:NZ	2.25	0.70
26:W:315:TYR:OH	26:W:348:THR:O	2.08	0.70
10:IN:28:N:O2'	18:O:190:THR:OG1	2.06	0.70
26:W:217:ASP:OD1	26:W:356:ARG:NH2	2.26	0.69
2:5:12:C:OP1	4:A:213:THR:OG1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DX:466:LEU:N	25:TF:164:MET:SD	2.67	0.68
21:Q:934:GLU:OE2	21:Q:1014:ARG:NH1	2.27	0.68
9:I:192:GLU:OE2	9:I:220:LYS:NZ	2.27	0.68
2:5:42:C:O2'	2:5:44:U:OP2	2.09	0.68
4:A:105:ASP:OD1	17:N:9:ARG:NH2	2.26	0.67
15:L2:445:TRP:NE1	15:L2:451:THR:OG1	2.28	0.67
2:5:10:U:O4	2:5:70:G:O6	2.13	0.66
9:I:543:GLN:NE2	11:J:306:LYS:O	2.28	0.66
6:D:109:ASP:OD1	6:D:122:LYS:NZ	2.28	0.66
4:A:1479:GLU:OE1	4:A:1484:ARG:NE	2.28	0.66
11:J:582:ASN:ND2	11:J:619:MET:SD	2.69	0.66
4:A:133:GLN:NE2	4:A:197:PHE:O	2.30	0.65
13:L:27:GLY:HA2	13:L:34:ILE:HD11	1.79	0.64
14:L1:365:ILE:O	14:L1:409:LEU:N	2.29	0.64
18:O:231:ASP:O	18:O:284:ARG:NH1	2.31	0.64
4:A:824:TYR:OH	4:A:921:GLU:OE2	2.15	0.63
3:6:20:C:O4'	18:O:57:ARG:NH1	2.32	0.63
17:N:125:PRO:O	17:N:127:SER:N	2.33	0.62
2:5:27:G:OP1	2:5:61:U:O2'	2.17	0.61
4:A:68:SER:O	4:A:70:LYS:N	2.34	0.61
13:L:316:ARG:NH2	13:L:320:ASP:OD2	2.34	0.60
3:6:78:A:OP1	11:J:91:LYS:NZ	2.34	0.60
15:L2:291:GLU:OE2	15:L2:373:ARG:NH1	2.35	0.60
4:A:1857:THR:OG1	4:A:1858:ARG:NH2	2.35	0.60
5:C:154:GLU:OE1	5:C:162:ARG:NE	2.34	0.60
3:6:39:G:O2'	3:6:40:A:O5'	2.20	0.59
21:Q:802:ASN:ND2	21:Q:839:GLN:OE1	2.36	0.59
11:J:506:ARG:NH1	11:J:537:GLU:OE2	2.34	0.59
1:2:11:C:H42	3:6:82:C:H42	1.51	0.59
3:6:39:G:O3'	13:L:170:ARG:NH2	2.35	0.59
1:2:1:A:OP1	16:M:99:LYS:NZ	2.35	0.59
9:I:201:ASP:OD2	9:I:205:LYS:NZ	2.35	0.58
26:W:104:ASN:O	26:W:106:PHE:N	2.36	0.58
9:I:26:ASP:OD2	9:I:50:LYS:NZ	2.30	0.58
11:J:456:ARG:NH2	41:J:3000:IHP:O35	2.36	0.58
25:TF:438:TRP:O	25:TF:496:ARG:NH1	2.35	0.58
28:Z:87:ASP:OD2	28:Z:91:ARG:NH1	2.36	0.58
6:D:161:TYR:OH	9:I:152:HIS:ND1	2.32	0.58
7:DX:220:ILE:O	7:DX:224:VAL:HG23	2.03	0.57
4:A:1392:GLN:O	4:A:1394:ARG:N	2.36	0.57
25:TF:405:ARG:NH2	25:TF:409:GLU:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1760:ASN:ND2	4:A:1881:GLU:OE2	2.37	0.57
24:T:315:ASP:OD2	24:T:358:LEU:N	2.36	0.56
5:C:145:LYS:NZ	42:C:1101:GTP:O1B	2.22	0.56
6:D:90:GLN:OE1	6:D:93:ARG:NH1	2.38	0.56
14:L1:343:CYS:N	14:L1:378:GLU:OE1	2.38	0.56
21:Q:724:ASP:OD2	21:Q:789:ARG:NH1	2.38	0.56
7:DX:396:ARG:NH1	7:DX:659:ASP:OD2	2.38	0.56
13:L:49:ARG:NH2	13:L:134:GLU:O	2.38	0.56
26:W:341:ARG:NH1	26:W:360:GLY:O	2.37	0.56
5:C:162:ARG:NH1	5:C:318:ASN:OD1	2.39	0.56
9:I:396:GLN:OE1	9:I:400:VAL:HG23	2.06	0.56
5:C:406:ARG:O	5:C:426:ARG:NH2	2.39	0.55
14:L1:336:VAL:HG11	14:L1:339:ILE:HD11	1.88	0.55
14:L1:383:LYS:HG2	14:L1:399:THR:HG21	1.89	0.55
1:2:13:G:H22	16:M:187:TYR:HD1	1.54	0.55
5:C:391:ASP:O	5:C:393:ASP:N	2.38	0.55
26:W:361:HIS:ND1	26:W:383:GLN:OE1	2.40	0.54
4:A:694:LYS:O	4:A:696:ASN:N	2.40	0.54
5:C:183:SER:N	42:C:1101:GTP:O3G	2.36	0.54
25:TF:388:PHE:O	25:TF:392:ARG:NH2	2.41	0.54
13:L:228:ASN:O	13:L:230:SER:N	2.39	0.54
21:Q:1140:ARG:NH2	21:Q:1269:GLN:OE1	2.40	0.54
4:A:1454:ASP:O	4:A:1456:LYS:N	2.40	0.54
20:PX:524:GLU:OE2	20:PX:534:ARG:NH1	2.40	0.54
4:A:545:LEU:HD13	4:A:577:VAL:CG2	2.37	0.54
4:A:793:ILE:HD13	4:A:984:LEU:HD22	1.89	0.54
26:W:120:TYR:OH	26:W:143:GLU:OE1	2.18	0.54
4:A:967:VAL:HG11	4:A:1145:VAL:HG21	1.90	0.54
7:DX:408:ALA:O	7:DX:411:MET:N	2.41	0.54
12:K:130:ARG:NH1	13:L:653:GLU:OE1	2.38	0.53
4:A:1049:ARG:NH2	4:A:1052:GLU:OE1	2.41	0.53
5:C:483:THR:HG22	5:C:566:THR:HG22	1.91	0.53
22:R:131:ASN:OD1	24:T:422:ARG:NE	2.38	0.53
18:O:79:LYS:O	18:O:98:ARG:NH2	2.39	0.53
18:O:366:ARG:NE	21:Q:1340:HIS:O	2.40	0.53
4:A:1048:ARG:NH2	4:A:1052:GLU:OE2	2.42	0.53
4:A:1328:PRO:O	4:A:1330:SER:N	2.41	0.53
26:W:215:LYS:NZ	26:W:223:GLU:OE1	2.32	0.53
5:C:262:LYS:HG2	42:C:1101:GTP:C6	2.44	0.53
7:DX:665:LEU:CD2	7:DX:694:VAL:HG11	2.38	0.53
5:C:714:ASN:OD1	5:C:715:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:89:VAL:O	13:L:91:ARG:N	2.42	0.52
21:Q:1268:GLN:O	21:Q:1298:ARG:NH2	2.42	0.52
4:A:865:ASN:O	4:A:868:GLU:N	2.42	0.52
8:E:231:VAL:HG23	8:E:252:HIS:CE1	2.45	0.52
8:E:181:ILE:HG13	8:E:191:VAL:HG13	1.91	0.52
4:A:587:LYS:O	4:A:589:LYS:N	2.43	0.52
13:L:266:LYS:O	13:L:269:LYS:NZ	2.37	0.52
21:Q:909:ARG:NH2	21:Q:1017:GLU:OE2	2.43	0.52
4:A:1742:LYS:NZ	15:L2:173:GLY:O	2.40	0.52
7:DX:565:ASP:HB2	7:DX:569:LEU:HD12	1.92	0.52
11:J:119:SER:O	11:J:122:ILE:N	2.41	0.51
13:L:23:ILE:HA	13:L:27:GLY:HA3	1.92	0.51
18:O:164:ALA:HB3	18:O:165:PRO:HD3	1.93	0.51
22:R:140:PRO:HG3	24:T:321:VAL:HG21	1.91	0.51
4:A:545:LEU:HD13	4:A:577:VAL:HG21	1.93	0.51
4:A:585:ARG:NH2	15:L2:197:ASP:OD1	2.42	0.51
7:DX:488:ASN:OD1	25:TF:153:ASN:ND2	2.42	0.51
4:A:1450:HIS:O	4:A:1452:ARG:N	2.43	0.51
13:L:24:MET:O	22:R:270:ARG:NH2	2.43	0.51
7:DX:330:ILE:HD12	7:DX:360:LYS:HD2	1.93	0.51
7:DX:397:VAL:HG22	7:DX:683:PHE:CE1	2.45	0.51
4:A:95:ASN:O	4:A:104:ARG:NH2	2.44	0.51
7:DX:443:TYR:OH	25:TF:204:THR:N	2.39	0.51
1:2:30:A:OP2	4:A:853:ARG:NH1	2.43	0.51
25:TF:161:MET:O	25:TF:166:TYR:N	2.43	0.51
3:6:19:A:N3	3:6:21:U:O2'	2.37	0.51
4:A:1519:LEU:O	4:A:1521:GLN:N	2.43	0.51
1:2:18:U:H3	3:6:77:A:HO2'	1.59	0.51
5:C:669:THR:OG1	5:C:832:MET:SD	2.54	0.51
7:DX:215:ILE:HD11	7:DX:454:VAL:HG13	1.92	0.51
4:A:142:ARG:NH2	4:A:608:PHE:O	2.44	0.50
4:A:801:ILE:HD11	4:A:984:LEU:HD21	1.93	0.50
5:C:431:PHE:O	5:C:434:PHE:N	2.42	0.50
4:A:1497:GLU:O	4:A:1526:ARG:NH2	2.44	0.50
11:J:82:ASN:O	11:J:84:MET:N	2.45	0.50
26:W:445:ASN:ND2	26:W:483:ARG:O	2.42	0.50
5:C:146:THR:OG1	42:C:1101:GTP:O2B	2.29	0.50
4:A:1885:PRO:O	4:A:1888:ALA:N	2.45	0.50
11:J:186:PRO:O	11:J:217:HIS:NE2	2.45	0.50
5:C:600:ASN:ND2	5:C:603:GLU:OE1	2.42	0.49
13:L:497:GLU:O	13:L:500:SER:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:197:ARG:NH2	14:L1:199:PRO:O	2.45	0.49
19:P:67:GLU:OE1	24:T:456:ARG:NH2	2.45	0.49
4:A:743:THR:HG22	4:A:774:LEU:HD21	1.94	0.49
4:A:240:ASP:OD1	4:A:240:ASP:N	2.41	0.49
41:J:3000:IHP:O14	13:L:307:LYS:NZ	2.38	0.49
16:M:214:ASP:OD1	22:R:269:LYS:NZ	2.40	0.49
4:A:1628:TYR:N	4:A:1651:GLN:OE1	2.45	0.49
24:T:190:VAL:HG22	24:T:447:ALA:HB1	1.95	0.49
26:W:441:LYS:NZ	26:W:480:ASP:OD2	2.35	0.49
3:6:95:A:O2'	3:6:96:A:OP1	2.25	0.48
4:A:989:LEU:O	4:A:993:VAL:HG12	2.13	0.48
21:Q:567:LEU:HB3	21:Q:609:VAL:HG11	1.95	0.48
24:T:447:ALA:HB3	24:T:460:ALA:HB3	1.95	0.48
18:O:262:TYR:O	18:O:289:ARG:NH1	2.41	0.48
2:5:3:A:N6	2:5:81:G:N3	2.61	0.48
7:DX:540:VAL:HG21	7:DX:601:ALA:HB2	1.95	0.48
16:M:213:LEU:HD11	22:R:265:VAL:HG13	1.96	0.48
19:P:89:ARG:NH2	19:P:93:ASP:OD2	2.46	0.48
4:A:915:ASP:OD2	4:A:1432:ARG:NE	2.47	0.48
4:A:1551:THR:HG22	4:A:1553:ILE:H	1.78	0.48
9:I:418:ASP:OD1	9:I:419:ALA:N	2.46	0.48
14:L1:102:THR:HG1	14:L1:104:SER:HG	1.61	0.48
8:E:187:ASN:O	8:E:210:ILE:HD11	2.14	0.48
9:I:688:ALA:HA	9:I:691:ILE:HD12	1.94	0.48
16:M:213:LEU:CD1	22:R:265:VAL:HG13	2.44	0.48
4:A:663:THR:O	4:A:668:ARG:NH2	2.40	0.48
14:L1:156:ASP:OD1	14:L1:156:ASP:N	2.47	0.48
4:A:1939:ASN:O	4:A:1942:LYS:N	2.47	0.48
11:J:202:GLU:O	11:J:204:ASP:N	2.47	0.48
11:J:257:ASN:O	11:J:259:THR:N	2.47	0.48
4:A:1337:GLN:NE2	4:A:1705:TYR:O	2.46	0.48
7:DX:698:ARG:NH1	27:X:253:GLU:OE1	2.45	0.48
14:L1:97:LYS:NZ	14:L1:131:GLU:OE1	2.47	0.48
20:PX:706:ILE:HD13	20:PX:709:ILE:HD12	1.94	0.48
5:C:243:GLU:OE2	5:C:247:ARG:NH1	2.46	0.48
9:I:232:CYS:HA	9:I:235:ILE:HG22	1.95	0.48
4:A:760:ASP:O	4:A:763:VAL:N	2.47	0.47
4:A:1327:ILE:HD11	4:A:1358:ILE:HG23	1.96	0.47
9:I:388:VAL:HG21	9:I:404:TRP:CZ2	2.48	0.47
5:C:212:VAL:HG23	5:C:902:MET:SD	2.55	0.47
5:C:730:LEU:HA	5:C:733:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1486:THR:O	4:A:1488:PHE:N	2.43	0.47
22:R:265:VAL:HG12	22:R:265:VAL:O	2.14	0.47
4:A:790:GLY:O	4:A:792:TYR:N	2.47	0.47
16:M:203:ASN:OD1	16:M:204:GLU:N	2.48	0.47
18:O:168:CYS:O	18:O:171:PHE:N	2.41	0.47
13:L:66:GLU:N	13:L:66:GLU:OE1	2.47	0.47
2:5:4:C:O2	2:5:81:G:N2	2.28	0.47
13:L:146:ASP:OD1	13:L:147:ASP:N	2.48	0.47
18:O:238:TYR:N	18:O:308:ARG:O	2.47	0.47
25:TF:626:LEU:HD22	25:TF:660:ILE:HG22	1.95	0.47
26:W:433:GLU:HG3	26:W:440:THR:HG21	1.97	0.47
3:6:50:C:OP2	3:6:69:U:O2'	2.32	0.47
4:A:1313:GLU:OE2	4:A:1464:ARG:NH2	2.47	0.47
4:A:936:ASP:OD1	4:A:936:ASP:N	2.48	0.47
16:M:77:ALA:O	16:M:81:GLY:N	2.44	0.47
26:W:419:ARG:HH21	26:W:431:ILE:HG21	1.80	0.47
3:6:25:A:N1	10:IN:24:N:O2'	2.35	0.46
3:6:94:C:O2'	3:6:95:A:OP1	2.24	0.46
5:C:850:VAL:HG22	5:C:891:LEU:HD11	1.97	0.46
14:L1:441:THR:O	15:L2:435:LYS:NZ	2.47	0.46
3:6:56:C:OP1	4:A:658:LYS:NZ	2.40	0.46
4:A:1312:LYS:NZ	15:L2:361:MET:O	2.42	0.46
26:W:220:GLN:NE2	26:W:317:GLY:O	2.44	0.46
4:A:1858:ARG:O	4:A:1860:ALA:N	2.48	0.46
2:5:56:U:OP1	19:P:39:THR:OG1	2.30	0.46
4:A:1773:VAL:HG22	4:A:1856:VAL:HG22	1.98	0.46
2:5:60:G:H2'	2:5:61:U:H5'	1.98	0.46
5:C:267:LEU:HD13	5:C:267:LEU:H	1.80	0.46
5:C:600:ASN:OD1	5:C:600:ASN:N	2.48	0.46
25:TF:786:ARG:NE	25:TF:798:LEU:O	2.45	0.46
4:A:1007:VAL:HG22	4:A:1008:LEU:H	1.80	0.45
6:D:225:GLU:OE2	6:D:239:ARG:NE	2.48	0.45
2:5:9:G:H3'	2:5:10:U:H5"	1.98	0.45
22:R:274:ASP:OD2	22:R:276:ARG:NE	2.44	0.45
25:TF:614:ILE:HG21	25:TF:652:THR:HG22	1.98	0.45
4:A:1369:GLU:O	4:A:1373:VAL:HG22	2.16	0.45
21:Q:716:LEU:O	21:Q:768:ARG:NH1	2.47	0.45
23:S:66:THR:HG21	26:W:55:VAL:HG22	1.98	0.45
7:DX:369:GLU:O	7:DX:416:ARG:NH1	2.49	0.45
6:D:113:ARG:NH2	9:I:216:ASN:OD1	2.47	0.45
7:DX:187:ARG:NH1	7:DX:508:GLU:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DX:645:VAL:O	7:DX:657:VAL:HG23	2.16	0.45
4:A:1512:THR:O	4:A:1514:ALA:N	2.50	0.45
9:I:576:LYS:NZ	11:J:314:GLU:OE1	2.46	0.45
14:L1:201:ARG:NH1	14:L1:254:ALA:O	2.49	0.45
4:A:373:PRO:O	5:C:358:ARG:NH2	2.50	0.45
11:J:85:GLN:O	11:J:87:ALA:N	2.50	0.45
13:L:467:LYS:NZ	13:L:469:ASP:OD1	2.43	0.45
24:T:389:LEU:HD22	24:T:424:GLY:HA2	1.98	0.45
26:W:414:PHE:HA	26:W:477:LEU:HD23	1.98	0.45
26:W:507:ASP:O	26:W:509:SER:N	2.50	0.45
4:A:1640:ASP:O	4:A:1716:LYS:NZ	2.39	0.45
16:M:83:ASP:O	16:M:85:GLU:N	2.50	0.45
21:Q:852:ARG:NH1	21:Q:1030:LEU:O	2.46	0.45
25:TF:794:LEU:HD23	25:TF:805:VAL:HG21	1.98	0.45
4:A:181:ILE:HG13	4:A:563:ALA:HB1	1.99	0.45
7:DX:395:ILE:HD12	7:DX:397:VAL:HG21	1.98	0.45
9:I:703:VAL:HG23	9:I:704:HIS:CD2	2.51	0.44
11:J:169:ASN:O	11:J:172:GLY:N	2.48	0.44
14:L1:111:LEU:HD23	14:L1:175:LEU:HD21	1.98	0.44
17:N:88:ASP:O	17:N:90:ALA:N	2.50	0.44
20:PX:410:LYS:NZ	20:PX:520:ASP:OD1	2.50	0.44
26:W:290:LEU:HD21	26:W:302:LEU:HD13	1.98	0.44
9:I:547:LYS:HB2	11:J:306:LYS:HE3	1.99	0.44
9:I:416:ASP:O	9:I:420:ALA:N	2.48	0.44
14:L1:66:THR:N	14:L1:90:ASN:O	2.46	0.44
20:PX:407:LEU:O	20:PX:411:VAL:HG23	2.18	0.44
23:S:44:ASN:OD1	23:S:47:ASN:ND2	2.50	0.44
4:A:1988:ASN:O	4:A:1990:VAL:N	2.51	0.44
14:L1:338:ALA:O	14:L1:345:ALA:N	2.41	0.44
2:5:26:C:N4	4:A:457:LYS:O	2.49	0.44
4:A:994:ASP:O	4:A:996:ASN:N	2.50	0.44
2:5:75:C:O2'	2:5:76:A:O5'	2.35	0.44
5:C:817:ARG:NE	5:C:821:TYR:OH	2.51	0.44
21:Q:467:LEU:O	21:Q:1124:ARG:NH2	2.48	0.44
9:I:562:ASN:O	9:I:566:VAL:HG22	2.18	0.43
11:J:364:ILE:HG23	11:J:383:TRP:CZ2	2.53	0.43
25:TF:619:VAL:HG13	25:TF:660:ILE:HD11	2.00	0.43
4:A:388:ASP:OD1	4:A:388:ASP:N	2.50	0.43
5:C:600:ASN:O	5:C:602:SER:N	2.51	0.43
24:T:274:LEU:HB2	24:T:285:THR:HG22	2.00	0.43
5:C:182:CYS:HG	5:C:639:PHE:HE2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:262:LYS:HG2	42:C:1101:GTP:C5	2.53	0.43
9:I:290:ILE:HG21	9:I:350:LEU:HD13	1.99	0.43
10:IN:10:N:H2'	10:IN:11:N:H4'	2.00	0.43
21:Q:433:GLU:OE1	21:Q:649:ARG:NH1	2.51	0.43
7:DX:607:GLN:O	7:DX:611:VAL:HG23	2.19	0.43
21:Q:168:VAL:HG22	21:Q:217:LEU:HD11	2.01	0.43
18:O:245:SER:OG	18:O:272:THR:O	2.35	0.43
3:6:101:U:H2'	7:DX:510:PRO:HB3	2.00	0.43
4:A:1654:TRP:NE1	4:A:1690:SER:O	2.48	0.43
4:A:65:ASP:OD1	4:A:67:THR:N	2.50	0.43
26:W:524:ASP:OD2	26:W:527:THR:N	2.46	0.43
5:C:640:TYR:O	5:C:644:VAL:HG23	2.18	0.43
11:J:462:GLU:OE2	11:J:470:ARG:NH2	2.49	0.43
26:W:445:ASN:OD1	26:W:446:VAL:N	2.51	0.43
4:A:1482:LEU:O	4:A:1485:GLY:N	2.51	0.42
5:C:846:CYS:O	5:C:850:VAL:HG23	2.18	0.42
20:PX:459:ALA:O	20:PX:463:ALA:N	2.45	0.42
21:Q:581:ARG:NE	21:Q:596:SER:O	2.45	0.42
4:A:756:GLY:O	4:A:758:THR:N	2.52	0.42
11:J:309:GLU:HA	11:J:313:ILE:HD12	2.02	0.42
14:L1:527:THR:O	15:L2:87:LYS:NZ	2.50	0.42
17:N:18:TRP:NE1	17:N:22:GLU:OE2	2.49	0.42
5:C:116:VAL:HG23	5:C:156:THR:O	2.19	0.42
5:C:212:VAL:HG22	5:C:241:ASN:OD1	2.19	0.42
25:TF:176:GLY:O	25:TF:178:GLY:N	2.52	0.42
4:A:148:ARG:NH1	4:A:562:ASP:OD2	2.47	0.42
4:A:443:LEU:O	4:A:447:VAL:HG23	2.20	0.42
4:A:1518:GLY:O	15:L2:194:ARG:NH1	2.50	0.42
4:A:1893:GLU:O	4:A:1897:ASP:N	2.53	0.42
4:A:1926:PHE:O	4:A:1930:VAL:HG23	2.20	0.42
7:DX:198:TYR:O	7:DX:227:ARG:NH1	2.52	0.42
4:A:550:VAL:O	4:A:554:VAL:HG23	2.19	0.42
4:A:1046:GLY:HA2	4:A:1050:ALA:HB3	2.01	0.42
5:C:859:GLY:O	25:TF:532:GLN:NE2	2.45	0.42
17:N:120:CYS:SG	17:N:121:ILE:N	2.92	0.42
4:A:1224:VAL:HB	4:A:1273:THR:HG21	2.01	0.42
16:M:75:LYS:O	16:M:79:ASP:N	2.46	0.42
3:6:90:G:H3'	3:6:91:U:H5"	2.02	0.42
4:A:875:ARG:NH2	13:L:128:GLU:OE2	2.53	0.42
21:Q:315:GLU:OE2	21:Q:424:ARG:NH2	2.50	0.42
8:E:97:VAL:HG12	8:E:129:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:9:GLY:O	13:L:41:LYS:NZ	2.53	0.42
20:PX:742:ARG:O	20:PX:746:LYS:NZ	2.41	0.42
22:R:3:MET:SD	22:R:4:LYS:N	2.93	0.42
25:TF:155:ASN:OD1	25:TF:155:ASN:N	2.52	0.42
15:L2:76:ASP:OD1	15:L2:76:ASP:N	2.53	0.41
4:A:1310:THR:HG22	4:A:1310:THR:O	2.20	0.41
4:A:1392:GLN:OE1	4:A:1394:ARG:NH2	2.46	0.41
23:S:82:ASP:OD1	23:S:106:ASN:ND2	2.46	0.41
25:TF:626:LEU:HD23	25:TF:665:PHE:HB2	2.02	0.41
4:A:670:GLU:OE2	4:A:770:ARG:NH1	2.53	0.41
7:DX:272:GLU:OE2	7:DX:281:ARG:NH1	2.48	0.41
10:IN:27:N:H5"	18:O:162:ARG:CG	2.51	0.41
4:A:286:ASP:O	4:A:287:ILE:HG22	2.20	0.41
7:DX:317:ILE:HD13	7:DX:320:LEU:HD12	2.02	0.41
15:L2:152:ARG:NH1	15:L2:214:ASP:OD1	2.49	0.41
20:PX:614:GLU:HA	20:PX:618:ILE:HD12	2.02	0.41
27:X:254:GLU:O	27:X:257:ASN:ND2	2.54	0.41
9:I:454:ARG:O	9:I:457:ALA:N	2.48	0.41
17:N:124:VAL:HG12	17:N:124:VAL:O	2.21	0.41
24:T:322:ASP:N	24:T:322:ASP:OD1	2.53	0.41
13:L:438:GLN:OE1	13:L:439:MET:N	2.49	0.41
20:PX:435:ARG:NH1	20:PX:494:GLU:O	2.49	0.41
21:Q:1071:GLU:OE2	21:Q:1124:ARG:NE	2.50	0.41
5:C:445:PRO:O	5:C:449:ALA:N	2.50	0.41
11:J:89:TRP:CD1	11:J:112:ALA:HB2	2.56	0.41
25:TF:569:ILE:O	25:TF:572:VAL:HG22	2.21	0.41
26:W:194:GLN:O	26:W:198:ASP:N	2.49	0.41
14:L1:14:VAL:HA	14:L1:222:ILE:HD12	2.01	0.41
20:PX:339:ASP:N	20:PX:339:ASP:OD1	2.54	0.41
4:A:933:LYS:HA	4:A:933:LYS:HE2	2.03	0.40
14:L1:106:LEU:HD23	14:L1:238:PRO:HB3	2.03	0.40
20:PX:401:ARG:NH1	25:TF:330:ASN:OD1	2.46	0.40
1:2:9:U:O2'	1:2:10:U:O4'	2.39	0.40
4:A:468:PHE:O	4:A:471:THR:HG22	2.21	0.40
4:A:1325:VAL:HB	4:A:1358:ILE:HD11	2.03	0.40
5:C:522:ASP:O	5:C:524:GLU:N	2.54	0.40
9:I:543:GLN:HB2	11:J:306:LYS:HA	2.04	0.40
18:O:40:ASP:O	18:O:54:THR:HG23	2.21	0.40
14:L1:399:THR:HG22	14:L1:413:MET:HG2	2.03	0.40
18:O:98:ARG:NH1	18:O:99:ASP:OD1	2.51	0.40
20:PX:469:ARG:NH2	20:PX:487:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:91:MET:O	21:Q:95:VAL:HG23	2.22	0.40
4:A:880:GLN:O	4:A:882:ALA:N	2.55	0.40
4:A:1641:SER:OG	20:PX:367:GLN:NE2	2.55	0.40
4:A:1863:ASP:OD2	15:L2:132:ASN:ND2	2.55	0.40
8:E:64:PHE:O	8:E:73:ASN:ND2	2.49	0.40
9:I:41:ASN:OD1	9:I:45:ARG:NH2	2.54	0.40
9:I:215:GLN:NE2	9:I:217:VAL:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1976/2329 (85%)	1789 (90%)	101 (5%)	86 (4%)	2 15
5	C	896/974 (92%)	800 (89%)	66 (7%)	30 (3%)	4 21
6	D	192/267 (72%)	185 (96%)	7 (4%)	0	100 100
7	DX	680/739 (92%)	634 (93%)	36 (5%)	10 (2%)	10 42
8	E	310/331 (94%)	295 (95%)	13 (4%)	2 (1%)	25 64
9	I	743/855 (87%)	702 (94%)	37 (5%)	4 (0%)	29 68
11	J	570/744 (77%)	531 (93%)	22 (4%)	17 (3%)	4 24
12	K	201/238 (84%)	196 (98%)	4 (2%)	1 (0%)	29 68
13	L	611/755 (81%)	570 (93%)	28 (5%)	13 (2%)	7 33
14	L1	468/533 (88%)	435 (93%)	26 (6%)	7 (2%)	10 42
15	L2	358/460 (78%)	336 (94%)	16 (4%)	6 (2%)	9 39
16	M	190/234 (81%)	179 (94%)	6 (3%)	5 (3%)	5 27
17	N	140/147 (95%)	123 (88%)	10 (7%)	7 (5%)	2 12
18	O	334/408 (82%)	302 (90%)	23 (7%)	9 (3%)	5 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	P	146/230 (64%)	130 (89%)	10 (7%)	6 (4%)	3 16
20	PX	470/809 (58%)	468 (100%)	2 (0%)	0	100 100
21	Q	1376/1467 (94%)	1336 (97%)	39 (3%)	1 (0%)	51 85
22	R	274/535 (51%)	243 (89%)	26 (10%)	5 (2%)	8 37
23	S	167/169 (99%)	158 (95%)	9 (5%)	0	100 100
24	T	385/494 (78%)	342 (89%)	35 (9%)	8 (2%)	7 33
25	TF	551/830 (66%)	507 (92%)	35 (6%)	9 (2%)	9 40
26	W	490/567 (86%)	435 (89%)	40 (8%)	15 (3%)	4 23
27	X	78/500 (16%)	75 (96%)	2 (3%)	1 (1%)	12 45
28	Z	67/69 (97%)	64 (96%)	3 (4%)	0	100 100
29	a	79/136 (58%)	78 (99%)	1 (1%)	0	100 100
29	h	79/136 (58%)	69 (87%)	8 (10%)	2 (2%)	5 28
30	b	92/160 (58%)	87 (95%)	5 (5%)	0	100 100
30	i	75/160 (47%)	69 (92%)	5 (7%)	1 (1%)	12 45
31	c	78/127 (61%)	76 (97%)	2 (3%)	0	100 100
31	j	78/127 (61%)	72 (92%)	6 (8%)	0	100 100
32	d	90/118 (76%)	86 (96%)	4 (4%)	0	100 100
32	k	75/118 (64%)	72 (96%)	3 (4%)	0	100 100
33	e	78/90 (87%)	74 (95%)	1 (1%)	3 (4%)	3 18
33	l	78/90 (87%)	73 (94%)	3 (4%)	2 (3%)	5 27
34	f	70/85 (82%)	68 (97%)	2 (3%)	0	100 100
34	m	70/85 (82%)	66 (94%)	3 (4%)	1 (1%)	11 43
35	g	75/77 (97%)	72 (96%)	3 (4%)	0	100 100
35	n	75/77 (97%)	68 (91%)	5 (7%)	2 (3%)	5 26
36	o	160/253 (63%)	154 (96%)	5 (3%)	1 (1%)	25 64
37	p	74/217 (34%)	70 (95%)	4 (5%)	0	100 100
38	q	117/492 (24%)	115 (98%)	2 (2%)	0	100 100
38	r	129/492 (26%)	127 (98%)	1 (1%)	1 (1%)	19 57
38	s	465/492 (94%)	450 (97%)	14 (3%)	1 (0%)	47 82
38	t	124/492 (25%)	121 (98%)	3 (2%)	0	100 100
39	y	77/79 (98%)	76 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	13911/18787 (74%)	12978 (93%)	677 (5%)	256 (2%)	12 37

All (256) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	68	SER
4	A	69	ARG
4	A	167	ASP
4	A	287	ILE
4	A	305	PRO
4	A	588	TYR
4	A	690	PRO
4	A	694	LYS
4	A	695	GLN
4	A	757	ALA
4	A	934	PRO
4	A	980	MET
4	A	995	HIS
4	A	1067	GLN
4	A	1135	MET
4	A	1310	THR
4	A	1311	PRO
4	A	1393	ASN
4	A	1394	ARG
4	A	1451	GLN
4	A	1455	GLY
4	A	1456	LYS
4	A	1487	TYR
4	A	1489	PRO
4	A	1513	ASN
4	A	1520	ASN
4	A	1730	ASN
4	A	1745	GLN
4	A	1846	PRO
4	A	1858	ARG
4	A	1873	PRO
4	A	1990	VAL
5	C	158	PRO
5	C	181	GLY
5	C	308	GLY
5	C	309	ASN
5	C	392	VAL

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Mol	Chain	Res	Type
5	C	404	GLY
5	C	405	ILE
5	C	444	SER
5	C	539	ALA
5	C	619	PRO
5	C	636	THR
5	C	737	TRP
5	C	782	PRO
5	C	843	PRO
7	DX	225	ARG
7	DX	226	ASN
7	DX	241	ALA
8	E	128	ALA
9	I	414	ASN
13	L	79	PRO
13	L	81	GLN
13	L	90	GLY
13	L	137	PRO
13	L	228	ASN
13	L	349	MET
14	L1	227	LYS
14	L1	228	GLN
15	L2	327	ASN
16	M	54	PRO
16	M	83	ASP
17	N	124	VAL
17	N	125	PRO
17	N	126	LYS
18	O	130	ASP
18	O	135	ILE
18	O	165	PRO
18	O	183	PRO
18	O	194	ASP
19	P	36	PRO
22	R	10	PRO
25	TF	151	ASP
25	TF	168	PRO
25	TF	546	ASP
26	W	105	GLU
26	W	176	PRO
26	W	190	THR
26	W	191	PRO

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Mol	Chain	Res	Type
26	W	508	GLN
27	X	219	LYS
4	A	36	SER
4	A	432	PRO
4	A	453	HIS
4	A	581	THR
4	A	725	THR
4	A	881	ARG
4	A	982	LEU
4	A	1007	VAL
4	A	1084	ILE
4	A	1094	SER
4	A	1225	ASP
4	A	1328	PRO
4	A	1329	GLN
4	A	1571	ARG
4	A	1859	LYS
4	A	1965	SER
4	A	1989	ASN
5	C	97	VAL
5	C	371	ARG
5	C	415	ASN
5	C	431	PHE
5	C	600	ASN
5	C	729	ASP
5	C	929	PRO
7	DX	242	GLY
7	DX	247	TYR
9	I	415	GLY
11	J	83	ARG
11	J	85	GLN
11	J	101	GLU
11	J	102	ILE
11	J	169	ASN
11	J	186	PRO
11	J	203	ILE
11	J	258	GLU
11	J	273	GLU
13	L	39	HIS
13	L	92	THR
13	L	268	LYS
14	L1	151	SER

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Mol	Chain	Res	Type
16	M	163	HIS
17	N	88	ASP
17	N	89	ALA
17	N	104	CYS
18	O	111	GLN
19	P	206	LYS
22	R	16	ASP
24	T	481	PRO
25	TF	148	MET
25	TF	180	VAL
26	W	84	SER
33	e	32	TYR
33	l	72	ARG
4	A	248	ASP
4	A	454	ARG
4	A	464	LEU
4	A	523	THR
4	A	559	ASN
4	A	562	ASP
4	A	724	PRO
4	A	794	SER
4	A	849	ASN
4	A	865	ASN
4	A	994	ASP
4	A	1012	LYS
4	A	1068	ASP
4	A	1273	THR
4	A	1450	HIS
4	A	1481	THR
4	A	1767	ASN
5	C	239	MET
5	C	730	LEU
7	DX	258	GLY
11	J	34	THR
11	J	86	LEU
11	J	99	ILE
11	J	202	GLU
11	J	257	ASN
13	L	42	SER
15	L2	268	ASP
16	M	84	TYR
17	N	74	SER

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Mol	Chain	Res	Type
18	O	169	SER
19	P	48	GLN
19	P	49	GLU
21	Q	349	ASN
22	R	21	GLN
24	T	248	LYS
26	W	68	PHE
29	h	46	GLU
38	r	22	GLY
4	A	232	ASN
4	A	297	ARG
4	A	1247	THR
4	A	1274	GLN
5	C	443	LYS
7	DX	240	ASP
7	DX	658	LYS
12	K	71	PHE
13	L	146	ASP
13	L	440	ARG
14	L1	191	LEU
14	L1	206	LEU
14	L1	229	LYS
15	L2	160	SER
15	L2	199	SER
15	L2	210	LYS
18	O	168	CYS
18	O	182	CYS
22	R	113	VAL
24	T	444	GLY
24	T	483	VAL
25	TF	176	GLY
26	W	67	LYS
26	W	360	GLY
33	e	13	PRO
30	i	4	SER
35	n	59	MET
4	A	426	HIS
4	A	665	THR
4	A	939	PRO
4	A	940	PRO
4	A	993	VAL
4	A	1136	LYS

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Mol	Chain	Res	Type
4	A	1668	ASP
5	C	65	ASP
5	C	273	PRO
7	DX	168	GLU
7	DX	239	LEU
13	L	229	PRO
14	L1	2	ALA
15	L2	209	GLY
16	M	152	TYR
19	P	30	TYR
24	T	438	SER
25	TF	154	SER
26	W	136	ASP
26	W	317	GLY
26	W	406	GLN
26	W	484	PHE
26	W	537	HIS
33	e	12	GLN
29	h	54	GLY
38	s	56	LYS
4	A	981	ASP
4	A	1296	ASN
4	A	1939	ASN
11	J	218	GLY
11	J	288	LEU
19	P	22	ASP
25	TF	196	ALA
4	A	296	ILE
4	A	759	VAL
5	C	601	PRO
5	C	803	GLU
11	J	100	GLY
24	T	167	LYS
34	m	74	VAL
35	n	68	VAL
4	A	1318	GLY
5	C	828	THR
5	C	866	PRO
8	E	205	GLY
22	R	12	PRO
26	W	531	VAL
24	T	182	GLY

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Mol	Chain	Res	Type
4	A	417	PRO
4	A	1190	PRO
36	o	32	PRO
4	A	659	GLY
9	I	360	PRO
9	I	799	GLY
24	T	261	ILE
25	TF	195	GLY
33	l	44	ILE

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	
4	A	1790/2100 (85%)	1730 (97%)	60 (3%)	37	72
5	C	793/861 (92%)	774 (98%)	19 (2%)	49	79
6	D	173/230 (75%)	170 (98%)	3 (2%)	60	85
7	DX	604/652 (93%)	597 (99%)	7 (1%)	71	90
8	E	275/291 (94%)	268 (98%)	7 (2%)	47	79
9	I	660/754 (88%)	641 (97%)	19 (3%)	42	76
11	J	508/650 (78%)	501 (99%)	7 (1%)	67	88
12	K	183/214 (86%)	181 (99%)	2 (1%)	73	90
13	L	543/645 (84%)	523 (96%)	20 (4%)	34	70
14	L1	406/452 (90%)	393 (97%)	13 (3%)	39	74
15	L2	331/417 (79%)	327 (99%)	4 (1%)	71	90
16	M	178/212 (84%)	169 (95%)	9 (5%)	24	60
17	N	125/129 (97%)	121 (97%)	4 (3%)	39	74
18	O	295/351 (84%)	290 (98%)	5 (2%)	60	85
19	P	129/197 (66%)	124 (96%)	5 (4%)	32	69
20	PX	423/724 (58%)	419 (99%)	4 (1%)	78	92
21	Q	1235/1311 (94%)	1222 (99%)	13 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	R	235/447 (53%)	219 (93%)	16 (7%)	16 48
23	S	137/137 (100%)	134 (98%)	3 (2%)	52 81
24	T	335/421 (80%)	319 (95%)	16 (5%)	25 62
25	TF	493/718 (69%)	479 (97%)	14 (3%)	43 77
26	W	444/502 (88%)	427 (96%)	17 (4%)	33 69
27	X	69/443 (16%)	64 (93%)	5 (7%)	14 45
28	Z	63/63 (100%)	62 (98%)	1 (2%)	62 86
29	a	71/106 (67%)	70 (99%)	1 (1%)	67 88
29	h	71/106 (67%)	70 (99%)	1 (1%)	67 88
30	b	79/116 (68%)	78 (99%)	1 (1%)	69 89
30	i	70/116 (60%)	68 (97%)	2 (3%)	42 76
31	c	73/98 (74%)	73 (100%)	0	100 100
31	j	73/98 (74%)	73 (100%)	0	100 100
32	d	84/103 (82%)	81 (96%)	3 (4%)	35 70
32	k	72/103 (70%)	71 (99%)	1 (1%)	67 88
33	e	71/81 (88%)	71 (100%)	0	100 100
33	l	71/81 (88%)	70 (99%)	1 (1%)	67 88
34	f	61/71 (86%)	61 (100%)	0	100 100
34	m	61/71 (86%)	59 (97%)	2 (3%)	38 73
35	g	69/69 (100%)	69 (100%)	0	100 100
35	n	69/69 (100%)	68 (99%)	1 (1%)	67 88
36	o	151/225 (67%)	150 (99%)	1 (1%)	84 94
37	p	68/192 (35%)	67 (98%)	1 (2%)	65 87
38	q	108/417 (26%)	107 (99%)	1 (1%)	78 92
38	r	114/417 (27%)	111 (97%)	3 (3%)	46 78
38	s	396/417 (95%)	393 (99%)	3 (1%)	81 93
38	t	115/417 (28%)	115 (100%)	0	100 100
39	y	64/64 (100%)	64 (100%)	0	100 100
All	All	12438/16358 (76%)	12143 (98%)	295 (2%)	51 79

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	GLU
4	A	68	SER
4	A	87	HIS
4	A	120	ASN
4	A	129	VAL
4	A	178	LEU
4	A	209	VAL
4	A	213	THR
4	A	227	LEU
4	A	240	ASP
4	A	246	LEU
4	A	298	THR
4	A	305	PRO
4	A	327	VAL
4	A	406	ARG
4	A	532	PHE
4	A	560	ASN
4	A	577	VAL
4	A	587	LYS
4	A	603	LEU
4	A	669	VAL
4	A	690	PRO
4	A	767	ASN
4	A	801	ILE
4	A	836	GLU
4	A	840	GLU
4	A	876	HIS
4	A	934	PRO
4	A	952	ASN
4	A	961	SER
4	A	969	MET
4	A	1020	PHE
4	A	1048	ARG
4	A	1097	GLU
4	A	1153	LEU
4	A	1177	MET
4	A	1267	ARG
4	A	1274	GLN
4	A	1312	LYS
4	A	1329	GLN
4	A	1358	ILE
4	A	1377	ARG
4	A	1480	HIS

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Mol	Chain	Res	Type
4	A	1487	TYR
4	A	1489	PRO
4	A	1494	LEU
4	A	1497	GLU
4	A	1512	THR
4	A	1630	TRP
4	A	1651	GLN
4	A	1668	ASP
4	A	1715	MET
4	A	1738	GLU
4	A	1828	GLN
4	A	1846	PRO
4	A	1873	PRO
4	A	1877	ILE
4	A	1893	GLU
4	A	1899	ILE
4	A	1924	THR
5	C	68	TYR
5	C	76	TYR
5	C	92	LEU
5	C	233	ASP
5	C	235	HIS
5	C	258	LEU
5	C	267	LEU
5	C	326	PHE
5	C	380	PRO
5	C	392	VAL
5	C	501	MET
5	C	619	PRO
5	C	698	LYS
5	C	728	TRP
5	C	737	TRP
5	C	796	LEU
5	C	807	ARG
5	C	835	TYR
5	C	930	THR
6	D	35	LYS
6	D	155	ARG
6	D	243	LEU
7	DX	66	TYR
7	DX	243	LYS
7	DX	272	GLU

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Mol	Chain	Res	Type
7	DX	367	ILE
7	DX	681	ASN
7	DX	708	GLN
7	DX	715	PHE
8	E	53	LEU
8	E	127	ASN
8	E	186	ASP
8	E	187	ASN
8	E	255	ASN
8	E	293	TYR
8	E	314	MET
9	I	118	ARG
9	I	159	TYR
9	I	176	TYR
9	I	215	GLN
9	I	250	ILE
9	I	351	MET
9	I	395	ILE
9	I	399	LYS
9	I	417	LEU
9	I	487	SER
9	I	551	LEU
9	I	578	GLU
9	I	628	ASP
9	I	639	TYR
9	I	663	LEU
9	I	735	GLU
9	I	791	LYS
9	I	798	ARG
9	I	802	LYS
11	J	89	TRP
11	J	117	HIS
11	J	119	SER
11	J	144	ASP
11	J	309	GLU
11	J	458	TYR
11	J	603	CYS
12	K	48	HIS
12	K	79	GLU
13	L	13	ASN
13	L	53	TRP
13	L	122	ARG

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Mol	Chain	Res	Type
13	L	132	THR
13	L	137	PRO
13	L	162	ASN
13	L	269	LYS
13	L	318	TYR
13	L	347	THR
13	L	355	GLN
13	L	361	LEU
13	L	366	ASN
13	L	438	GLN
13	L	451	GLU
13	L	452	GLN
13	L	504	GLU
13	L	508	LYS
13	L	585	LYS
13	L	611	LEU
13	L	704	LYS
14	L1	3	THR
14	L1	10	CYS
14	L1	118	SER
14	L1	121	LEU
14	L1	134	ILE
14	L1	156	ASP
14	L1	176	SER
14	L1	193	VAL
14	L1	226	GLU
14	L1	235	ASN
14	L1	269	LYS
14	L1	449	LEU
14	L1	532	SER
15	L2	76	ASP
15	L2	96	LEU
15	L2	184	ARG
15	L2	210	LYS
16	M	27	ARG
16	M	54	PRO
16	M	55	LYS
16	M	63	ARG
16	M	83	ASP
16	M	92	MET
16	M	151	PHE
16	M	183	ARG

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Mol	Chain	Res	Type
16	M	206	ASN
17	N	111	THR
17	N	125	PRO
17	N	126	LYS
17	N	135	ILE
18	O	40	ASP
18	O	42	TYR
18	O	115	ARG
18	O	188	LYS
18	O	199	GLN
19	P	3	THR
19	P	59	LEU
19	P	89	ARG
19	P	90	GLN
19	P	92	MET
20	PX	344	LEU
20	PX	357	PHE
20	PX	443	GLN
20	PX	447	CYS
21	Q	37	HIS
21	Q	209	ASN
21	Q	318	ASP
21	Q	346	ARG
21	Q	627	GLU
21	Q	669	ARG
21	Q	780	ARG
21	Q	979	LYS
21	Q	1118	GLU
21	Q	1269	GLN
21	Q	1308	ARG
21	Q	1337	PHE
21	Q	1389	GLU
22	R	3	MET
22	R	4	LYS
22	R	21	GLN
22	R	24	ARG
22	R	53	PHE
22	R	90	ASN
22	R	91	THR
22	R	130	TRP
22	R	156	LEU
22	R	160	VAL

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Mol	Chain	Res	Type
22	R	200	ILE
22	R	204	GLU
22	R	205	GLU
22	R	241	THR
22	R	243	LYS
22	R	290	LEU
23	S	53	ARG
23	S	100	ASN
23	S	147	ASN
24	T	92	MET
24	T	177	TYR
24	T	272	GLN
24	T	289	ASP
24	T	322	ASP
24	T	344	SER
24	T	345	MET
24	T	346	CYS
24	T	387	GLN
24	T	388	ASN
24	T	389	LEU
24	T	404	ASP
24	T	435	GLN
24	T	436	PRO
24	T	446	TYR
24	T	451	ASP
25	TF	153	ASN
25	TF	155	ASN
25	TF	200	GLU
25	TF	202	THR
25	TF	368	LEU
25	TF	388	PHE
25	TF	392	ARG
25	TF	496	ARG
25	TF	590	MET
25	TF	645	CYS
25	TF	682	VAL
25	TF	777	PRO
25	TF	779	LYS
25	TF	829	GLN
26	W	58	LYS
26	W	69	ASP
26	W	133	PHE

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Mol	Chain	Res	Type
26	W	282	GLN
26	W	294	CYS
26	W	299	LYS
26	W	312	VAL
26	W	343	VAL
26	W	354	LYS
26	W	369	HIS
26	W	385	LYS
26	W	410	SER
26	W	417	ASN
26	W	434	TRP
26	W	454	MET
26	W	481	LYS
26	W	504	PHE
27	X	243	PHE
27	X	246	GLN
27	X	247	ASP
27	X	257	ASN
27	X	258	LYS
28	Z	124	LYS
29	a	47	THR
30	b	38	MET
32	d	48	ASN
32	d	65	MET
32	d	73	MET
29	h	77	MET
30	i	35	ASP
30	i	89	ASP
32	k	49	ASN
33	l	54	PHE
34	m	72	LEU
34	m	73	TYR
35	n	32	ARG
36	o	106	ILE
37	p	34	GLN
38	q	129	ARG
38	r	32	LYS
38	r	104	LEU
38	r	115	CYS
38	s	24	ILE
38	s	390	GLU
38	s	432	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	47	GLN
4	A	449	ASN
4	A	729	ASN
4	A	1568	GLN
5	C	235	HIS
5	C	772	GLN
8	E	252	HIS
8	E	254	HIS
8	E	255	ASN
9	I	52	GLN
13	L	366	ASN
19	P	221	HIS
21	Q	209	ASN
23	S	147	ASN
24	T	238	HIS
25	TF	543	ASN
26	W	282	GLN
33	e	37	HIS
34	f	70	ASN
32	k	69	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/228 (16%)	18 (47%)	4 (10%)
10	IN	1/51 (1%)	1 (100%)	0
2	5	110/112 (98%)	32 (29%)	12 (10%)
3	6	100/101 (99%)	45 (45%)	13 (13%)
All	All	249/492 (50%)	96 (38%)	29 (11%)

All (96) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	U
1	2	19	U
1	2	21	G
1	2	25	A
1	2	26	G
1	2	30	A
1	2	31	A

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Mol	Chain	Res	Type
1	2	32	A
1	2	33	G
1	2	34	U
1	2	35	G
1	2	36	U
1	2	37	A
1	2	38	G
1	2	39	U
1	2	40	A
1	2	41	U
1	2	42	C
2	5	4	C
2	5	6	C
2	5	8	G
2	5	9	G
2	5	10	U
2	5	20	U
2	5	23	A
2	5	24	A
2	5	26	C
2	5	28	U
2	5	43	U
2	5	60	G
2	5	73	U
2	5	74	A
2	5	76	A
2	5	77	U
2	5	79	G
2	5	80	A
2	5	81	G
2	5	82	U
2	5	83	A
2	5	94	U
2	5	96	U
2	5	100	G
2	5	101	A
2	5	105	C
2	5	110	G
2	5	112	G
2	5	113	A
2	5	114	G
2	5	115	A

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Mol	Chain	Res	Type
2	5	117	C
3	6	4	C
3	6	5	U
3	6	6	U
3	6	7	C
3	6	8	C
3	6	9	G
3	6	10	A
3	6	20	C
3	6	21	U
3	6	22	A
3	6	23	A
3	6	24	A
3	6	29	G
3	6	32	C
3	6	34	A
3	6	37	C
3	6	39	G
3	6	40	A
3	6	41	G
3	6	43	A
3	6	44	G
3	6	46	U
3	6	49	G
3	6	54	G
3	6	56	C
3	6	62	G
3	6	64	A
3	6	69	U
3	6	74	C
3	6	77	A
3	6	79	A
3	6	81	U
3	6	82	C
3	6	84	U
3	6	85	G
3	6	86	A
3	6	89	C
3	6	90	G
3	6	91	U
3	6	92	U
3	6	93	C

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Mol	Chain	Res	Type
3	6	95	A
3	6	96	A
3	6	97	A
3	6	101	U
10	IN	2	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	18	U
1	2	25	A
1	2	29	C
1	2	34	U
2	5	3	A
2	5	5	U
2	5	9	G
2	5	19	A
2	5	25	C
2	5	27	G
2	5	79	G
2	5	82	U
2	5	109	C
2	5	111	A
2	5	112	G
2	5	114	G
3	6	23	A
3	6	28	G
3	6	32	C
3	6	38	A
3	6	39	G
3	6	41	G
3	6	43	A
3	6	45	A
3	6	48	A
3	6	53	G
3	6	81	U
3	6	85	G
3	6	90	G

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 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
42	GTP	C	1101	40	26,34,34	1.49	2 (7%)	32,54,54	2.20	7 (21%)
41	IHP	A	3000	-	36,36,36	2.02	6 (16%)	54,60,60	1.22	7 (12%)
41	IHP	J	3000	-	36,36,36	2.27	10 (27%)	54,60,60	0.97	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	C	1101	40	-	0/18/38/38	0/3/3/3
41	IHP	A	3000	-	-	3/30/54/54	0/1/1/1
41	IHP	J	3000	-	-	4/30/54/54	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	J	3000	IHP	C3-C2	-5.48	1.40	1.52
41	A	3000	IHP	P5-O15	5.03	1.68	1.59
41	A	3000	IHP	P4-O14	4.82	1.68	1.59
41	A	3000	IHP	P6-O16	4.76	1.68	1.59
41	J	3000	IHP	P3-O13	4.73	1.68	1.59
41	A	3000	IHP	P2-O12	4.68	1.68	1.59
42	C	1101	GTP	C5-C6	-4.64	1.38	1.47
41	J	3000	IHP	P2-O12	4.52	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	J	3000	IHP	P4-O14	4.41	1.67	1.59
41	J	3000	IHP	P1-O11	4.31	1.67	1.59
41	J	3000	IHP	P5-O15	4.16	1.67	1.59
41	A	3000	IHP	P3-O13	4.04	1.66	1.59
41	J	3000	IHP	P6-O16	3.87	1.66	1.59
41	A	3000	IHP	P1-O11	3.53	1.66	1.59
41	J	3000	IHP	O12-C2	-3.24	1.32	1.44
42	C	1101	GTP	C5-C4	-2.67	1.36	1.43
41	J	3000	IHP	C2-C1	-2.65	1.46	1.52
41	J	3000	IHP	O13-C3	-2.64	1.34	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	C	1101	GTP	PB-O3B-PG	-6.27	111.31	132.83
42	C	1101	GTP	C5-C6-N1	5.20	123.14	113.95
42	C	1101	GTP	C2-N1-C6	-4.87	116.14	125.10
42	C	1101	GTP	O6-C6-C5	-3.72	117.10	124.37
42	C	1101	GTP	O3G-PG-O3B	3.35	115.87	104.64
41	A	3000	IHP	C5-C6-C1	3.20	117.41	110.41
41	A	3000	IHP	O16-C6-C5	-2.93	101.79	108.69
41	J	3000	IHP	C4-C3-C2	2.89	116.73	110.41
41	A	3000	IHP	O11-C1-C2	-2.78	102.14	108.69
42	C	1101	GTP	PA-O3A-PB	-2.73	123.46	132.83
41	A	3000	IHP	C6-C1-C2	2.60	116.09	110.41
42	C	1101	GTP	C8-N7-C5	2.48	107.72	102.99
41	J	3000	IHP	C3-C2-C1	2.43	115.74	110.41
41	A	3000	IHP	C6-C5-C4	2.42	115.71	110.41
41	A	3000	IHP	O11-P1-O21	-2.08	101.38	109.39
41	J	3000	IHP	O46-P6-O36	2.06	115.49	107.64
41	A	3000	IHP	O11-C1-C6	2.02	113.44	108.69

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C2-O12-P2-O22
41	J	3000	IHP	C5-O15-P5-O25
41	A	3000	IHP	C4-O14-P4-O44
41	A	3000	IHP	C5-O15-P5-O35
41	J	3000	IHP	C4-O14-P4-O34
41	J	3000	IHP	C5-O15-P5-O35

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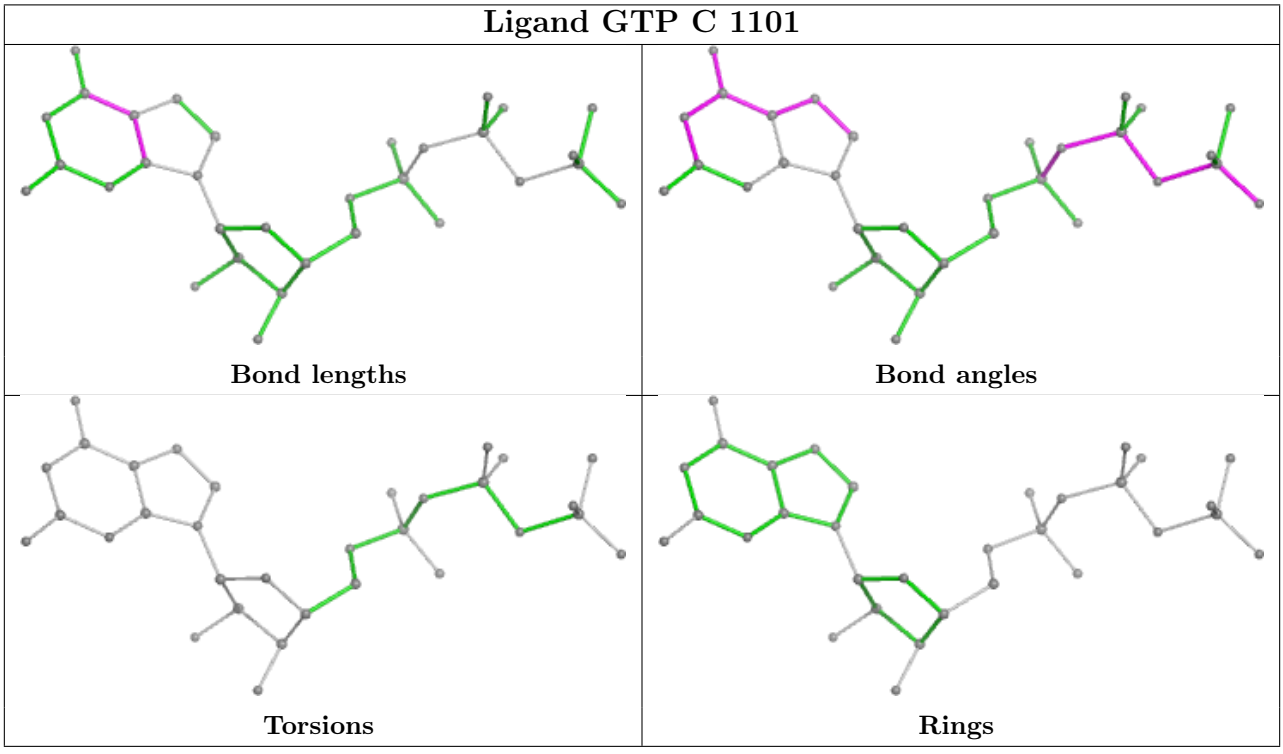
Mol	Chain	Res	Type	Atoms
41	J	3000	IHP	C5-O15-P5-O45

There are no ring outliers.

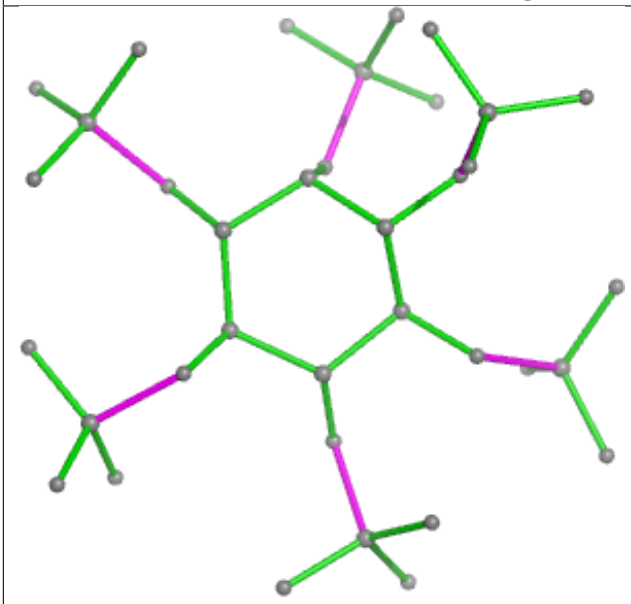
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	C	1101	GTP	6	0
41	J	3000	IHP	2	0

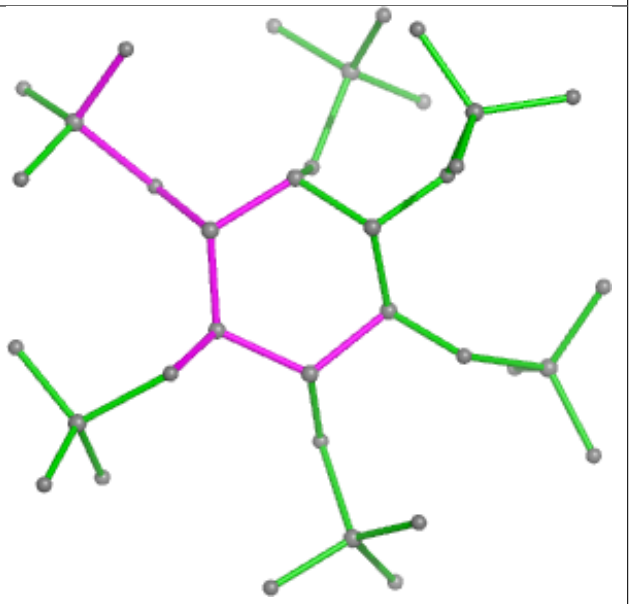
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



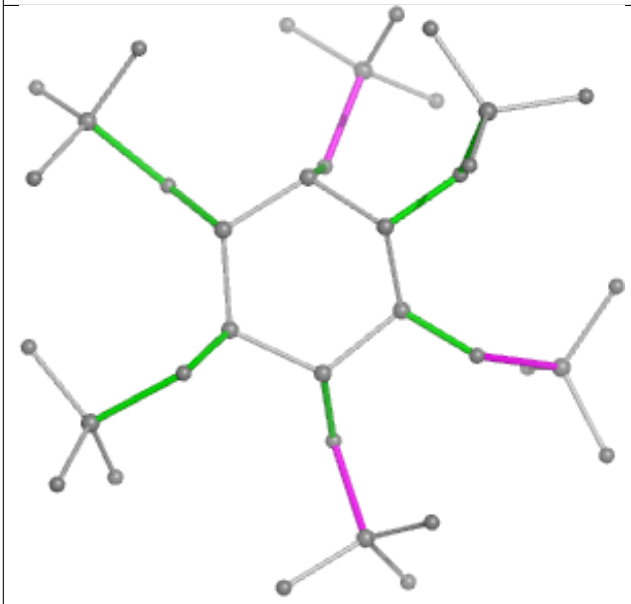
Ligand IHP A 3000



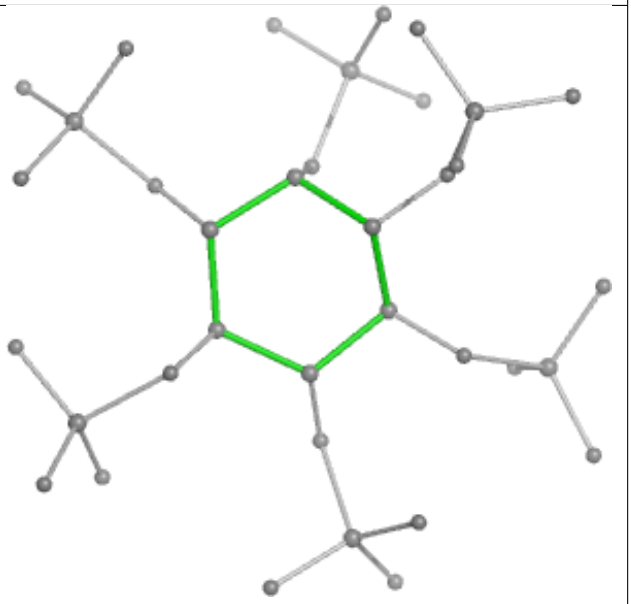
Bond lengths



Bond angles

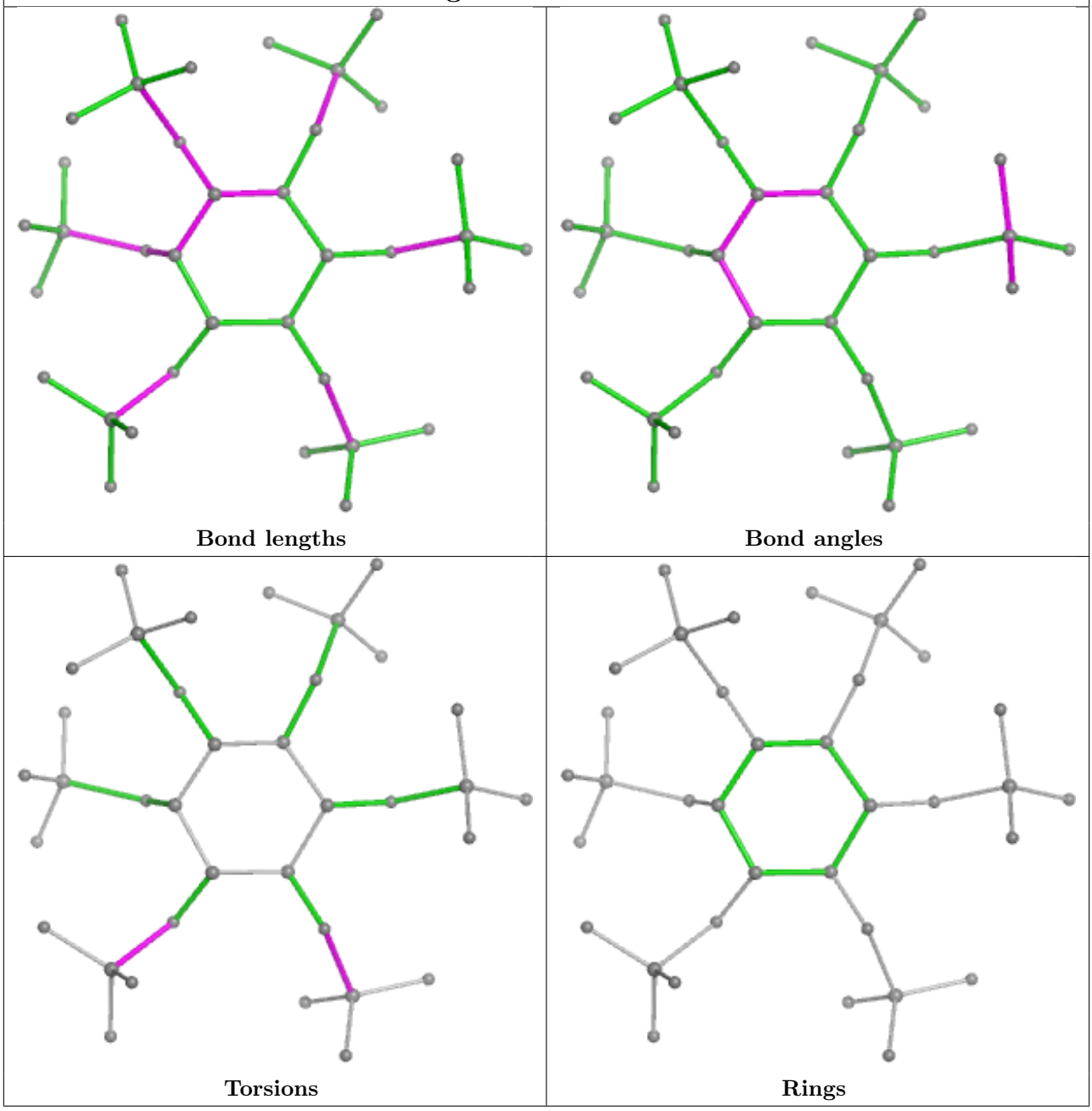


Torsions



Rings

Ligand IHP J 3000



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.

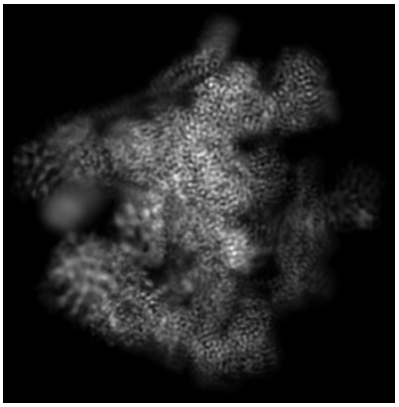
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19398. These allow visual inspection of the internal detail of the map and identification of artifacts.

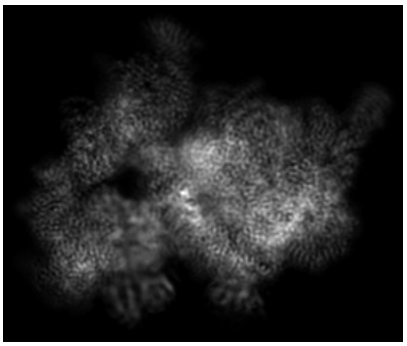
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

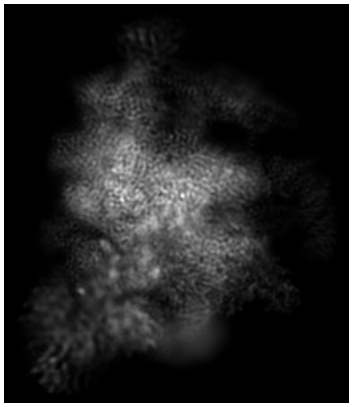
6.1.1 Primary map



X



Y

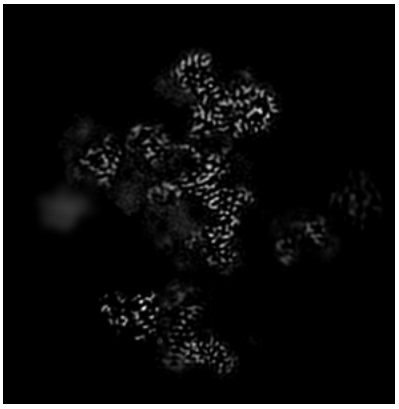


Z

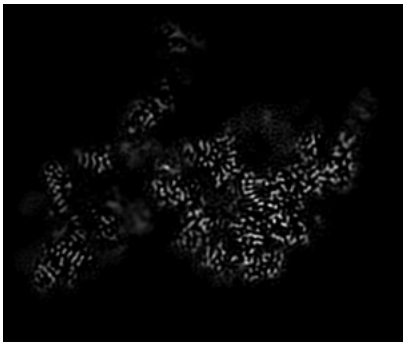
The images above show the map projected in three orthogonal directions.

6.2 Central slices

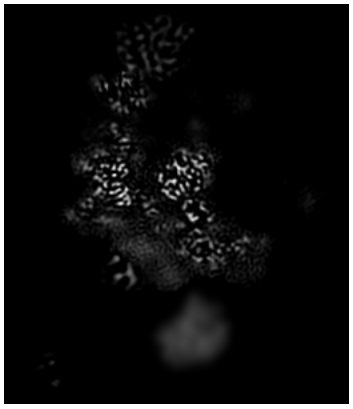
6.2.1 Primary map



X Index: 99



Y Index: 115

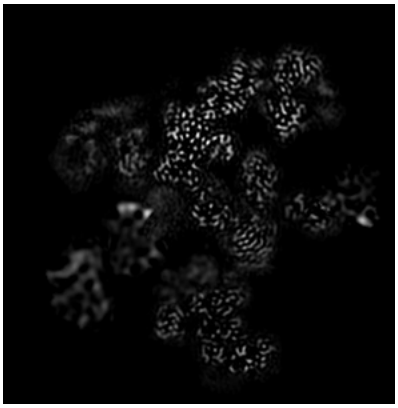


Z Index: 118

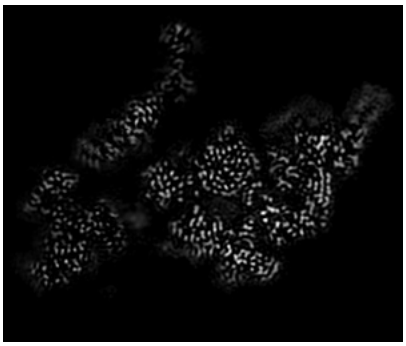
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

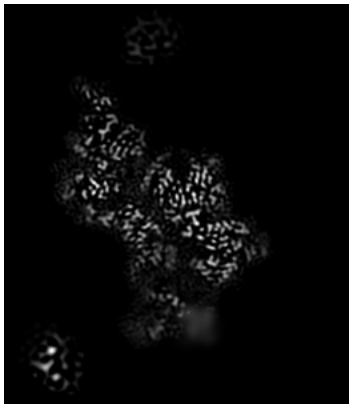
6.3.1 Primary map



X Index: 73



Y Index: 122

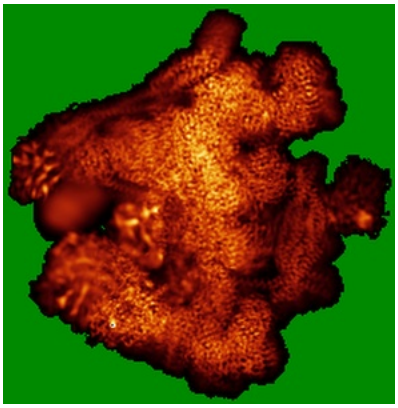


Z Index: 132

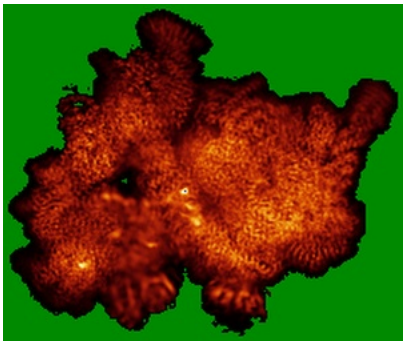
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

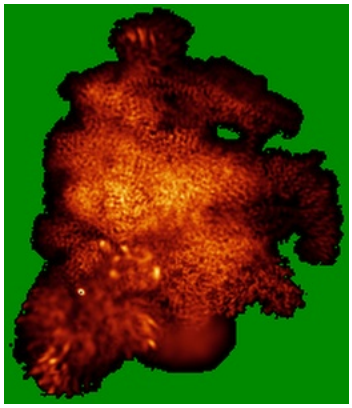
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

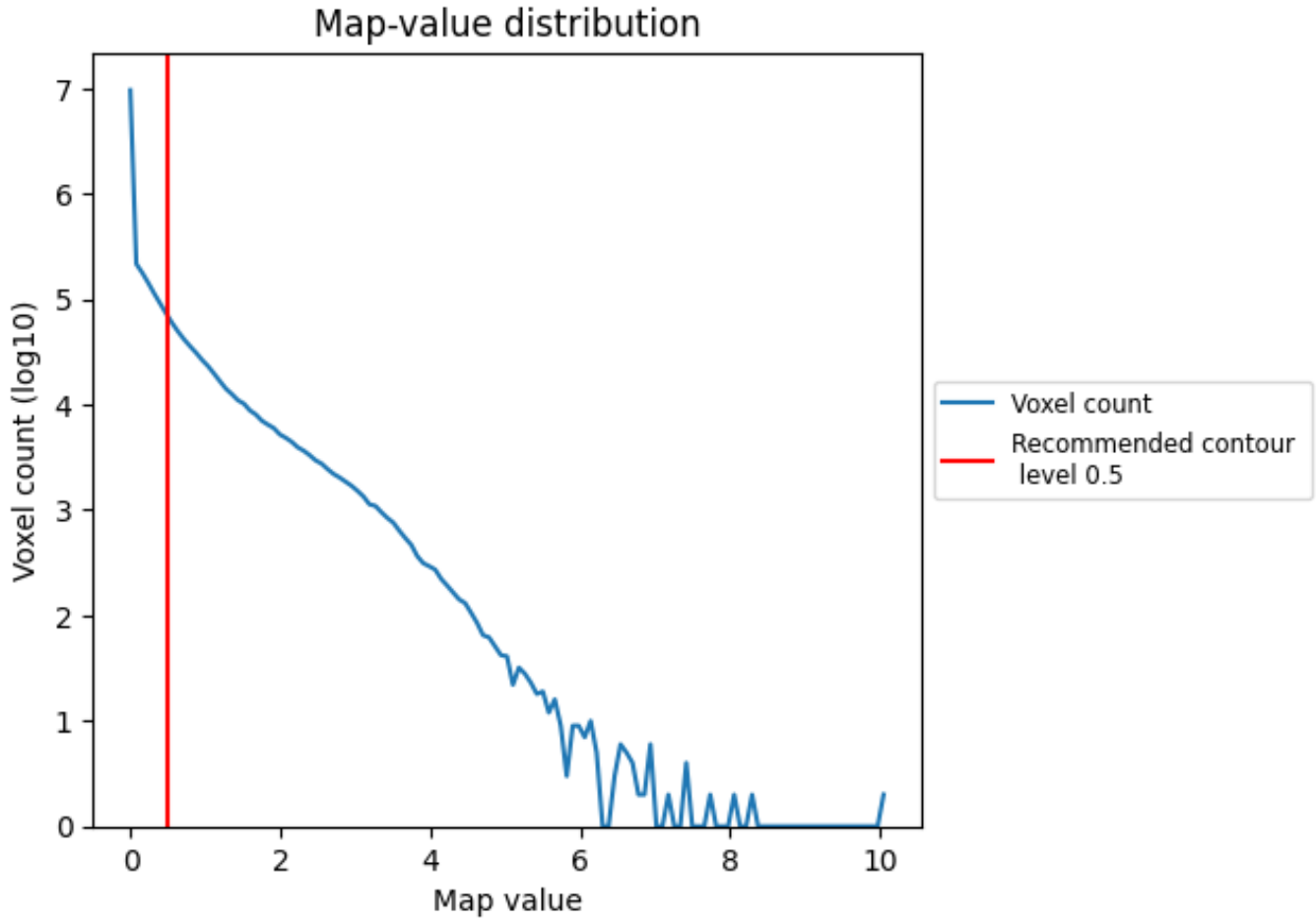
6.6 Mask visualisation (i)

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

7 Map analysis

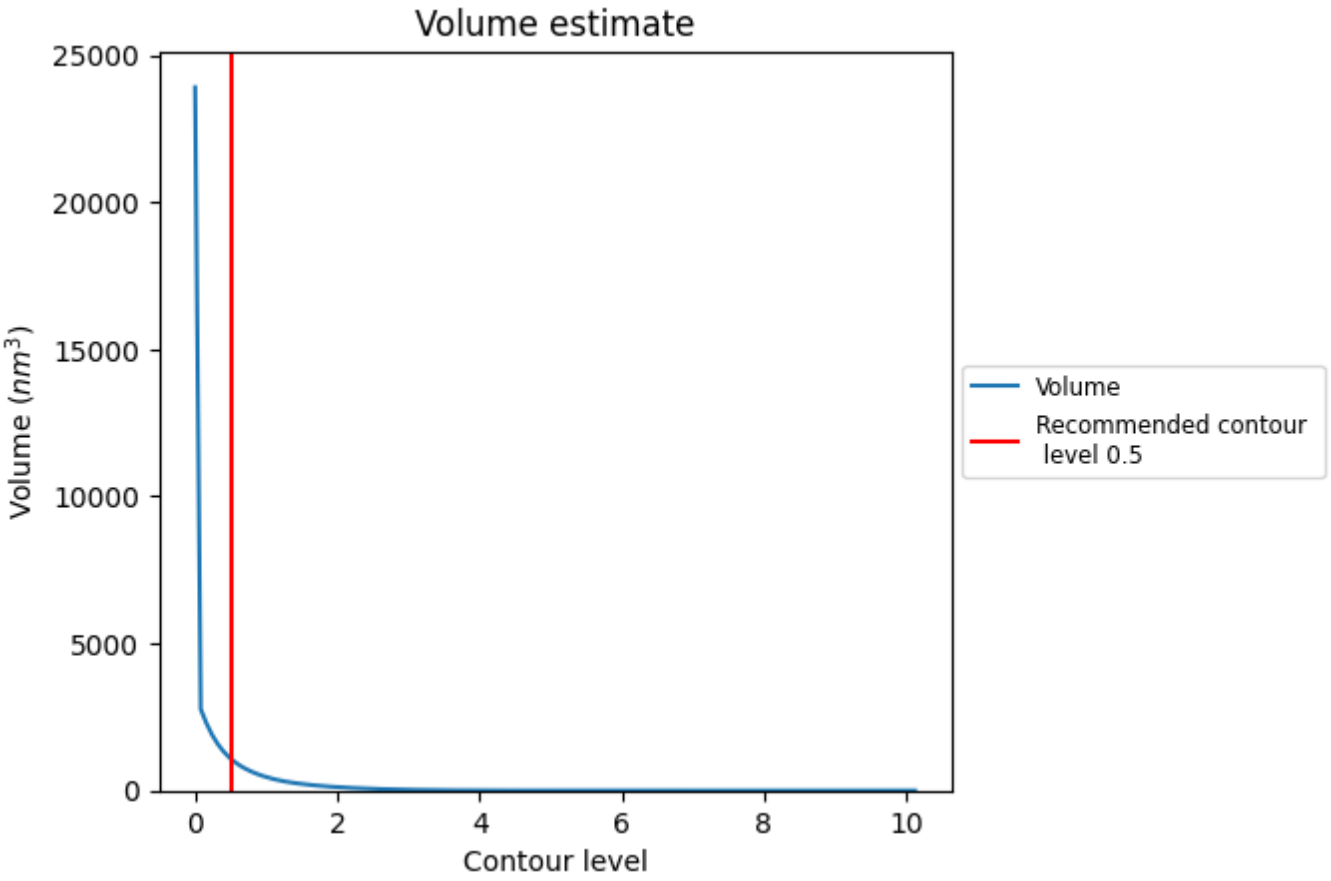
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 1088 nm^3; this corresponds to an approximate mass of 983 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

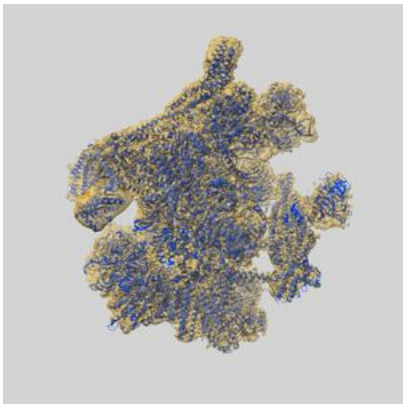
8 Fourier-Shell correlation

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

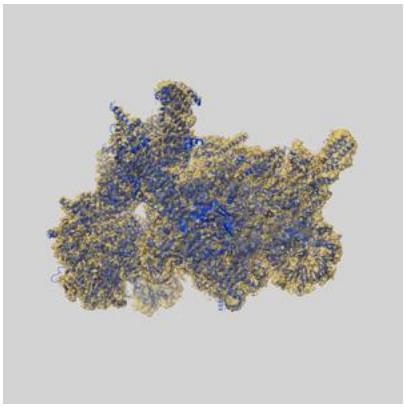
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19398 and PDB model 8RO1. Per-residue inclusion information can be found in section 3 on page 13.

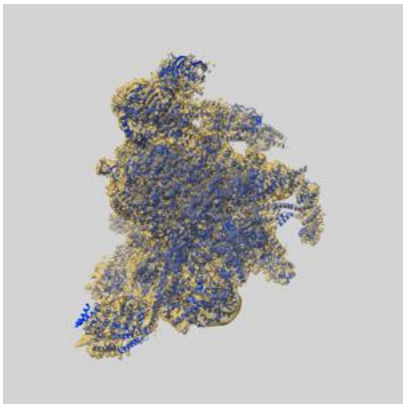
9.1 Map-model overlay



X



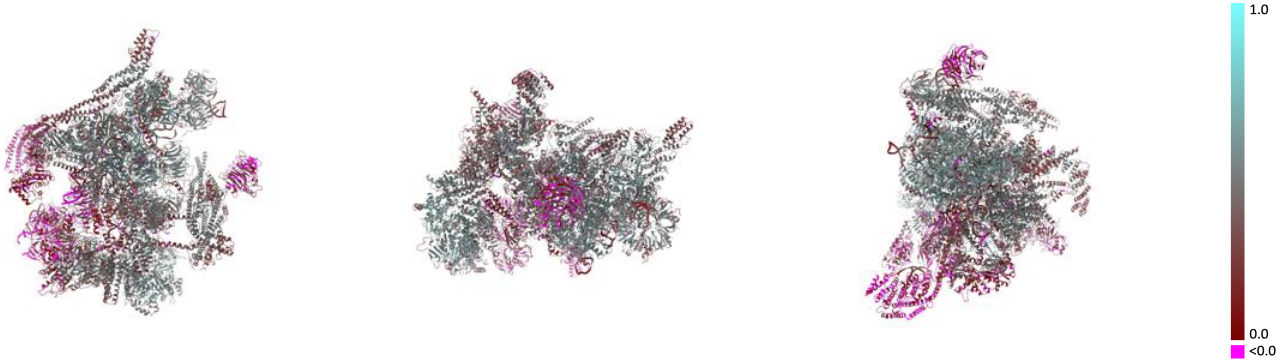
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

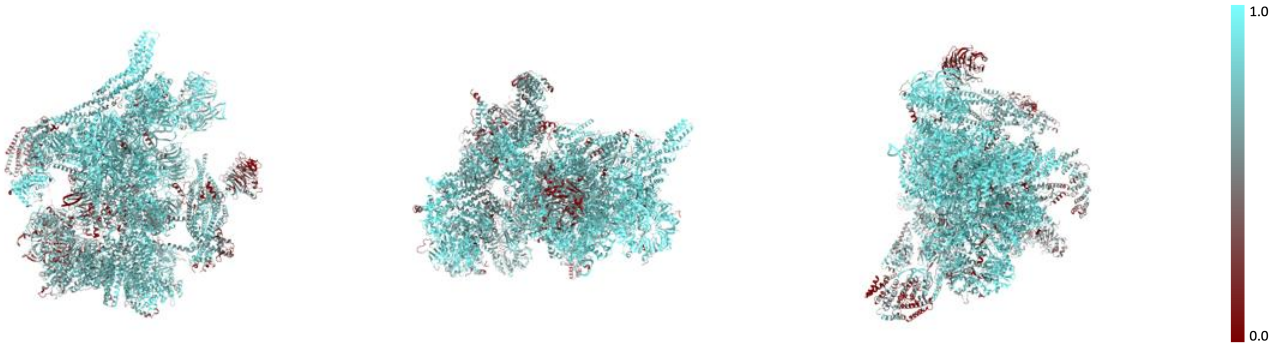
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

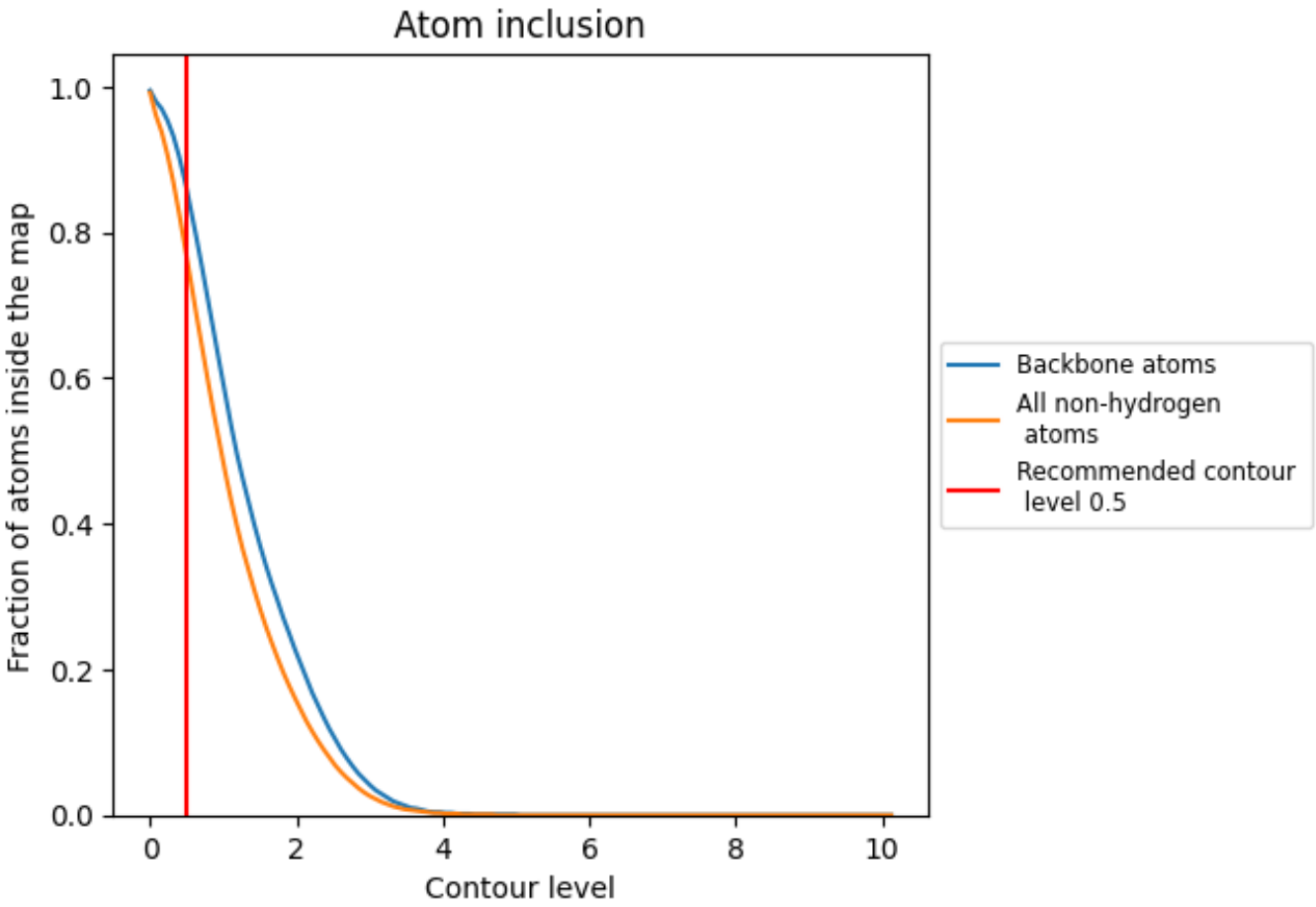
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.3730
2	0.7910	0.1990
5	0.9250	0.3860
6	0.9140	0.3690
A	0.8850	0.4550
C	0.9180	0.5080
D	0.5890	0.2280
DX	0.6750	0.3620
E	0.8960	0.5150
I	0.8270	0.4520
IN	0.6210	0.1200
J	0.7830	0.4420
K	0.6830	0.4120
L	0.6470	0.3620
L1	0.6700	0.1440
L2	0.8300	0.3910
M	0.7920	0.3580
N	0.9560	0.5340
O	0.8550	0.4330
P	0.5210	0.2890
PX	0.4250	0.0570
Q	0.8260	0.5110
R	0.8360	0.4130
S	0.7870	0.4330
T	0.9160	0.5250
TF	0.8020	0.3470
W	0.6480	0.1480
X	0.6800	0.3030
Z	0.5270	0.3770
a	0.9090	0.4940
b	0.8700	0.4320
c	0.9090	0.4700
d	0.7610	0.3600
e	0.8350	0.4480
f	0.8730	0.4600

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Chain	Atom inclusion	Q-score
g	0.7800	0.4020
h	0.7000	0.0770
i	0.6120	0.0830
j	0.5460	0.0620
k	0.5100	0.0410
l	0.5990	0.0350
m	0.6370	0.0790
n	0.6310	0.0690
o	0.6180	0.0970
p	0.6400	0.0810
q	0.7330	0.4560
r	0.4840	0.3560
s	0.4260	0.1830
t	0.5390	0.3670
y	0.6720	0.4330