



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:01 AM UTC

PDB ID : 8RO0 / pdb_00008ro0
EMDB ID : EMD-19397
Title : Structure of the C. elegans Intron Lariat Spliceosome primed for disassembly (ILS')
Authors : Vorlaender, M.K.; Rothe, P.; Plaschka, C.
Deposited on : 2024-01-11
Resolution : 2.90 Å(reported)
Based on initial model : .

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:

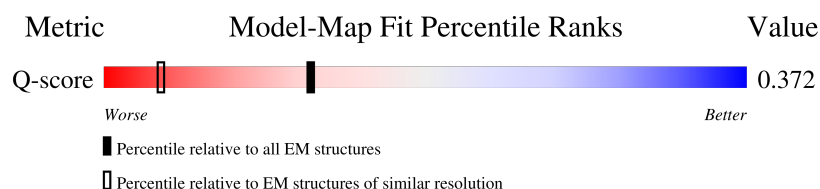
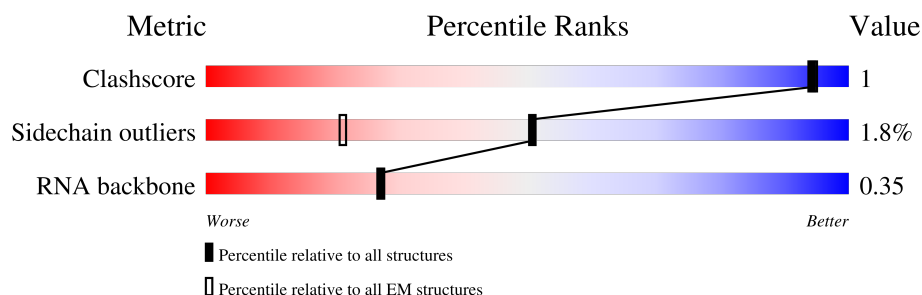
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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.



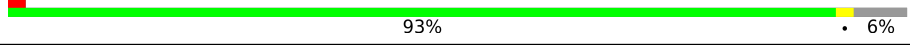
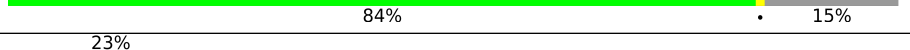
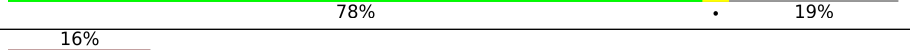
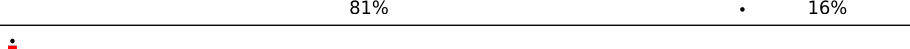
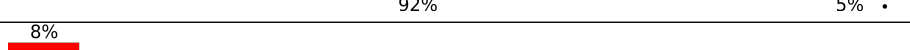
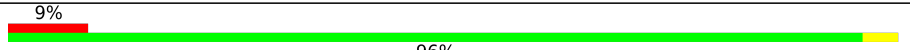
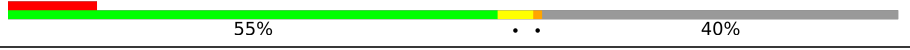
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	2	191	
2	5	121	
3	6	101	
4	A	2329	

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Mol	Chain	Length	Quality of chain
5	B	2145	
6	C	974	
7	D	267	
8	E	331	
9	I	855	
10	J	744	
11	K	238	
12	L	755	
13	M	234	
14	N	147	
15	O	408	
16	P	230	
17	PX	809	
18	Q	1467	
19	R	535	
20	S	169	
21	T	494	
22	TF	830	
23	W	567	
24	Z	169	
25	a	136	
25	h	136	
26	b	160	
26	i	160	
27	c	127	

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Mol	Chain	Length	Quality of chain
27	j	127	
28	d	118	
28	k	118	
29	e	90	
29	l	90	
30	f	85	
30	m	85	
31	g	77	
31	n	77	
32	o	253	
33	p	217	
34	q	492	
34	r	492	
34	s	492	
34	t	492	
35	y	331	
36	In	19	

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 121370 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
1	2	61	Total	C	N	O	P	0	0
			947	410	82	394	61		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	111	Total	C	N	O	P	0	0
			2349	1052	405	781	111		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	90	Total	C	N	O	P	0	0
			1927	863	358	616	90		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2231	Total	C	N	O	S	0	0
			18444	11870	3216	3272	86		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1806	Total	C	N	O	S	0	0
			14404	9175	2476	2669	84		

- Molecule 6 is a protein called Tr-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	898	Total	C	N	O	S	0	0
			7152	4558	1211	1337	46		

- Molecule 7 is a protein called Protein isy-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	88	Total	C	N	O	S	0	0
			726	458	122	143	3		

- 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
			2443	1528	429	466	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	724	Total	C	N	O	S	0	0
			5995	3813	1047	1092	43		

- Molecule 10 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	574	Total	C	N	O	S	0	0
			4893	3122	855	896	20		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	203	Total	C	N	O	S	0	0
			1665	1041	298	309	17		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	609	Total	C	N	O	S	0	0
			4898	3039	902	934	23		

- Molecule 13 is a protein called Pre-mRNA-splicing factor syf-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	196	Total	C	N	O	S	0	0
			1652	1021	308	317	6		

- Molecule 14 is a protein called Protein BUD31 homolog.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	342	Total	C	N	O	S	0	0
			2717	1703	493	502	19		

- Molecule 16 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	150	Total	C	N	O	S	0	0
			1204	729	232	237	6		

- Molecule 17 is a protein called GCF C-terminal domain-containing protein.

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

- Molecule 18 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	1378	Total	C	N	O	S	0	0
			11292	7218	1964	2063	47		

- Molecule 19 is a protein called Uncharacterized protein T27F2.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	282	Total	C	N	O	S	0	0
			2207	1379	404	414	10		

- Molecule 20 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	169	Total	C	N	O	S	0	0
			1301	818	233	243	7		

- Molecule 21 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	387	Total	C	N	O	S	0	0
			3066	1937	555	555	19		

- Molecule 22 is a protein called Septin and tuftelin-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	TF	497	Total	C	N	O	S	0	0
			4094	2637	685	750	22		

- Molecule 23 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	496	Total	C	N	O	S	0	0
			4071	2584	726	746	15		

- Molecule 24 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	69	Total	C	N	O	S	0	0
			567	356	104	105	2		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	81	Total	C	N	O	S	0	0
			634	396	113	119	6		
25	h	81	Total	C	N	O	S	0	0
			634	396	113	119	6		

- Molecule 26 is a protein called Probable small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	98	Total	C	N	O	S	0	0
			754	475	141	130	8		
26	i	79	Total	C	N	O	S	0	0
			638	405	117	110	6		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	80	Total	C	N	O	S	0	0
			621	396	109	112	4		
27	j	80	Total	C	N	O	S	0	0
			621	396	109	112	4		

- Molecule 28 is a protein called Probable small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	94	Total	C	N	O	S	0	0
			747	469	135	138	5		
28	k	79	Total	C	N	O	S	0	0
			630	398	118	109	5		

- Molecule 29 is a protein called Probable small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	80	Total	C	N	O	S	0	0
			663	424	118	119	2		
29	l	80	Total	C	N	O	S	0	0
			663	424	118	119	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	72	Total	C	N	O	S	0	0
			557	359	93	101	4		
30	m	72	Total	C	N	O	S	0	0
			557	359	93	101	4		

- Molecule 31 is a protein called Probable small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	77	Total	C	N	O	S	0	0
			606	379	107	113	7		
31	n	77	Total	C	N	O	S	0	0
			606	379	107	113	7		

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

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

- Molecule 33 is a protein called RRM domain-containing protein.

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

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	q	121	Total	C	N	O	S	0	0
			939	585	165	184	5		
34	r	131	Total	C	N	O	S	0	0
			1003	621	179	198	5		
34	s	469	Total	C	N	O	S	0	0
			3570	2239	620	702	9		
34	t	128	Total	C	N	O	S	0	0
			991	620	173	193	5		

- Molecule 35 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	y	79	Total	C	N	O	S	0	0
			618	396	100	117	5		

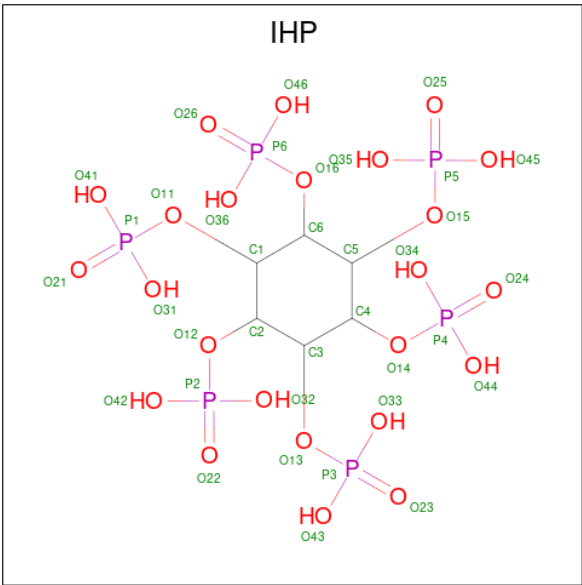
- Molecule 36 is a DNA chain called Intron lariat RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	In	19	Total	C	O	P	0	0
			225	95	112	18		

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

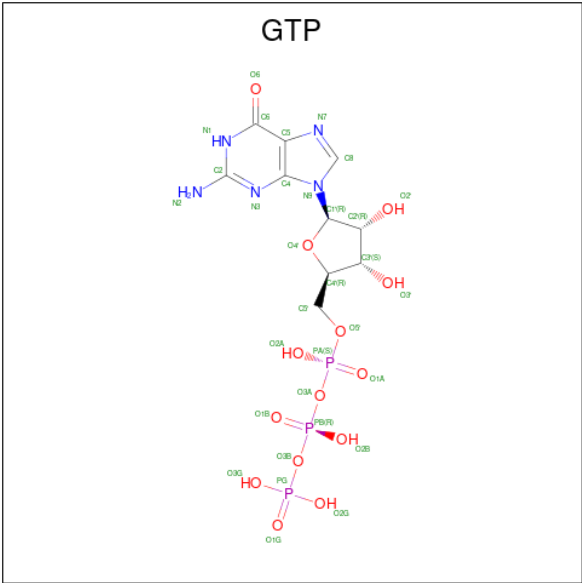
Mol	Chain	Residues	Atoms		AltConf
37	6	6	Total	Mg	0
			6	6	
37	C	1	Total	Mg	0
			1	1	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

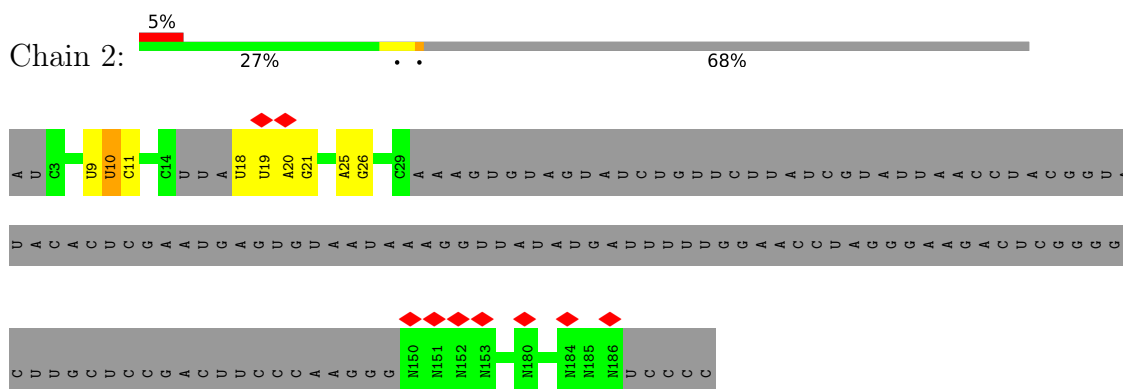
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	N	3	Total 3	Zn 3	0
40	O	3	Total 3	Zn 3	0

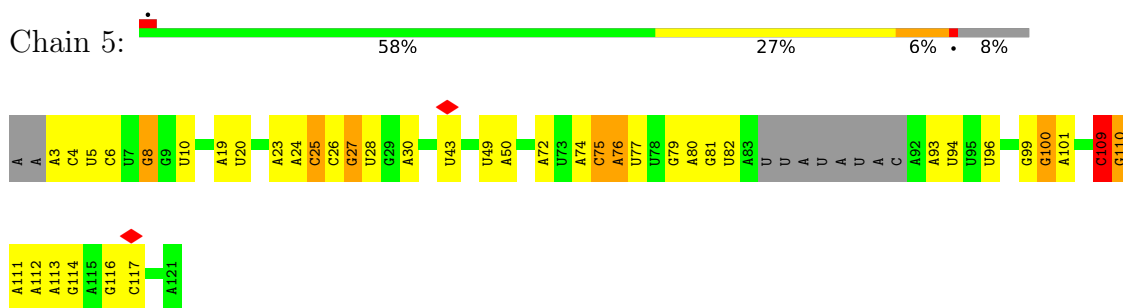
3 Residue-property plots [i](#)

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.

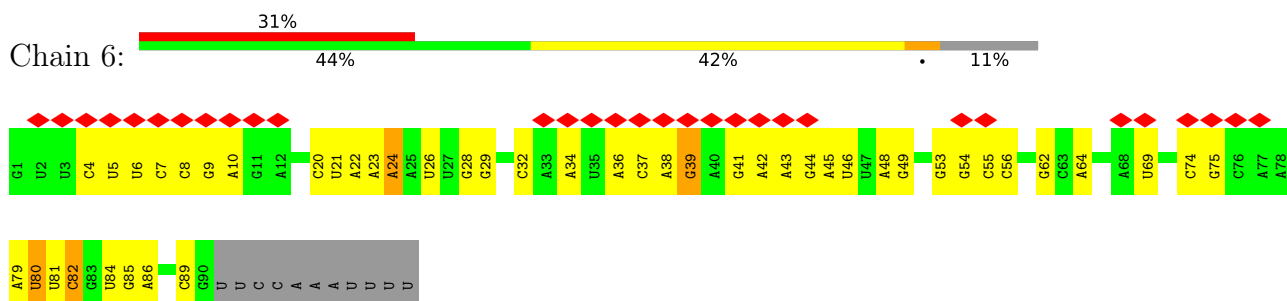
• Molecule 1: U2 snRNA



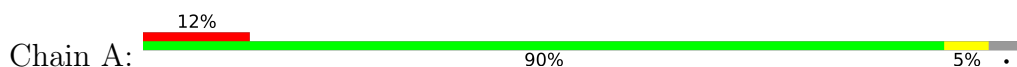
• Molecule 2: U5 snRNA

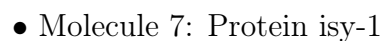
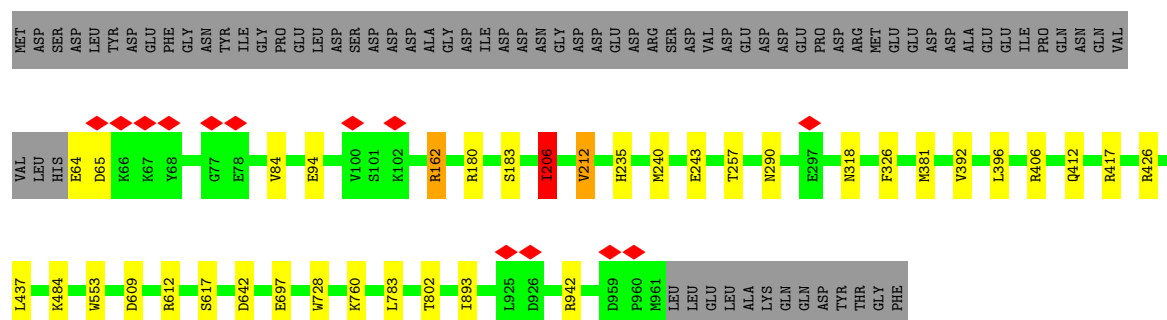
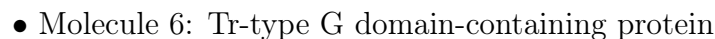


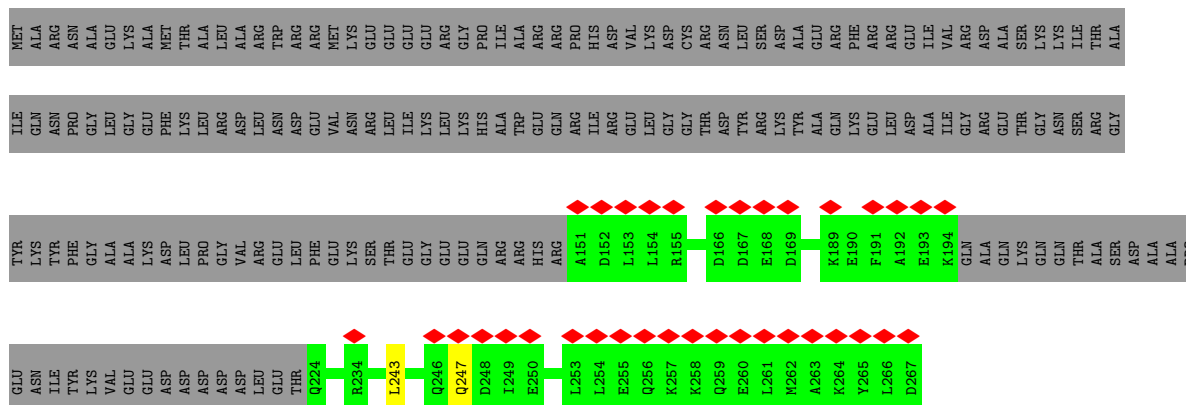
• Molecule 3: U6 snRNA



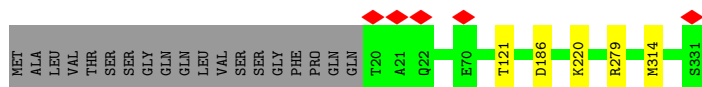
• Molecule 4: Pre-mRNA-splicing factor 8 homolog



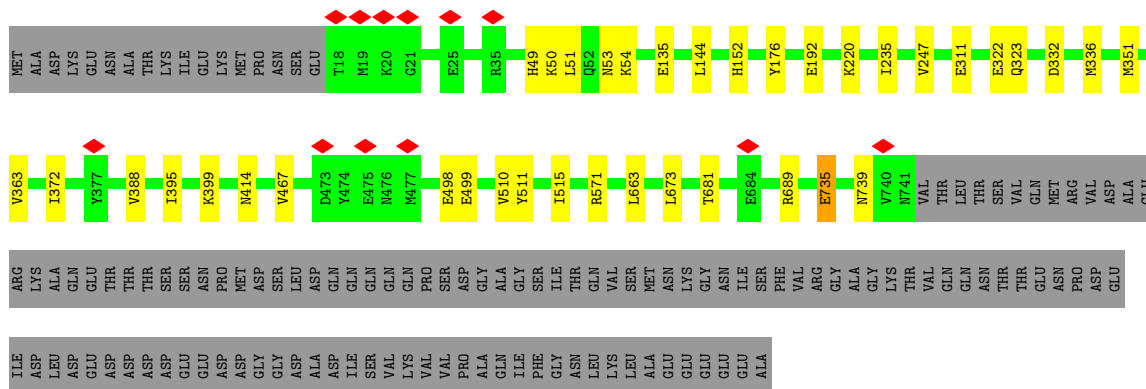
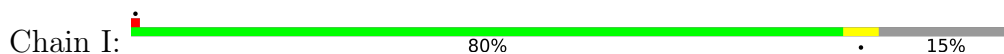




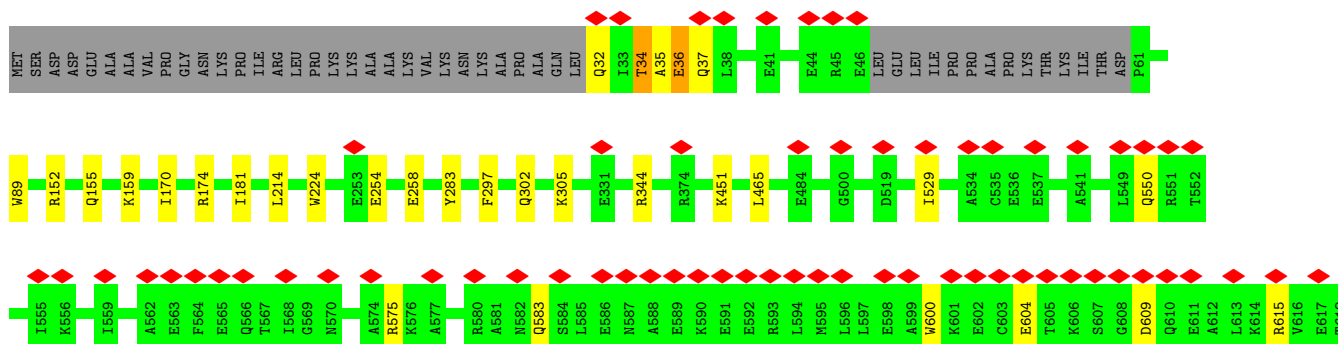
- Molecule 8: WD REPEATS REGION domain-containing protein.

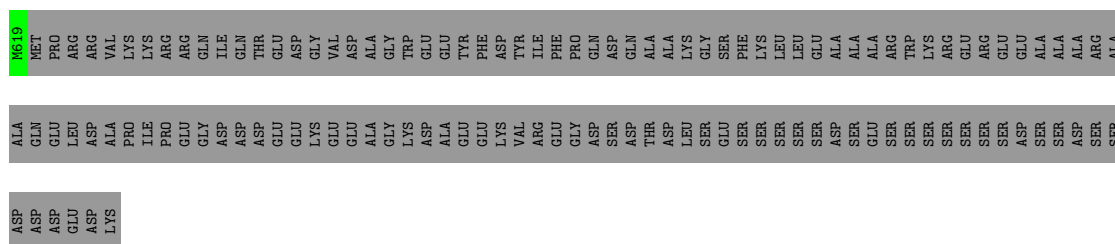


- Molecule 9: Pre-mRNA-splicing factor SYF1

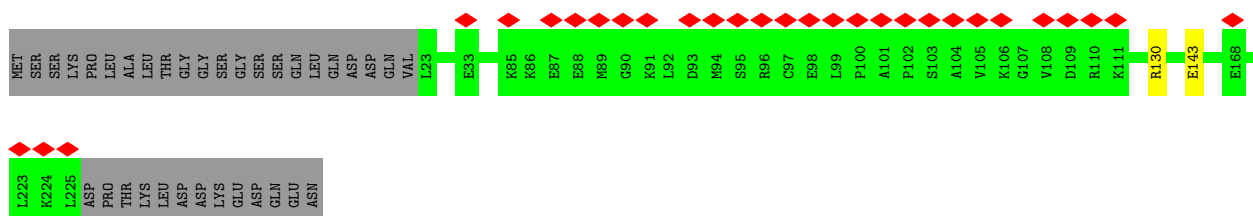
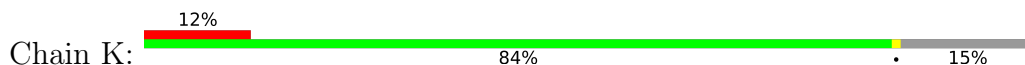


- Molecule 10: TPR REGION domain-containing protein

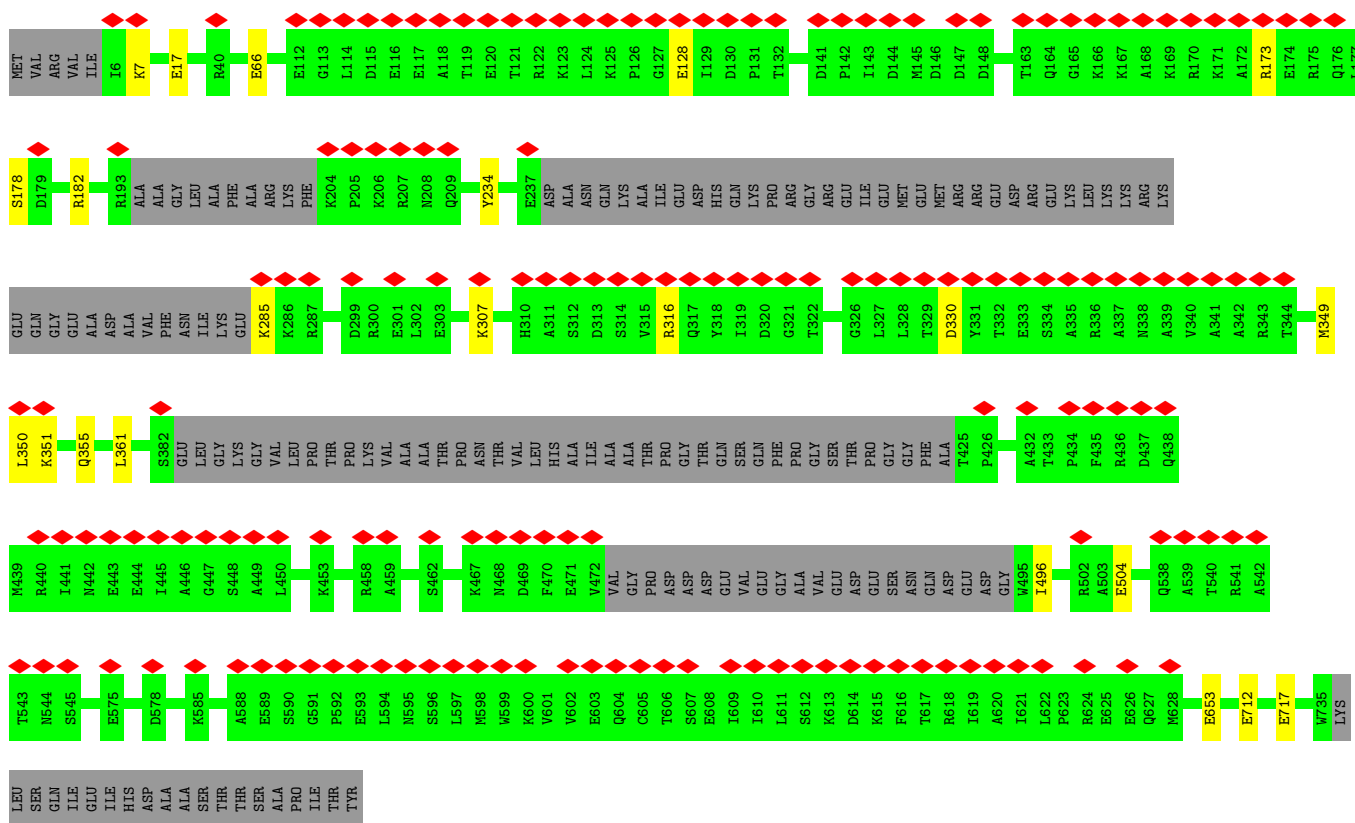
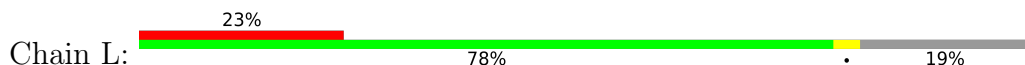




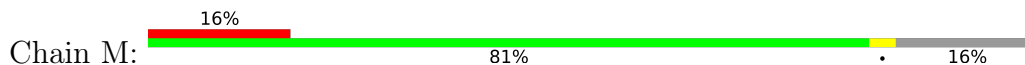
- Molecule 11: Pre-mRNA-splicing factor SPF27

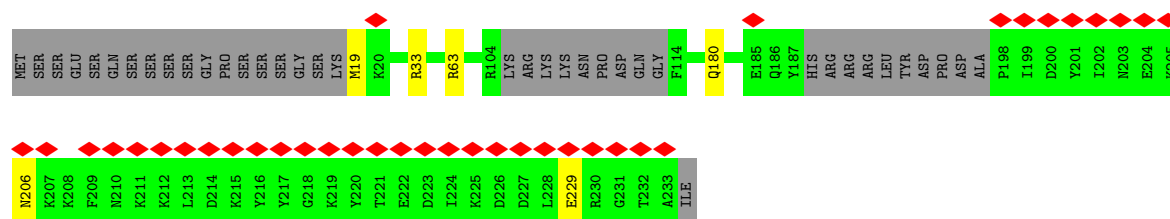


- Molecule 12: Cell division cycle 5-like protein

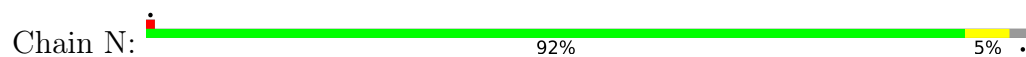


- Molecule 13: Pre-mRNA-splicing factor syf-2

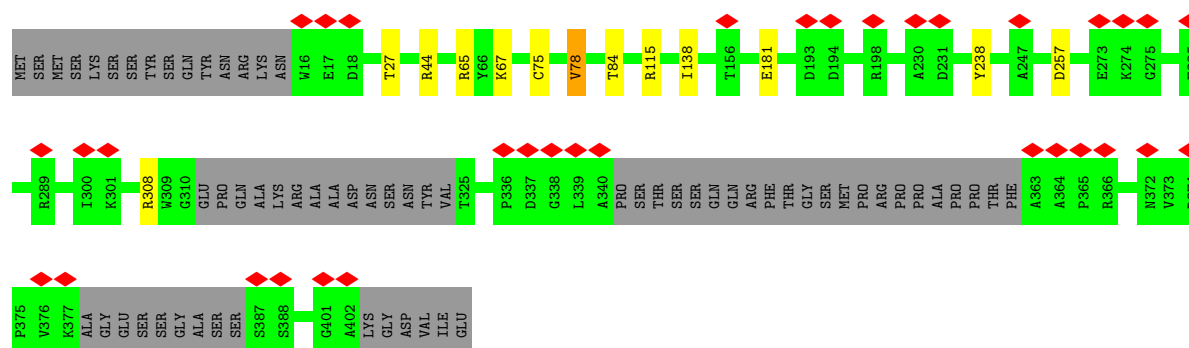
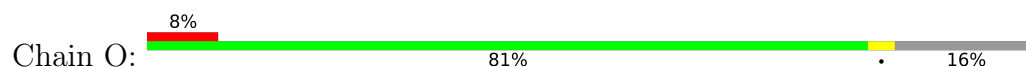




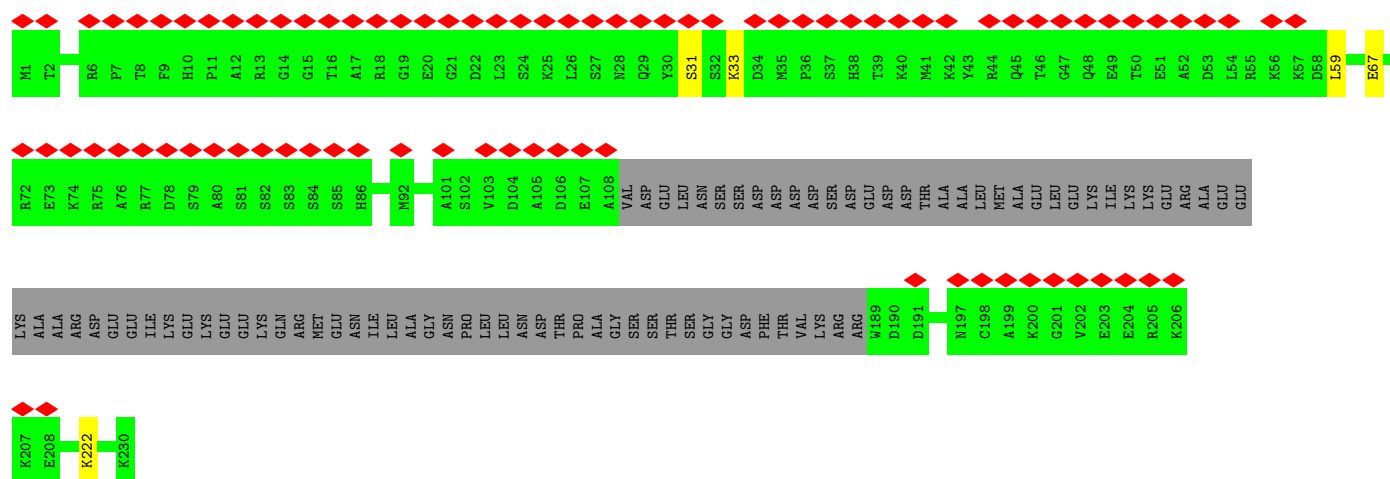
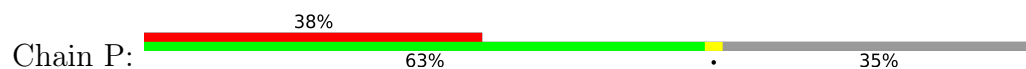
- Molecule 14: Protein BUD31 homolog



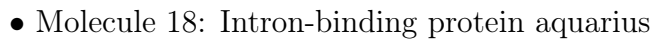
- Molecule 15: Pre-mRNA-splicing factor RBM22



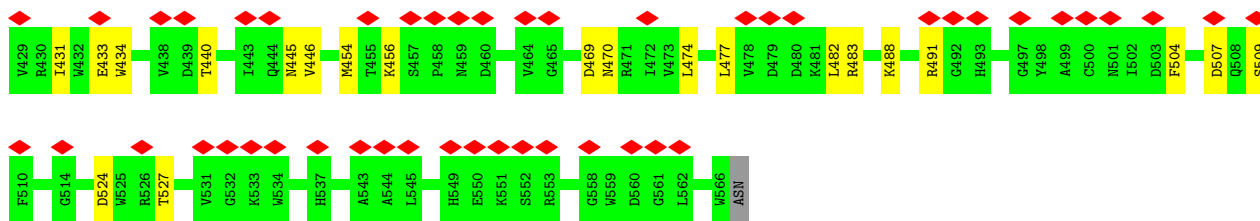
- Molecule 16: Spliceosome-associated protein CWC15 homolog



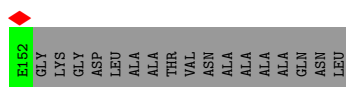
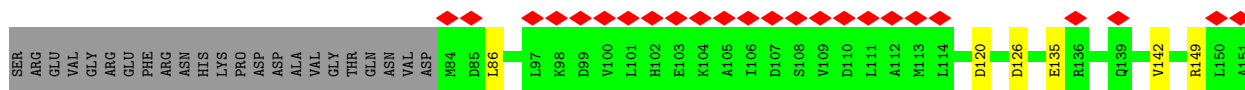
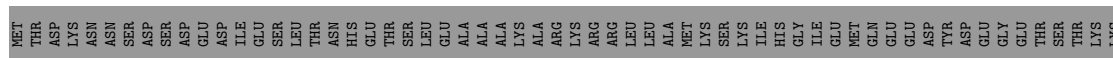
- Molecule 17: GCF C-terminal domain-containing protein



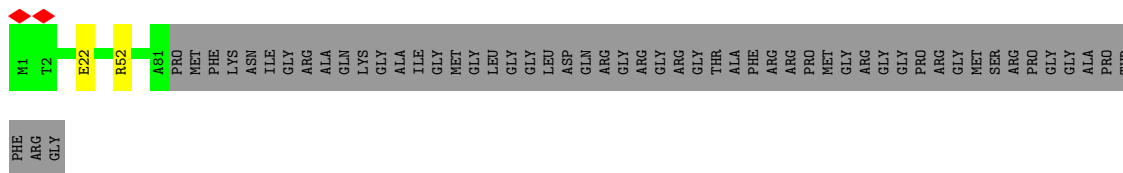




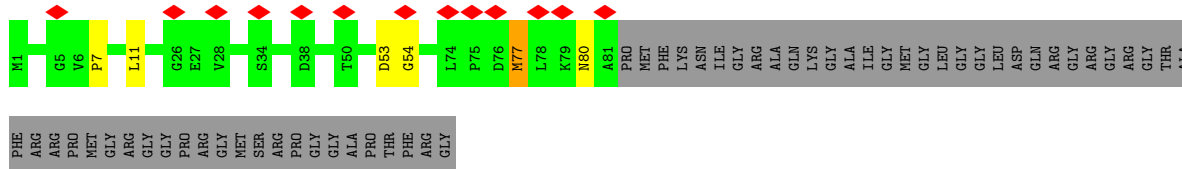
- Molecule 24: Coiled-coil domain-containing protein 12



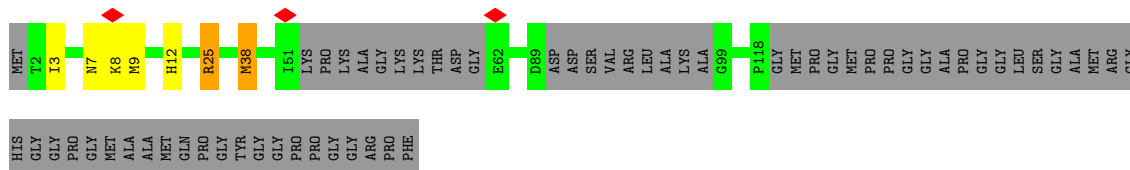
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



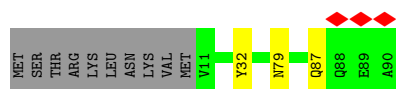
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



- Molecule 26: Probable small nuclear ribonucleoprotein-associated protein B

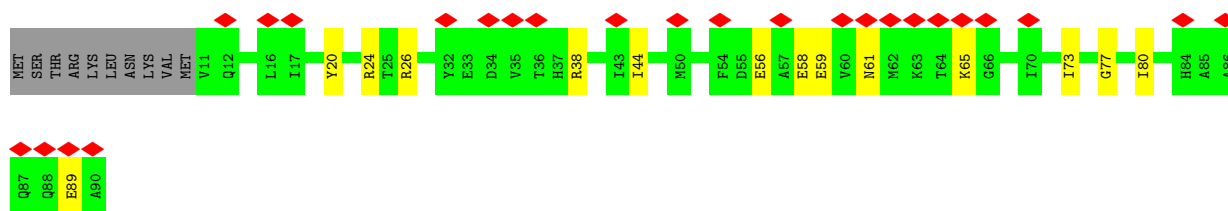


Chain e:  86% 11%



- Molecule 29: Probable small nuclear ribonucleoprotein E

Chain l:  28% 73% 16% 11%



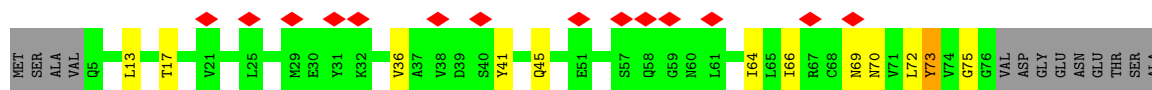
- Molecule 30: Probable small nuclear ribonucleoprotein F

Chain f:  79% 6% 15%

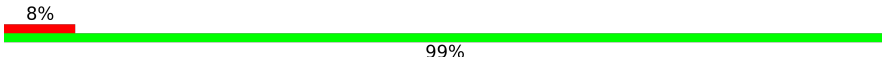


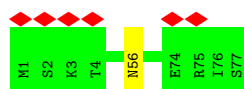
- Molecule 30: Probable small nuclear ribonucleoprotein F

Chain m:  16% 71% 13% 15%

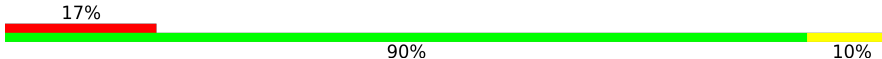


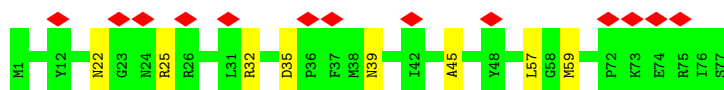
- Molecule 31: Probable small nuclear ribonucleoprotein G

Chain g:  8% 99%



- Molecule 31: Probable small nuclear ribonucleoprotein G

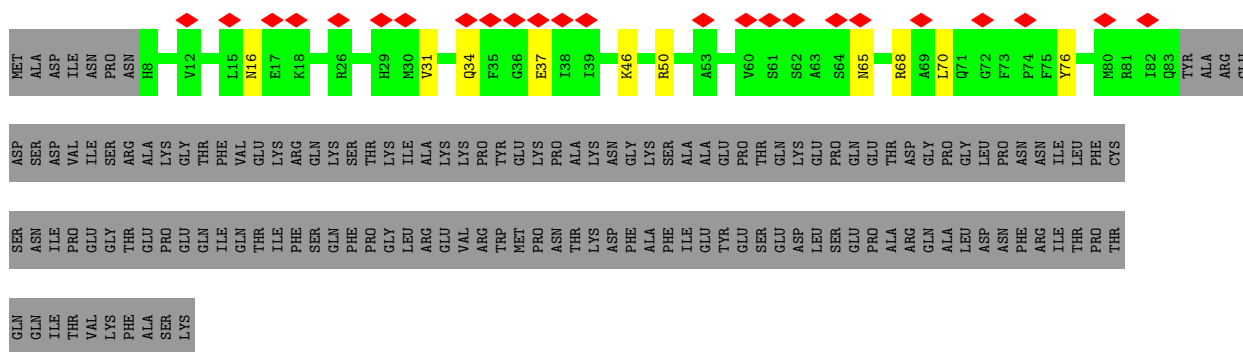
Chain n:  17% 90% 10%



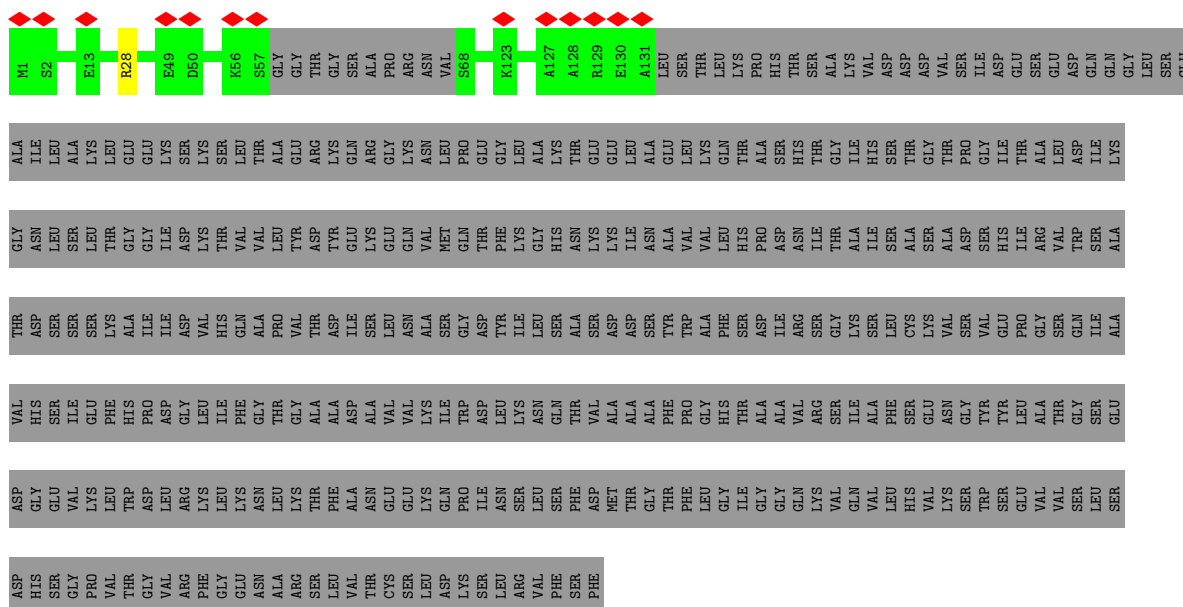
- Molecule 32: Probable U2 small nuclear ribonucleoprotein A'

Chain o:  26% 59% 36%

- Molecule 33: RRM domain-containing protein



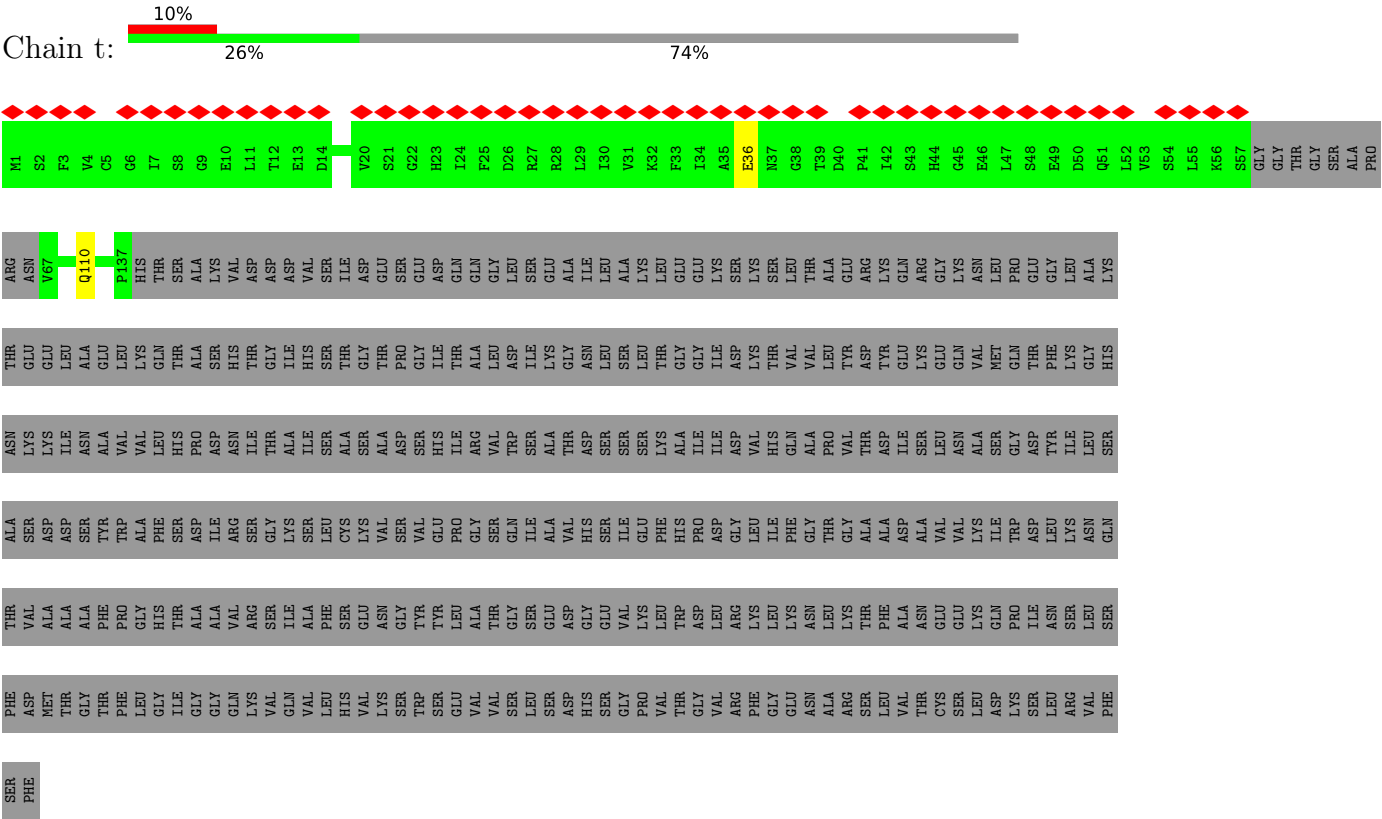
- Molecule 34: Pre-mRNA-processing factor 19



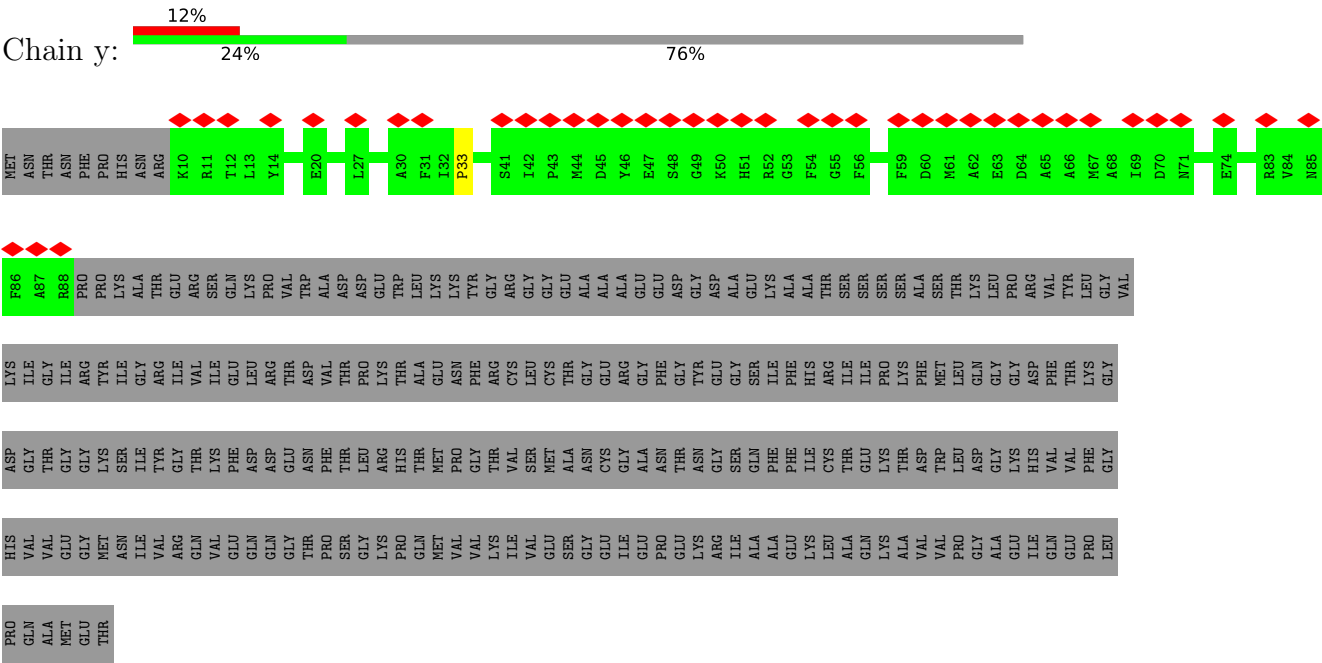
- Molecule 34: Pre-mRNA-processing factor 19



● Molecule 34: Pre-mRNA-processing factor 19

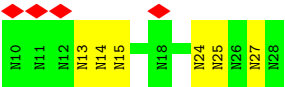


● Molecule 35: Peptidyl-prolyl cis-trans isomerase E



● Molecule 36: Intron lariat RNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	879523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.985	Depositor
Minimum map value	0.000	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	582.9824, 582.9824, 582.9824	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3013, 1.3013, 1.3013	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.34	0/558	0.67	0/863
2	5	0.62	0/2622	0.81	2/4077 (0.0%)
3	6	0.33	0/2159	0.73	0/3363
4	A	0.41	0/18943	0.59	0/25695
5	B	0.23	0/14697	0.48	0/19895
6	C	0.53	0/7309	0.62	1/9906 (0.0%)
7	D	0.26	0/734	0.54	0/984
8	E	0.35	0/2500	0.55	0/3384
9	I	0.34	0/6133	0.54	0/8286
10	J	0.35	0/5006	0.54	0/6735
11	K	0.24	0/1688	0.48	0/2260
12	L	0.25	0/4970	0.55	3/6673 (0.0%)
13	M	0.26	0/1678	0.53	0/2238
14	N	0.42	0/1190	0.58	0/1597
15	O	0.38	0/2779	0.55	0/3764
16	P	0.27	0/1220	0.63	0/1624
17	PX	0.30	0/3893	0.57	0/5223
18	Q	0.33	0/11554	0.51	0/15626
19	R	0.34	0/2252	0.63	0/3040
20	S	0.27	0/1330	0.58	0/1800
21	T	0.44	0/3144	0.62	0/4259
22	TF	0.48	0/4202	0.65	3/5711 (0.1%)
23	W	0.39	0/4179	0.73	0/5638
24	Z	0.22	0/571	0.51	0/765
25	a	0.42	0/642	0.60	0/864
25	h	0.31	0/642	0.65	0/864
26	b	0.38	0/766	0.64	0/1021
26	i	0.30	0/648	0.67	0/865
27	c	0.35	0/627	0.61	0/848
27	j	0.29	0/627	0.61	0/848
28	d	0.32	0/755	0.58	0/1013
28	k	0.39	0/637	0.81	0/854

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	e	0.34	0/674	0.55	0/909
29	l	0.31	0/674	0.70	0/909
30	f	0.30	0/568	0.56	0/769
30	m	0.40	0/568	0.78	0/769
31	g	0.36	0/614	0.65	0/820
31	n	0.33	0/614	0.69	0/820
32	o	0.28	0/1358	0.61	0/1837
33	p	0.31	0/638	0.65	0/850
34	q	0.25	0/951	0.47	0/1282
34	r	0.25	0/1017	0.47	0/1373
34	s	0.27	0/3632	0.56	0/4913
34	t	0.24	0/1004	0.47	0/1355
35	y	0.38	0/630	0.74	0/846
All	All	0.36	0/123597	0.58	9/168035 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	1
4	A	0	5
5	B	0	3
6	C	0	1
9	I	0	1
10	J	0	2
17	PX	0	1
19	R	0	1
22	TF	0	1
26	b	0	1
34	q	0	1
All	All	0	18

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	TF	392	ARG	CA-C-N	7.05	139.00	121.80
22	TF	392	ARG	C-N-CA	7.05	139.00	121.80
2	5	25	C	C2'-C3'-O3'	6.48	123.42	113.70
12	L	350	LEU	N-CA-C	5.86	123.28	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	27	G	O4'-C1'-N9	-5.75	99.57	108.20
22	TF	393	SER	N-CA-C	5.54	122.05	109.81
6	C	206	ILE	CA-CB-CG1	5.43	119.63	110.40
12	L	349	MET	CA-C-N	5.41	131.87	121.54
12	L	349	MET	C-N-CA	5.41	131.87	121.54

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	5	109	C	Sidechain
4	A	1409	ILE	Peptide
4	A	1432	ARG	Sidechain
4	A	229	ARG	Sidechain
4	A	655	ARG	Sidechain
4	A	933	LYS	Peptide
5	B	1513	ARG	Sidechain
5	B	1692	ARG	Sidechain
5	B	857	ARG	Sidechain
6	C	162	ARG	Sidechain
9	I	689	ARG	Sidechain
10	J	152	ARG	Sidechain
10	J	174	ARG	Sidechain
17	PX	469	ARG	Sidechain
19	R	190	ASN	Peptide
22	TF	392	ARG	Peptide
26	b	25	ARG	Sidechain
34	q	28	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	947	0	555	3	0
2	5	2349	0	1189	10	0
3	6	1927	0	973	7	0
4	A	18444	0	18399	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14404	0	14546	50	0
6	C	7152	0	7143	17	0
7	D	726	0	725	0	0
8	E	2443	0	2362	3	0
9	I	5995	0	5902	14	0
10	J	4893	0	4775	11	0
11	K	1665	0	1707	2	0
12	L	4898	0	4977	13	0
13	M	1652	0	1626	4	0
14	N	1163	0	1142	2	0
15	O	2717	0	2662	6	0
16	P	1204	0	1182	2	0
17	PX	3838	0	3889	12	0
18	Q	11292	0	11206	11	0
19	R	2207	0	2212	7	0
20	S	1301	0	1282	3	0
21	T	3066	0	3028	6	0
22	TF	4094	0	4038	12	0
23	W	4071	0	3967	17	0
24	Z	567	0	603	3	0
25	a	634	0	643	2	0
25	h	634	0	643	3	0
26	b	754	0	772	5	0
26	i	638	0	655	5	0
27	c	621	0	673	4	0
27	j	621	0	673	5	0
28	d	747	0	764	3	0
28	k	630	0	662	8	0
29	e	663	0	666	2	0
29	l	663	0	666	8	0
30	f	557	0	560	3	0
30	m	557	0	560	7	0
31	g	606	0	624	1	0
31	n	606	0	624	4	0
32	o	1335	0	1367	8	0
33	p	626	0	646	5	0
34	q	939	0	941	0	0
34	r	1003	0	1003	0	0
34	s	3570	0	3573	9	0
34	t	991	0	1004	0	0
35	y	618	0	598	0	0
36	In	225	0	153	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	6	6	0	0	0	0
37	C	1	0	0	0	0
38	A	36	0	6	0	0
38	J	36	0	6	1	0
39	C	32	0	12	1	0
40	N	3	0	0	0	0
40	O	3	0	0	0	0
All	All	121370	0	118584	292	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 1.

All (292) 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)
23:W:469:ASP:O	23:W:491:ARG:NH2	2.17	0.78
18:Q:934:GLU:OE2	18:Q:1014:ARG:NH2	2.19	0.75
9:I:53:ASN:O	26:i:88:ARG:NH2	2.21	0.73
3:6:36:A:C2	36:In:13:N:H1'	2.24	0.73
28:k:60:ASP:OD2	28:k:64:ASN:ND2	2.22	0.73
33:p:16:ASN:ND2	33:p:76:TYR:O	2.22	0.73
23:W:217:ASP:OD1	23:W:356:ARG:NH1	2.22	0.71
4:A:133:GLN:NE2	4:A:197:PHE:O	2.24	0.71
32:o:25:ASN:ND2	33:p:37:GLU:OE2	2.24	0.70
5:B:631:ARG:NH1	5:B:897:GLU:OE1	2.26	0.69
27:j:20:LYS:O	27:j:66:ARG:NH2	2.25	0.69
23:W:391:ASP:OD2	23:W:393:ARG:NH2	2.25	0.69
5:B:124:ARG:NH2	5:B:1024:ASP:OD2	2.25	0.69
29:l:20:TYR:OH	31:m:59:MET:O	2.11	0.68
3:6:26:U:OP1	23:W:205:GLN:NE2	2.27	0.68
29:l:59:GLU:OE1	30:m:73:TYR:OH	2.10	0.67
9:I:192:GLU:OE2	9:I:220:LYS:NZ	2.27	0.67
32:o:29:GLN:N	32:o:52:ASN:OD1	2.28	0.67
29:l:73:ILE:HG22	30:m:75:GLY:HA3	1.77	0.66
5:B:681:GLN:NE2	5:B:859:GLU:OE2	2.28	0.66
5:B:491:GLU:O	5:B:641:ARG:NE	2.27	0.66
9:I:322:GLU:OE1	13:M:19:MET:N	2.28	0.66
19:R:131:ASN:OD1	21:T:422:ARG:NE	2.27	0.65
15:O:238:TYR:N	15:O:308:ARG:O	2.30	0.63
5:B:897:GLU:OE1	5:B:902:THR:OG1	2.17	0.63
5:B:1402:LEU:O	5:B:1425:ARG:NH1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:147:ASN:O	23:W:83:LYS:NZ	2.32	0.62
5:B:674:ARG:NH2	5:B:846:LEU:O	2.32	0.62
4:A:1997:GLN:NE2	22:TF:346:GLN:OE1	2.32	0.62
5:B:1493:ASP:OD2	5:B:1762:ARG:NH1	2.32	0.62
28:d:60:ASP:OD2	28:d:64:ASN:ND2	2.33	0.62
3:6:80:U:O2	10:J:155:GLN:NE2	2.33	0.61
33:p:65:ASN:OD1	33:p:68:ARG:NH2	2.32	0.61
17:PX:772:ARG:NH2	17:PX:808:GLU:OE2	2.33	0.61
17:PX:614:GLU:OE1	17:PX:652:ASN:ND2	2.33	0.61
10:J:159:LYS:NZ	13:M:180:GLN:OE1	2.33	0.61
18:Q:133:GLU:OE1	18:Q:223:LYS:NZ	2.26	0.60
3:6:36:A:H2	36:In:13:N:H1'	1.66	0.60
28:k:64:ASN:OD1	28:k:103:GLY:N	2.34	0.60
1:2:11:C:H42	3:6:82:C:H42	1.50	0.60
5:B:591:THR:OG1	5:B:628:ARG:NH1	2.35	0.60
10:J:451:LYS:NZ	38:J:3000:IHP:O43	2.35	0.60
34:s:172:SER:O	34:s:176:GLU:N	2.35	0.60
5:B:484:ASP:OD1	5:B:488:ARG:NH1	2.34	0.60
2:5:93:A:OP1	28:d:61:ARG:NH1	2.35	0.59
9:I:311:GLU:OE1	13:M:33:ARG:NE	2.32	0.59
11:K:143:GLU:OE1	21:T:76:ASN:ND2	2.35	0.59
4:A:328:VAL:HG21	6:C:235:HIS:CD2	2.38	0.59
14:N:123:ARG:NH1	14:N:145:CYS:O	2.35	0.58
2:5:100:G:OP2	30:f:67:ARG:NH2	2.36	0.58
2:5:116:G:OP1	25:a:52:ARG:NH1	2.37	0.58
34:s:172:SER:OG	34:s:176:GLU:OE1	2.13	0.58
5:B:1382:LYS:NZ	5:B:1653:ILE:O	2.29	0.57
18:Q:1140:ARG:NH1	18:Q:1269:GLN:OE1	2.37	0.57
4:A:875:ARG:NH1	12:L:128:GLU:OE1	2.38	0.57
5:B:816:ALA:O	5:B:850:GLY:N	2.35	0.57
5:B:1853:GLU:O	5:B:1917:ARG:NH1	2.38	0.56
17:PX:641:THR:O	17:PX:645:SER:N	2.39	0.56
34:s:467:THR:OG1	34:s:481:CYS:SG	2.64	0.56
2:5:94:U:O5'	30:f:41:TYR:OH	2.23	0.55
10:J:600:TRP:NE1	10:J:604:GLU:OE2	2.39	0.55
27:c:56:ASP:OD1	27:c:57:THR:N	2.39	0.55
5:B:1398:THR:N	5:B:1417:GLN:OE1	2.40	0.55
11:K:130:ARG:NH2	12:L:653:GLU:OE1	2.40	0.55
4:A:2125:SER:OG	4:A:2133:LYS:NZ	2.37	0.55
4:A:249:MET:HE1	4:A:447:VAL:HA	1.88	0.54
27:c:20:LYS:NZ	27:c:65:ILE:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:498:GLU:HG3	9:I:510:VAL:HG21	1.88	0.54
4:A:142:ARG:NH1	4:A:608:PHE:O	2.40	0.54
30:f:51:GLU:OE1	30:f:58:GLN:NE2	2.41	0.54
6:C:609:ASP:OD1	6:C:612:ARG:NH1	2.39	0.54
2:5:8:G:O2'	2:5:75:C:N4	2.41	0.54
6:C:484:LYS:NZ	6:C:617:SER:O	2.40	0.54
10:J:32:GLN:NE2	10:J:36:GLU:OE1	2.40	0.54
4:A:1939:ASN:ND2	4:A:1941:ASP:OD1	2.40	0.53
6:C:697:GLU:OE2	6:C:728:TRP:NE1	2.40	0.53
25:a:22:GLU:OE2	26:b:25:ARG:NH1	2.41	0.53
9:I:50:LYS:O	26:i:88:ARG:NH2	2.42	0.53
30:m:36:VAL:O	30:m:45:GLN:NE2	2.40	0.53
5:B:415:HIS:NE2	5:B:868:GLU:OE1	2.39	0.53
18:Q:909:ARG:NH1	18:Q:1017:GLU:OE2	2.41	0.53
28:k:61:ARG:NH2	30:m:41:TYR:OH	2.41	0.53
5:B:1262:ARG:HG3	5:B:1274:VAL:HG22	1.91	0.52
32:o:120:PHE:N	32:o:146:ASP:OD1	2.42	0.52
19:R:47:TYR:OH	20:S:29:HIS:ND1	2.41	0.52
15:O:257:ASP:OD1	20:S:89:LYS:NZ	2.42	0.52
28:k:41:GLN:OE1	28:k:55:ARG:NH1	2.42	0.52
36:In:14:N:O2'	36:In:15:N:O5'	2.28	0.52
4:A:2222:LYS:O	4:A:2250:GLU:N	2.42	0.52
29:e:87:GLN:NE2	31:g:56:ASN:O	2.42	0.52
23:W:445:ASN:OD1	23:W:446:VAL:N	2.43	0.52
31:n:35:ASP:OD1	31:n:39:ASN:N	2.42	0.52
4:A:1956:GLU:OE1	4:A:1958:HIS:NE2	2.41	0.52
5:B:1376:MET:HE2	5:B:1452:MET:HE2	1.92	0.52
22:TF:619:VAL:HG13	22:TF:660:ILE:HD11	1.91	0.52
3:6:24:A:N6	36:In:25:N:OP2	2.43	0.51
18:Q:863:LEU:HD11	18:Q:1038:ALA:HB1	1.92	0.51
28:k:55:ARG:NH1	28:k:69:ASN:OD1	2.44	0.51
12:L:178:SER:O	12:L:182:ARG:N	2.37	0.51
2:5:49:U:O4	2:5:50:A:N6	2.44	0.51
17:PX:767:LEU:HD22	17:PX:807:LEU:HD12	1.91	0.51
30:m:13:LEU:O	30:m:17:THR:N	2.42	0.51
3:6:39:G:OP1	12:L:173:ARG:NH2	2.44	0.51
29:l:26:ARG:NH2	29:l:58:GLU:OE1	2.44	0.51
23:W:482:LEU:HD23	23:W:483:ARG:HG3	1.93	0.51
4:A:1611:LYS:NZ	4:A:1656:ASP:OD1	2.44	0.51
10:J:35:ALA:N	12:L:17:GLU:OE1	2.44	0.50
27:j:36:MET:SD	28:k:102:ARG:NH1	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:246:LEU:HD12	6:C:893:ILE:HD11	1.94	0.50
5:B:1638:ASN:OD1	5:B:1692:ARG:NH2	2.44	0.50
22:TF:667:PRO:O	22:TF:671:ASN:ND2	2.42	0.50
4:A:155:ARG:NH2	4:A:157:PRO:O	2.43	0.50
4:A:1941:ASP:OD1	4:A:1942:LYS:N	2.44	0.50
6:C:65:ASP:O	16:P:222:LYS:NZ	2.43	0.50
23:W:359:THR:OG1	23:W:361:HIS:O	2.26	0.50
26:i:79:SER:HB3	27:j:58:LEU:HD11	1.93	0.50
10:J:344:ARG:NH2	24:Z:126:ASP:OD2	2.44	0.49
4:A:1322:MET:HE1	4:A:1361:LEU:HB3	1.94	0.49
4:A:2097:TYR:O	4:A:2255:LEU:N	2.40	0.49
5:B:1978:VAL:HG21	5:B:1987:LEU:HD11	1.94	0.49
5:B:1469:ARG:NH1	5:B:1497:TRP:O	2.45	0.49
4:A:964:GLU:OE1	4:A:1092:ARG:NH2	2.44	0.49
5:B:1115:GLN:HB2	5:B:1119:LEU:HD12	1.94	0.49
5:B:2009:PHE:O	5:B:2013:TYR:N	2.45	0.49
15:O:67:LYS:HE2	15:O:84:THR:HG21	1.94	0.49
4:A:824:TYR:OH	4:A:921:GLU:OE2	2.22	0.49
25:h:77:MET:O	25:h:80:ASN:ND2	2.45	0.49
32:o:53:ASP:HB3	32:o:75:ARG:HE	1.77	0.49
9:I:51:LEU:O	26:i:88:ARG:NH1	2.45	0.49
5:B:2064:GLU:OE2	5:B:2066:TRP:NE1	2.44	0.49
32:o:146:ASP:O	32:o:148:ASN:ND2	2.46	0.49
17:PX:468:ARG:NH1	17:PX:492:ASP:OD2	2.45	0.48
23:W:433:GLU:HG3	23:W:440:THR:HG21	1.95	0.48
9:I:735:GLU:OE1	9:I:739:ASN:ND2	2.45	0.48
23:W:220:GLN:OE1	23:W:356:ARG:NH2	2.43	0.48
18:Q:1058:TYR:OH	18:Q:1077:PRO:O	2.31	0.48
27:j:77:ASP:OD1	28:k:57:LYS:NZ	2.47	0.48
6:C:212:VAL:HG21	6:C:240:MET:HE3	1.94	0.48
2:5:100:G:O6	27:c:66:ARG:NH2	2.41	0.48
29:l:24:ARG:NE	29:l:56:GLU:OE2	2.47	0.48
23:W:419:ARG:HH11	23:W:431:ILE:HG21	1.78	0.47
5:B:705:ILE:O	5:B:709:ALA:N	2.48	0.47
32:o:132:ARG:NH2	32:o:154:GLU:OE2	2.47	0.47
10:J:465:LEU:O	24:Z:149:ARG:NH2	2.48	0.47
26:b:7:ASN:OD1	26:b:8:LYS:NZ	2.44	0.47
29:l:38:ARG:NH1	29:l:89:GLU:OE2	2.44	0.47
4:A:137:MET:HE1	4:A:181:ILE:HB	1.96	0.47
17:PX:746:LYS:O	17:PX:789:GLN:NE2	2.46	0.47
18:Q:1392:GLU:OE2	18:Q:1395:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:904:GLU:OE2	12:L:7:LYS:NZ	2.44	0.47
19:R:163:LYS:NZ	21:T:302:GLN:O	2.45	0.47
26:i:3:ILE:O	26:i:5:LYS:N	2.44	0.47
28:k:60:ASP:OD1	28:k:63:CYS:N	2.48	0.47
34:s:347:HIS:ND1	34:s:349:ASP:OD1	2.47	0.47
4:A:328:VAL:HG21	6:C:235:HIS:NE2	2.30	0.47
5:B:2013:TYR:O	5:B:2043:ASN:ND2	2.48	0.47
24:Z:120:ASP:N	24:Z:120:ASP:OD1	2.47	0.47
32:o:53:ASP:OD1	32:o:75:ARG:NH2	2.48	0.47
33:p:31:VAL:HG11	33:p:70:LEU:HD21	1.97	0.47
5:B:1195:LEU:HD21	5:B:1263:ILE:HD11	1.97	0.47
5:B:2102:GLY:N	5:B:2128:VAL:O	2.46	0.47
5:B:1338:GLU:O	5:B:1480:ARG:NE	2.39	0.46
8:E:186:ASP:OD1	8:E:186:ASP:N	2.49	0.46
25:h:53:ASP:OD1	25:h:54:GLY:N	2.46	0.46
33:p:46:LYS:O	33:p:50:ARG:N	2.45	0.46
4:A:842:TYR:OH	4:A:855:GLU:OE1	2.32	0.46
5:B:430:ARG:NH2	5:B:437:GLU:OE1	2.48	0.46
9:I:235:ILE:CG2	9:I:247:VAL:HG13	2.45	0.46
22:TF:379:LYS:NZ	22:TF:383:GLU:OE1	2.46	0.46
4:A:1309:TYR:CD2	4:A:1358:ILE:HD13	2.51	0.46
15:O:44:ARG:NH2	36:In:24:N:OP1	2.47	0.46
26:b:3:ILE:HD11	26:b:12:HIS:H	1.80	0.46
5:B:485:SER:O	5:B:641:ARG:NH2	2.46	0.46
6:C:406:ARG:O	6:C:426:ARG:NH1	2.49	0.46
23:W:474:LEU:HD12	23:W:488:LYS:HB2	1.98	0.46
8:E:220:LYS:NZ	12:L:717:GLU:OE1	2.48	0.46
10:J:575:ARG:NH2	10:J:609:ASP:OD2	2.47	0.46
1:2:9:U:O2'	1:2:10:U:O5'	2.34	0.45
4:A:1333:ARG:NH1	17:PX:350:GLU:OE2	2.43	0.45
23:W:524:ASP:OD2	23:W:527:THR:N	2.44	0.45
1:2:9:U:O2'	1:2:10:U:O4'	2.33	0.45
17:PX:522:LEU:O	17:PX:526:SER:N	2.42	0.45
23:W:507:ASP:O	23:W:509:SER:N	2.49	0.45
5:B:1854:PHE:HB3	5:B:1890:VAL:HG21	1.98	0.45
17:PX:706:ILE:HD13	17:PX:709:ILE:HD12	1.99	0.45
4:A:1715:MET:HE3	4:A:1715:MET:HA	1.98	0.45
4:A:745:SER:OG	4:A:770:ARG:NH1	2.50	0.45
9:I:571:ARG:NH2	12:L:496:ILE:O	2.49	0.45
34:s:177:ARG:NH1	34:s:390:GLU:O	2.48	0.45
9:I:144:LEU:O	9:I:152:HIS:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:TF:642:TRP:NE1	22:TF:646:MET:SD	2.90	0.45
22:TF:677:LEU:HD23	22:TF:682:VAL:HG11	1.99	0.45
6:C:783:LEU:O	6:C:942:ARG:NH1	2.45	0.44
34:s:384:ARG:NE	34:s:400:GLU:OE2	2.42	0.44
4:A:979:LYS:NZ	6:C:64:GLU:OE2	2.30	0.44
22:TF:565:LEU:O	22:TF:568:ARG:N	2.49	0.44
27:j:23:THR:HG23	27:j:47:VAL:HA	2.00	0.44
18:Q:864:ASN:OD1	18:Q:882:ARG:NH2	2.48	0.44
4:A:2120:PHE:O	4:A:2139:VAL:N	2.43	0.44
32:o:106:ILE:O	32:o:110:ALA:N	2.45	0.44
4:A:2275:ASN:ND2	4:A:2297:TYR:OH	2.50	0.44
6:C:396:LEU:HD23	6:C:412:GLN:HG2	2.00	0.44
21:T:322:ASP:N	21:T:322:ASP:OD1	2.49	0.44
29:e:32:TYR:N	29:e:79:ASN:O	2.47	0.44
29:l:77:GLY:HA2	29:l:80:ILE:HD12	2.00	0.44
4:A:1235:ARG:NH1	4:A:1238:GLN:OE1	2.47	0.44
5:B:162:ASP:N	5:B:162:ASP:OD1	2.49	0.44
15:O:65:ARG:NH2	36:In:27:N:OP2	2.47	0.44
34:s:355:THR:OG1	34:s:365:TRP:NE1	2.49	0.44
5:B:1692:ARG:NH1	5:B:1696:ASP:OD2	2.48	0.44
4:A:555:GLN:OE1	4:A:560:ASN:ND2	2.47	0.43
4:A:1486:THR:O	4:A:1741:ARG:NH2	2.49	0.43
12:L:66:GLU:OE1	12:L:66:GLU:N	2.52	0.43
17:PX:538:TRP:NE1	17:PX:545:SER:OG	2.49	0.43
18:Q:1232:TYR:HB2	18:Q:1278:VAL:HG21	2.01	0.43
29:l:61:ASN:O	29:l:65:LYS:N	2.50	0.43
5:B:465:ALA:HB1	5:B:512:LEU:HD13	2.01	0.43
5:B:1006:ASP:OD1	5:B:1042:LYS:NZ	2.51	0.43
5:B:1972:ARG:NH2	5:B:1995:ILE:O	2.49	0.43
5:B:1776:THR:OG1	5:B:1779:HIS:ND1	2.47	0.43
31:n:22:ASN:O	31:n:25:ARG:NE	2.46	0.43
4:A:2300:GLU:OE2	5:B:1118:SER:N	2.51	0.43
22:TF:507:MET:SD	22:TF:511:ILE:HD12	2.58	0.43
2:5:109:C:O2'	2:5:110:G:O5'	2.36	0.43
5:B:929:TYR:O	5:B:945:ARG:NH2	2.51	0.43
4:A:2065:GLU:O	4:A:2069:ARG:NE	2.52	0.43
6:C:162:ARG:NH2	6:C:318:ASN:OD1	2.50	0.43
26:b:38:MET:SD	27:c:61:ARG:NH1	2.92	0.43
28:d:47:ARG:HD2	28:d:107:ILE:HD11	2.01	0.43
4:A:1005:ASN:O	4:A:1018:ASN:ND2	2.48	0.43
8:E:279:ARG:NH1	23:W:99:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:75:C:O2'	2:5:76:A:O5'	2.37	0.42
5:B:807:THR:O	5:B:811:GLY:N	2.48	0.42
22:TF:686:GLU:O	22:TF:690:TRP:N	2.45	0.42
16:P:67:GLU:OE1	21:T:456:ARG:NH1	2.52	0.42
4:A:827:ASP:OD1	4:A:913:TYR:OH	2.36	0.42
23:W:456:LYS:HD2	23:W:477:LEU:HD21	2.00	0.42
4:A:739:ALA:O	4:A:743:THR:HG22	2.20	0.42
31:n:45:ALA:HB3	31:n:57:LEU:HB2	2.02	0.42
4:A:2147:HIS:ND1	4:A:2148:GLN:OE1	2.44	0.42
5:B:1989:ASN:OD1	5:B:1992:ARG:NH1	2.52	0.42
4:A:2243:GLY:N	4:A:2245:MET:SD	2.93	0.42
5:B:1984:LEU:HD12	5:B:1987:LEU:HD12	2.01	0.42
6:C:206:ILE:HG13	6:C:553:TRP:CH2	2.54	0.42
4:A:2084:TYR:O	4:A:2218:LEU:N	2.48	0.42
22:TF:629:MET:O	22:TF:668:ARG:NH2	2.44	0.42
25:h:7:PRO:O	25:h:11:LEU:N	2.48	0.42
10:J:283:TYR:CD2	19:R:5:LEU:HD21	2.55	0.42
21:T:274:LEU:HB3	21:T:285:THR:HG22	2.02	0.42
22:TF:396:MET:HE2	22:TF:430:LEU:HB3	2.01	0.42
15:O:75:CYS:HA	15:O:78:VAL:HG12	2.01	0.42
4:A:2181:LEU:O	4:A:2244:TYR:OH	2.37	0.41
9:I:235:ILE:HG21	9:I:247:VAL:HG13	2.02	0.41
4:A:1880:SER:O	4:A:1882:LEU:N	2.53	0.41
19:R:265:VAL:HG23	19:R:270:ARG:HG3	2.02	0.41
17:PX:472:ARG:NH2	17:PX:492:ASP:OD1	2.54	0.41
4:A:1768:GLN:O	4:A:1806:ARG:NH2	2.52	0.41
4:A:474:PHE:CZ	19:R:210:MET:HE3	2.56	0.41
6:C:180:ARG:NH2	6:C:642:ASP:OD2	2.49	0.41
5:B:1492:ARG:NH1	5:B:1500:CYS:O	2.48	0.41
5:B:2027:VAL:HG13	5:B:2033:LEU:HD21	2.03	0.41
9:I:332:ASP:OD1	18:Q:346:ARG:NH1	2.46	0.41
12:L:330:ASP:OD1	12:L:330:ASP:N	2.52	0.41
2:5:30:A:OP2	4:A:420:LYS:NZ	2.44	0.41
6:C:183:SER:N	39:C:1101:GTP:O3G	2.49	0.41
9:I:499:GLU:OE2	9:I:511:TYR:OH	2.34	0.41
14:N:130:ASP:OD1	14:N:130:ASP:N	2.50	0.41
22:TF:677:LEU:HD21	22:TF:687:VAL:HG11	2.02	0.41
5:B:138:LEU:O	5:B:148:LYS:NZ	2.40	0.41
5:B:1021:SER:O	5:B:1051:LYS:NZ	2.44	0.41
5:B:1860:ARG:NH1	5:B:1863:GLU:OE2	2.47	0.41
17:PX:403:LEU:HD21	17:PX:531:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:433:GLU:OE1	18:Q:649:ARG:NH2	2.54	0.41
4:A:2236:ASP:OD1	4:A:2237:LYS:N	2.54	0.41
19:R:133:ASP:OD1	19:R:133:ASP:N	2.53	0.41
23:W:470:ASN:O	23:W:491:ARG:NE	2.44	0.41
4:A:2185:ASP:N	4:A:2185:ASP:OD1	2.53	0.41
5:B:447:ARG:O	5:B:477:ARG:NH1	2.51	0.41
10:J:34:THR:N	12:L:17:GLU:OE1	2.52	0.41
30:m:64:ILE:HD12	30:m:66:ILE:HD11	2.03	0.41
4:A:2230:TRP:O	4:A:2234:ASN:N	2.43	0.40
5:B:1985:LEU:HD21	5:B:2010:CYS:HB3	2.04	0.40
4:A:1243:SER:O	4:A:1246:THR:OG1	2.36	0.40
6:C:257:THR:HB	6:C:437:LEU:HD11	2.03	0.40
26:b:3:ILE:HD13	26:b:9:MET:O	2.22	0.40
30:m:69:ASN:OD1	30:m:70:ASN:N	2.55	0.40
4:A:312:ILE:HG22	4:A:312:ILE:O	2.22	0.40
34:s:17:VAL:HG22	34:s:24:ILE:HG22	2.04	0.40
4:A:2089:ASP:OD1	4:A:2090:VAL:N	2.54	0.40
5:B:515:ILE:O	5:B:519:LEU:N	2.54	0.40
12:L:285:LYS:NZ	13:M:229:GLU:OE1	2.41	0.40
12:L:712:GLU:OE1	34:s:129:ARG:NH1	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	2018/2100 (96%)	1972 (98%)	46 (2%)	44 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	1593/1886 (84%)	1587 (100%)	6 (0%)	84	94
6	C	793/861 (92%)	781 (98%)	12 (2%)	57	84
7	D	80/230 (35%)	78 (98%)	2 (2%)	42	74
8	E	275/291 (94%)	273 (99%)	2 (1%)	76	92
9	I	641/754 (85%)	622 (97%)	19 (3%)	36	70
10	J	508/650 (78%)	491 (97%)	17 (3%)	33	67
11	K	183/214 (86%)	183 (100%)	0	100	100
12	L	529/645 (82%)	522 (99%)	7 (1%)	61	86
13	M	178/212 (84%)	176 (99%)	2 (1%)	65	88
14	N	125/129 (97%)	121 (97%)	4 (3%)	34	68
15	O	295/351 (84%)	290 (98%)	5 (2%)	53	82
16	P	129/197 (66%)	126 (98%)	3 (2%)	44	76
17	PX	423/724 (58%)	418 (99%)	5 (1%)	63	86
18	Q	1235/1311 (94%)	1225 (99%)	10 (1%)	73	90
19	R	235/447 (53%)	221 (94%)	14 (6%)	17	47
20	S	137/137 (100%)	133 (97%)	4 (3%)	37	71
21	T	333/421 (79%)	326 (98%)	7 (2%)	47	77
22	TF	451/718 (63%)	439 (97%)	12 (3%)	39	73
23	W	444/502 (88%)	430 (97%)	14 (3%)	34	68
24	Z	63/145 (43%)	60 (95%)	3 (5%)	23	55
25	a	71/106 (67%)	71 (100%)	0	100	100
25	h	71/106 (67%)	70 (99%)	1 (1%)	59	85
26	b	79/116 (68%)	78 (99%)	1 (1%)	61	86
26	i	70/116 (60%)	68 (97%)	2 (3%)	37	71
27	c	73/98 (74%)	73 (100%)	0	100	100
27	j	73/98 (74%)	72 (99%)	1 (1%)	59	85
28	d	84/103 (82%)	82 (98%)	2 (2%)	43	75
28	k	72/103 (70%)	72 (100%)	0	100	100
29	e	71/81 (88%)	71 (100%)	0	100	100
29	l	71/81 (88%)	70 (99%)	1 (1%)	59	85
30	f	61/71 (86%)	60 (98%)	1 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	m	61/71 (86%)	59 (97%)	2 (3%)	33	67
31	g	69/69 (100%)	69 (100%)	0	100	100
31	n	69/69 (100%)	68 (99%)	1 (1%)	59	85
32	o	151/225 (67%)	150 (99%)	1 (1%)	76	92
33	p	68/192 (35%)	67 (98%)	1 (2%)	57	84
34	q	108/417 (26%)	108 (100%)	0	100	100
34	r	114/417 (27%)	110 (96%)	4 (4%)	32	66
34	s	396/417 (95%)	386 (98%)	10 (2%)	42	74
34	t	115/417 (28%)	113 (98%)	2 (2%)	53	82
35	y	64/270 (24%)	63 (98%)	1 (2%)	55	83
All	All	12679/16568 (76%)	12454 (98%)	225 (2%)	51	80

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	69	ARG
4	A	87	HIS
4	A	103	ILE
4	A	209	VAL
4	A	311	LEU
4	A	317	VAL
4	A	443	LEU
4	A	519	VAL
4	A	560	ASN
4	A	561	VAL
4	A	636	ILE
4	A	743	THR
4	A	801	ILE
4	A	877	MET
4	A	934	PRO
4	A	961	SER
4	A	969	MET
4	A	1012	LYS
4	A	1177	MET
4	A	1203	ASP
4	A	1274	GLN
4	A	1347	ARG
4	A	1361	LEU

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Mol	Chain	Res	Type
4	A	1369	GLU
4	A	1397	THR
4	A	1464	ARG
4	A	1542	VAL
4	A	1564	ILE
4	A	1627	GLN
4	A	1671	ARG
4	A	1715	MET
4	A	1746	LEU
4	A	1997	GLN
4	A	2106	LYS
4	A	2131	GLN
4	A	2133	LYS
4	A	2149	GLN
4	A	2168	LEU
4	A	2170	TRP
4	A	2171	MET
4	A	2177	GLU
4	A	2178	LEU
4	A	2182	SER
4	A	2185	ASP
4	A	2245	MET
4	A	2276	PHE
5	B	162	ASP
5	B	164	ILE
5	B	720	SER
5	B	878	GLN
5	B	1026	GLU
5	B	1070	LEU
6	C	84	VAL
6	C	94	GLU
6	C	206	ILE
6	C	212	VAL
6	C	243	GLU
6	C	290	ASN
6	C	326	PHE
6	C	381	MET
6	C	392	VAL
6	C	417	ARG
6	C	760	LYS
6	C	802	THR
7	D	243	LEU

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Mol	Chain	Res	Type
7	D	247	GLN
8	E	121	THR
8	E	314	MET
9	I	49	HIS
9	I	54	LYS
9	I	135	GLU
9	I	176	TYR
9	I	323	GLN
9	I	336	MET
9	I	351	MET
9	I	363	VAL
9	I	372	ILE
9	I	388	VAL
9	I	395	ILE
9	I	399	LYS
9	I	414	ASN
9	I	467	VAL
9	I	515	ILE
9	I	663	LEU
9	I	673	LEU
9	I	681	THR
9	I	735	GLU
10	J	34	THR
10	J	36	GLU
10	J	37	GLN
10	J	89	TRP
10	J	170	ILE
10	J	181	ILE
10	J	214	LEU
10	J	224	TRP
10	J	254	GLU
10	J	258	GLU
10	J	297	PHE
10	J	302	GLN
10	J	305	LYS
10	J	529	ILE
10	J	550	GLN
10	J	583	GLN
10	J	615	ARG
12	L	234	TYR
12	L	307	LYS
12	L	316	ARG

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Mol	Chain	Res	Type
12	L	351	LYS
12	L	355	GLN
12	L	361	LEU
12	L	504	GLU
13	M	63	ARG
13	M	206	ASN
14	N	19	ASP
14	N	48	ILE
14	N	101	GLU
14	N	142	CYS
15	O	27	THR
15	O	78	VAL
15	O	115	ARG
15	O	138	ILE
15	O	181	GLU
16	P	31	SER
16	P	33	LYS
16	P	59	LEU
17	PX	344	LEU
17	PX	396	LEU
17	PX	440	MET
17	PX	443	GLN
17	PX	598	ILE
18	Q	237	GLN
18	Q	318	ASP
18	Q	357	VAL
18	Q	602	LEU
18	Q	825	VAL
18	Q	1096	ILE
18	Q	1118	GLU
18	Q	1285	HIS
18	Q	1291	ARG
18	Q	1308	ARG
19	R	6	ARG
19	R	16	ASP
19	R	53	PHE
19	R	54	ARG
19	R	91	THR
19	R	130	TRP
19	R	200	ILE
19	R	202	MET
19	R	210	MET

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Mol	Chain	Res	Type
19	R	241	THR
19	R	259	ASN
19	R	267	LEU
19	R	276	ARG
19	R	298	ASP
20	S	100	ASN
20	S	117	THR
20	S	153	ILE
20	S	158	LEU
21	T	190	VAL
21	T	220	LEU
21	T	345	MET
21	T	397	ASN
21	T	435	GLN
21	T	451	ASP
21	T	473	ASP
22	TF	326	ILE
22	TF	338	GLU
22	TF	341	ARG
22	TF	351	LYS
22	TF	360	ASP
22	TF	451	ILE
22	TF	485	ILE
22	TF	490	ILE
22	TF	548	MET
22	TF	572	VAL
22	TF	638	GLU
22	TF	778	GLN
23	W	158	LYS
23	W	282	GLN
23	W	294	CYS
23	W	299	LYS
23	W	305	VAL
23	W	312	VAL
23	W	343	VAL
23	W	354	LYS
23	W	369	HIS
23	W	410	SER
23	W	417	ASN
23	W	434	TRP
23	W	454	MET
23	W	504	PHE

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Mol	Chain	Res	Type
24	Z	86	LEU
24	Z	135	GLU
24	Z	142	VAL
26	b	38	MET
28	d	48	ASN
28	d	65	MET
30	f	65	LEU
25	h	77	MET
26	i	35	ASP
26	i	88	ARG
27	j	46	THR
29	l	44	ILE
30	m	72	LEU
30	m	73	TYR
31	n	32	ARG
32	o	106	ILE
33	p	34	GLN
34	r	28	ARG
34	r	46	GLU
34	r	115	CYS
34	r	121	LEU
34	s	174	THR
34	s	199	GLN
34	s	289	ILE
34	s	299	ILE
34	s	306	ASP
34	s	331	VAL
34	s	342	HIS
34	s	352	ILE
34	s	395	LEU
34	s	455	GLU
34	t	36	GLU
34	t	110	GLN
35	y	33	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	95	ASN
4	A	347	ASN
4	A	703	GLN
4	A	747	HIS

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Mol	Chain	Res	Type
4	A	986	ASN
4	A	1005	ASN
4	A	1027	GLN
4	A	1274	GLN
4	A	1285	ASN
4	A	1853	GLN
4	A	1997	GLN
4	A	2116	GLN
4	A	2234	ASN
4	A	2308	HIS
5	B	895	ASN
5	B	992	GLN
5	B	1861	HIS
6	C	287	GLN
6	C	290	ASN
6	C	333	GLN
6	C	387	GLN
6	C	508	ASN
8	E	168	GLN
9	I	342	HIS
9	I	348	ASN
9	I	523	GLN
9	I	610	HIS
10	J	515	GLN
12	L	13	ASN
12	L	365	GLN
12	L	366	ASN
12	L	452	GLN
12	L	565	ASN
14	N	58	GLN
14	N	139	HIS
15	O	166	HIS
15	O	199	GLN
15	O	249	GLN
16	P	94	GLN
17	PX	394	GLN
18	Q	161	HIS
18	Q	234	ASN
18	Q	237	GLN
18	Q	682	GLN
18	Q	1002	HIS
18	Q	1268	GLN

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Mol	Chain	Res	Type
19	R	71	HIS
19	R	189	GLN
19	R	196	GLN
19	R	234	HIS
20	S	39	GLN
20	S	61	GLN
21	T	249	GLN
21	T	304	HIS
21	T	330	HIS
22	TF	346	GLN
22	TF	819	ASN
23	W	459	ASN
23	W	508	GLN
25	a	17	HIS
26	b	50	GLN
28	d	38	ASN
26	i	12	HIS
27	j	37	ASN
30	m	48	HIS
31	n	56	ASN
32	o	20	ASN
34	s	263	ASN
34	s	342	HIS
34	s	370	GLN
34	s	424	GLN
34	t	89	ASN
34	t	106	HIS
35	y	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	23/191 (12%)	7 (30%)	0
2	5	110/121 (90%)	29 (26%)	13 (11%)
3	6	89/101 (88%)	41 (46%)	10 (11%)
All	All	222/413 (53%)	77 (34%)	23 (10%)

All (77) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	10	U

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Mol	Chain	Res	Type
1	2	18	U
1	2	19	U
1	2	20	A
1	2	21	G
1	2	25	A
1	2	26	G
2	5	4	C
2	5	6	C
2	5	8	G
2	5	10	U
2	5	20	U
2	5	23	A
2	5	24	A
2	5	25	C
2	5	26	C
2	5	27	G
2	5	28	U
2	5	43	U
2	5	72	A
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	96	U
2	5	99	G
2	5	100	G
2	5	101	A
2	5	110	G
2	5	112	A
2	5	113	A
2	5	114	G
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

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Mol	Chain	Res	Type
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	38	A
3	6	39	G
3	6	41	G
3	6	42	A
3	6	43	A
3	6	44	G
3	6	46	U
3	6	48	A
3	6	49	G
3	6	54	G
3	6	55	C
3	6	56	C
3	6	62	G
3	6	64	A
3	6	69	U
3	6	74	C
3	6	75	G
3	6	79	A
3	6	80	U
3	6	81	U
3	6	82	C
3	6	84	U
3	6	85	G
3	6	86	A
3	6	89	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	3	A
2	5	5	U
2	5	19	A
2	5	23	A

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Mol	Chain	Res	Type
2	5	25	C
2	5	75	C
2	5	79	G
2	5	81	G
2	5	100	G
2	5	109	C
2	5	111	A
2	5	112	A
2	5	113	A
3	6	23	A
3	6	28	G
3	6	37	C
3	6	41	G
3	6	45	A
3	6	48	A
3	6	53	G
3	6	79	A
3	6	81	U
3	6	85	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 13 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
38	IHP	A	3000	-	36,36,36	2.32	10 (27%)	60,60,60	1.62	11 (18%)
38	IHP	J	3000	-	36,36,36	2.33	10 (27%)	60,60,60	0.95	2 (3%)
39	GTP	C	1101	37	33,34,34	1.38	5 (15%)	50,54,54	1.78	11 (22%)

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
38	IHP	A	3000	-	-	4/30/54/54	0/1/1/1
38	IHP	J	3000	-	-	0/30/54/54	0/1/1/1
39	GTP	C	1101	37	-	0/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	3000	IHP	C3-C2	-5.38	1.41	1.52
38	J	3000	IHP	P3-O13	5.16	1.68	1.59
38	A	3000	IHP	P5-O15	5.08	1.68	1.59
38	A	3000	IHP	P2-O12	4.88	1.68	1.59
38	A	3000	IHP	P6-O16	4.71	1.67	1.59
38	J	3000	IHP	P6-O16	4.59	1.67	1.59
38	A	3000	IHP	P3-O13	4.52	1.67	1.59
38	J	3000	IHP	P2-O12	4.51	1.67	1.59
38	J	3000	IHP	P5-O15	4.34	1.67	1.59
38	A	3000	IHP	P4-O14	4.33	1.67	1.59
38	A	3000	IHP	C3-C2	-4.30	1.43	1.52
38	A	3000	IHP	P1-O11	4.26	1.67	1.59
38	J	3000	IHP	P1-O11	4.20	1.66	1.59
38	J	3000	IHP	P4-O14	4.17	1.66	1.59
39	C	1101	GTP	C5-N7	-3.32	1.32	1.39
38	A	3000	IHP	C5-C4	3.28	1.59	1.52
38	J	3000	IHP	O12-C2	-3.03	1.33	1.44
38	J	3000	IHP	O13-C3	-3.00	1.33	1.44
38	A	3000	IHP	O12-C2	-2.89	1.34	1.44
38	A	3000	IHP	O13-C3	-2.75	1.34	1.44
39	C	1101	GTP	C5-C6	-2.66	1.34	1.44
38	J	3000	IHP	C2-C1	-2.57	1.47	1.52
39	C	1101	GTP	C6-N1	-2.38	1.34	1.38
39	C	1101	GTP	PG-O3G	-2.15	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	1101	GTP	O4'-C4'	-2.02	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	3000	IHP	O15-C5-C4	5.65	120.78	108.76
39	C	1101	GTP	C5-C4-N3	-5.37	119.85	128.39
39	C	1101	GTP	C2-N3-C4	4.57	120.16	112.30
38	A	3000	IHP	O15-C5-C6	4.54	118.42	108.76
39	C	1101	GTP	N9-C4-N3	3.97	133.89	125.95
38	A	3000	IHP	P5-O15-C5	-3.76	113.39	123.43
39	C	1101	GTP	C2-N1-C6	-3.61	118.56	125.11
39	C	1101	GTP	C5-C6-N1	3.40	121.91	113.25
39	C	1101	GTP	O6-C6-C5	-3.18	118.15	126.53
38	A	3000	IHP	P1-O11-C1	-3.13	115.07	123.43
39	C	1101	GTP	O2B-PB-O3A	2.96	115.29	107.27
38	A	3000	IHP	C6-C5-C4	-2.76	104.37	110.43
38	A	3000	IHP	O11-C1-C2	2.56	114.21	108.76
39	C	1101	GTP	O3B-PB-O1B	-2.53	103.10	110.70
38	A	3000	IHP	O13-C3-C2	2.46	114.00	108.76
38	A	3000	IHP	P3-O13-C3	2.42	129.90	123.43
39	C	1101	GTP	O2A-PA-O3A	2.35	113.63	107.27
38	J	3000	IHP	C5-C4-C3	2.30	115.48	110.43
39	C	1101	GTP	N9-C8-N7	-2.25	109.22	113.40
38	J	3000	IHP	P4-O14-C4	-2.20	117.56	123.43
38	A	3000	IHP	O12-C2-C1	2.18	113.39	108.76
38	A	3000	IHP	C5-C6-C1	-2.13	105.74	110.43
39	C	1101	GTP	O4'-C1'-N9	2.13	113.18	108.36
38	A	3000	IHP	C3-C2-C1	2.10	115.04	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

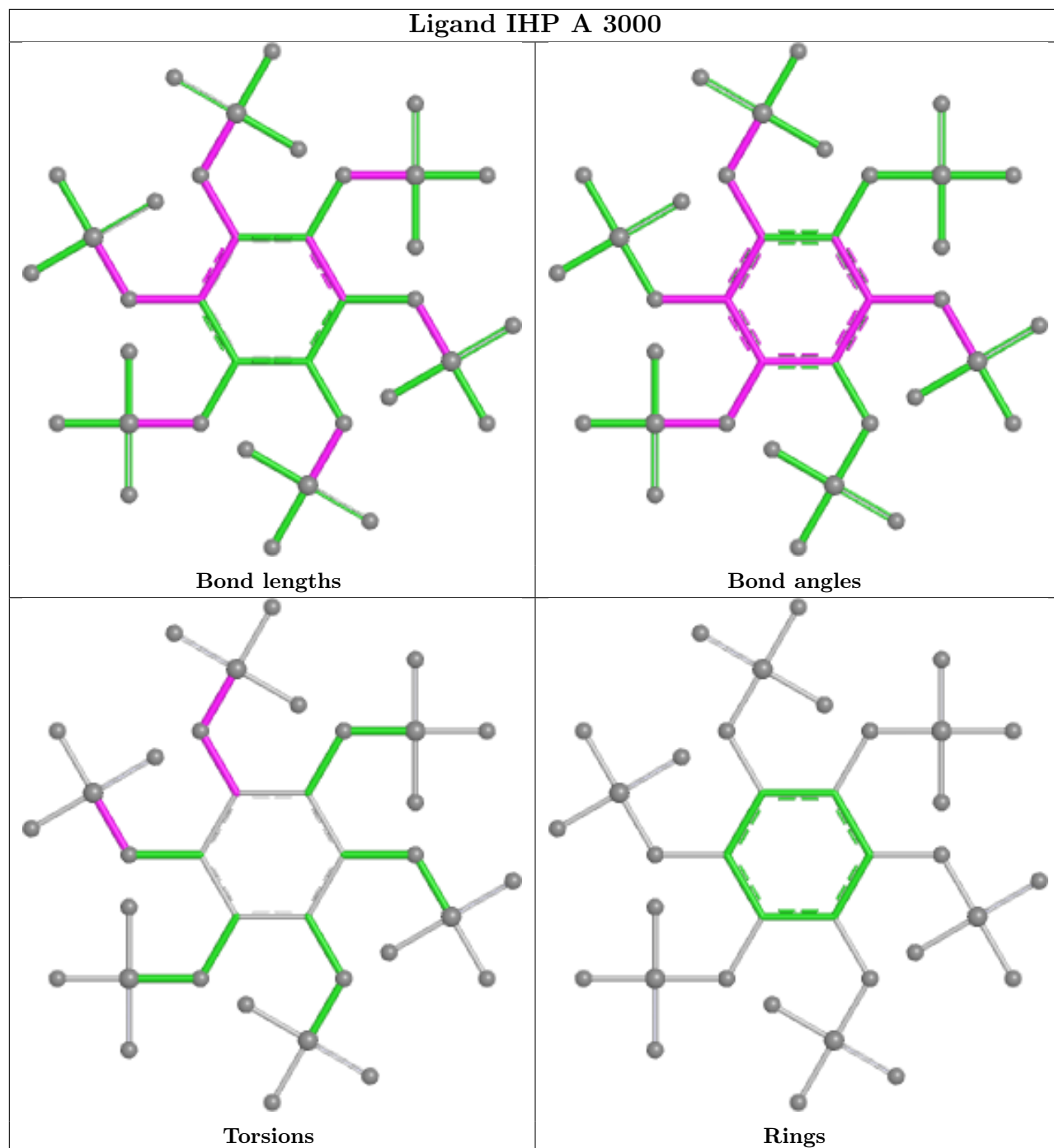
Mol	Chain	Res	Type	Atoms
38	A	3000	IHP	C4-C3-O13-P3
38	A	3000	IHP	C2-C3-O13-P3
38	A	3000	IHP	C3-O13-P3-O23
38	A	3000	IHP	C2-O12-P2-O32

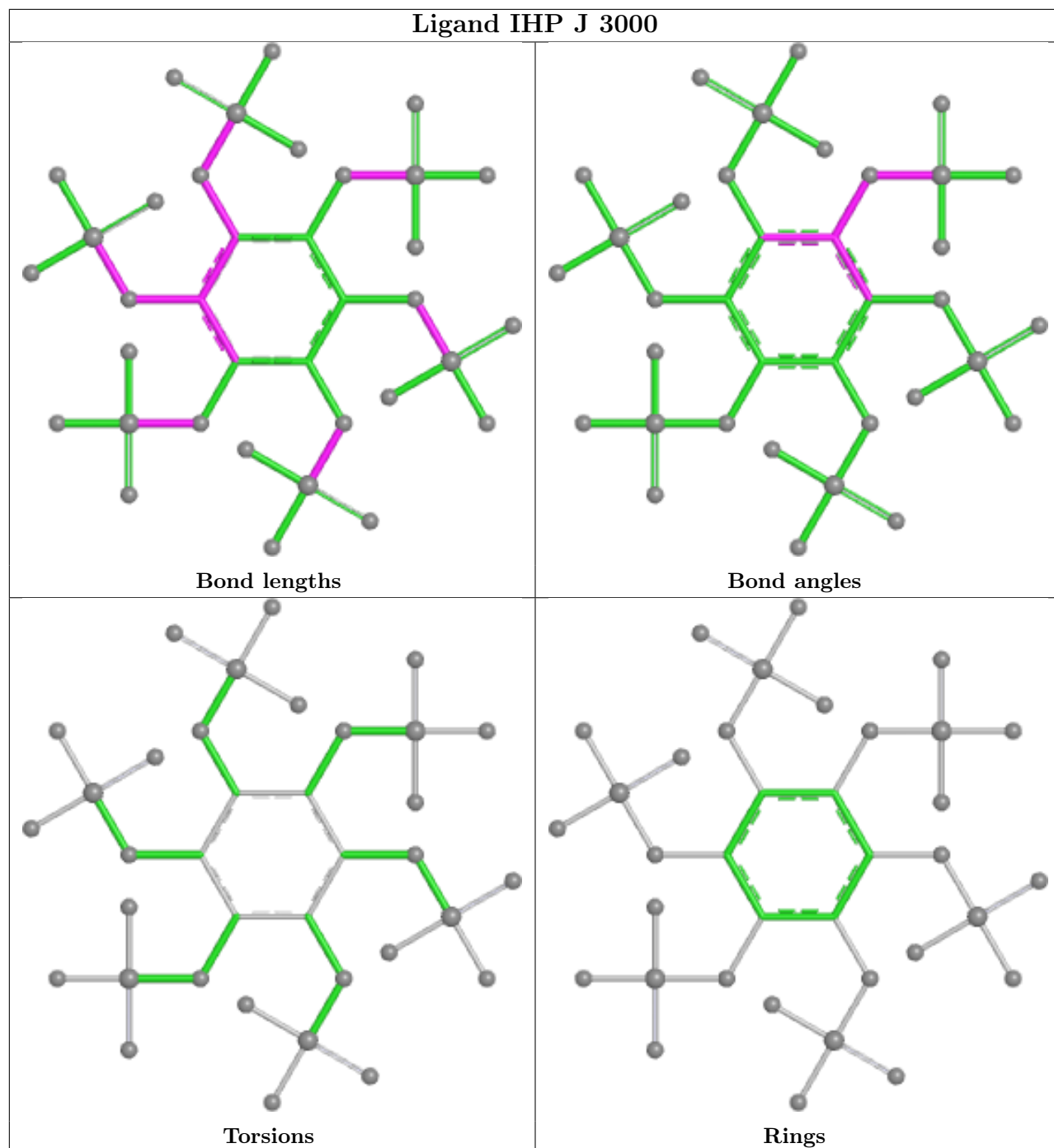
There are no ring outliers.

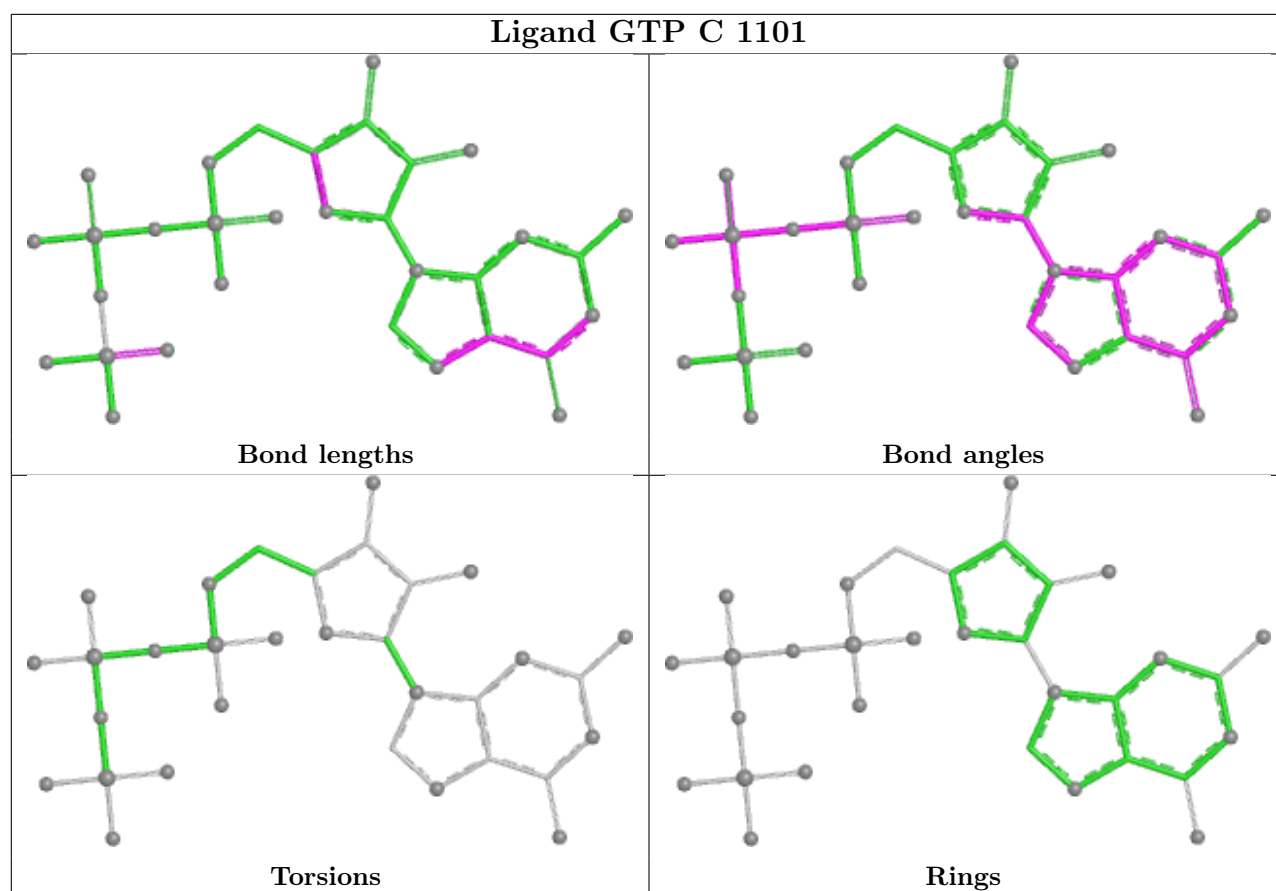
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	J	3000	IHP	1	0
39	C	1101	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

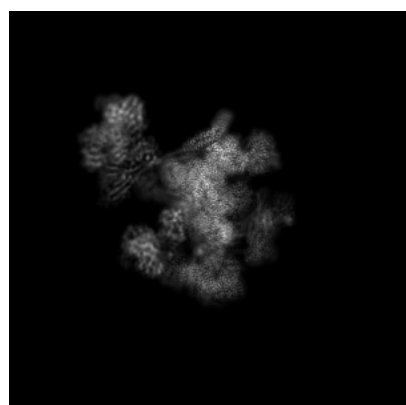
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19397. These allow visual inspection of the internal detail of the map and identification of artifacts.

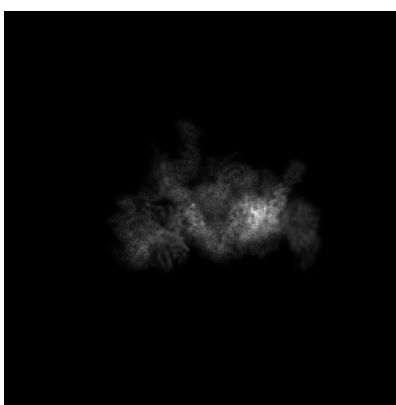
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

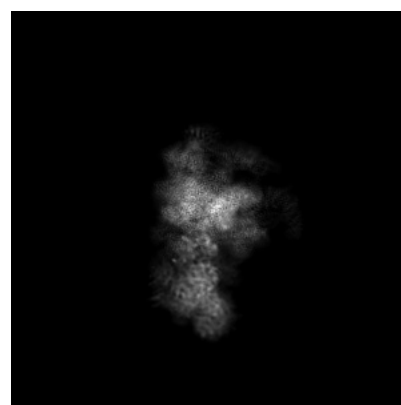
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

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: 221



Y Index: 228

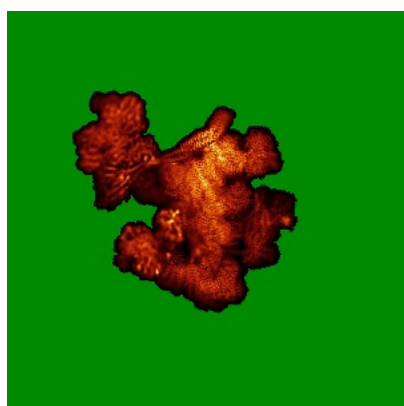


Z Index: 282

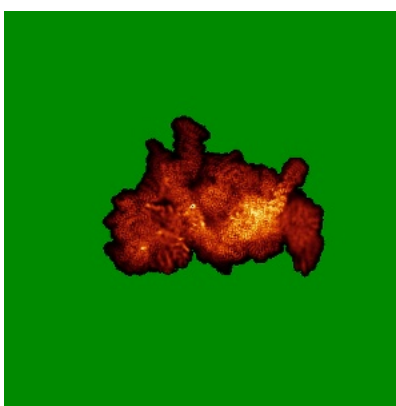
The images above show the largest variance slices of the map in three orthogonal directions.

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

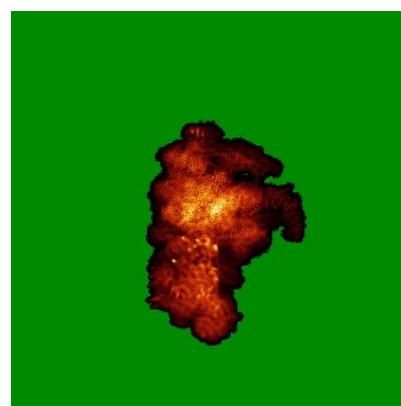
6.4.1 Primary map



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

This section was not generated.

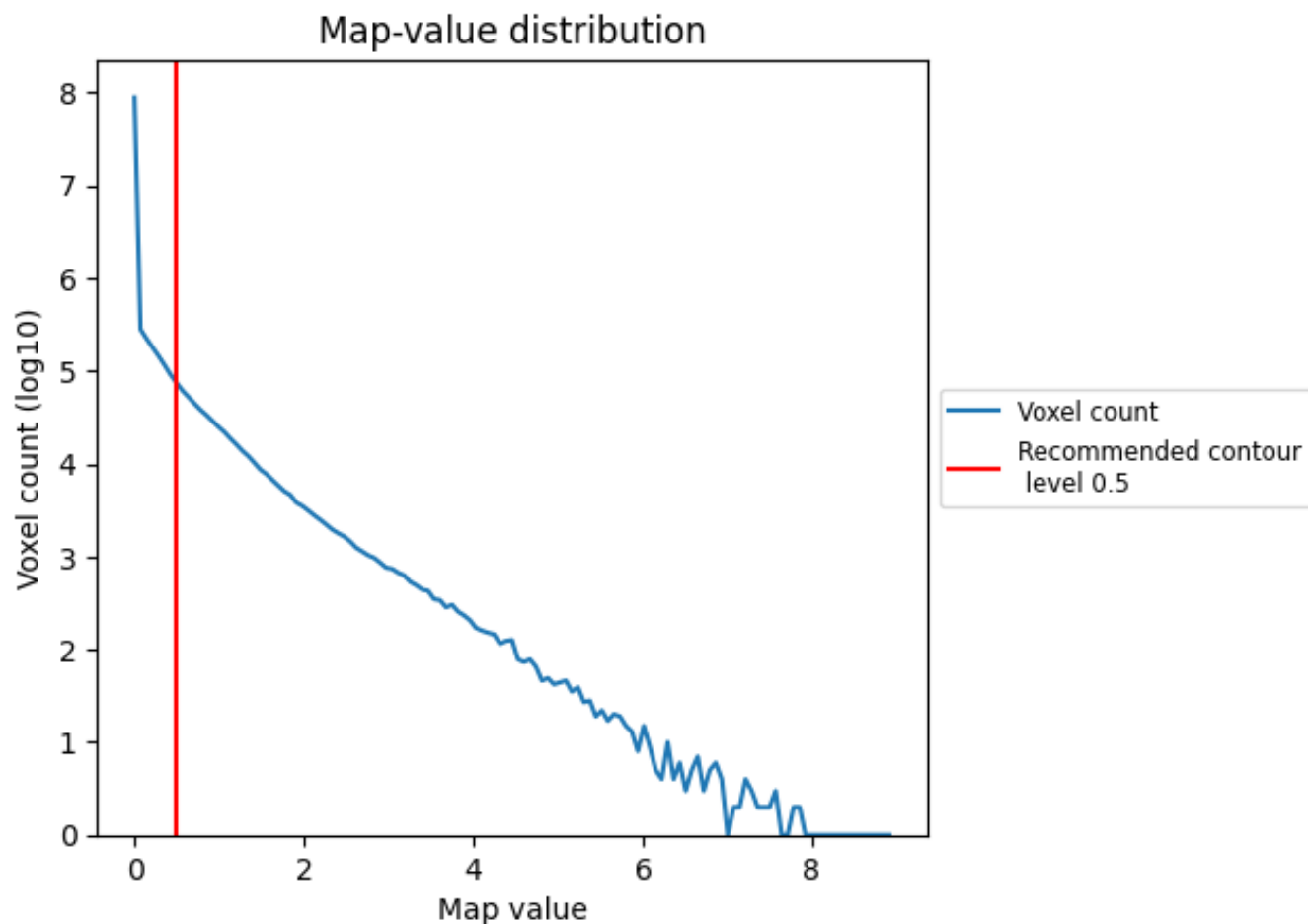
6.6 Mask visualisation

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

7 Map analysis [i](#)

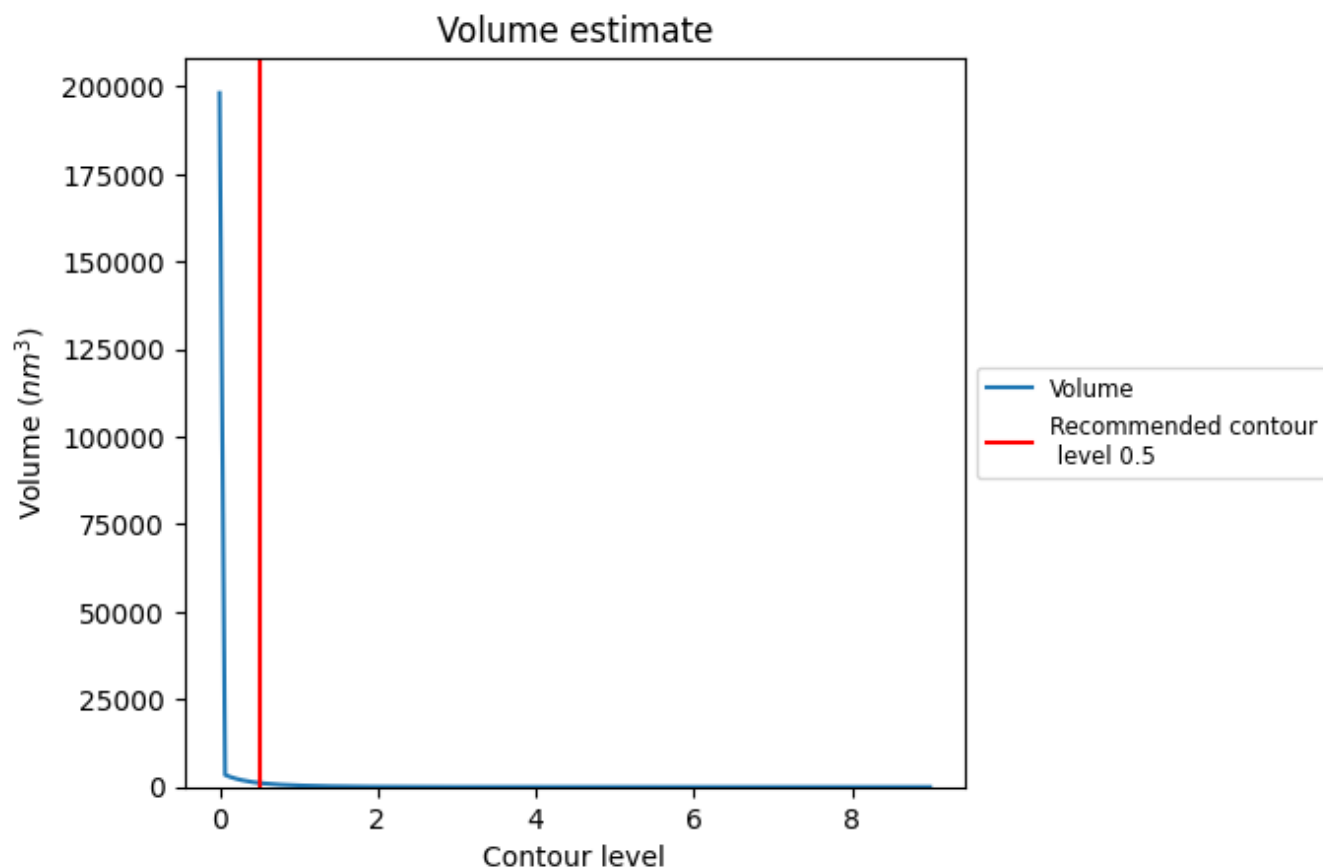
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

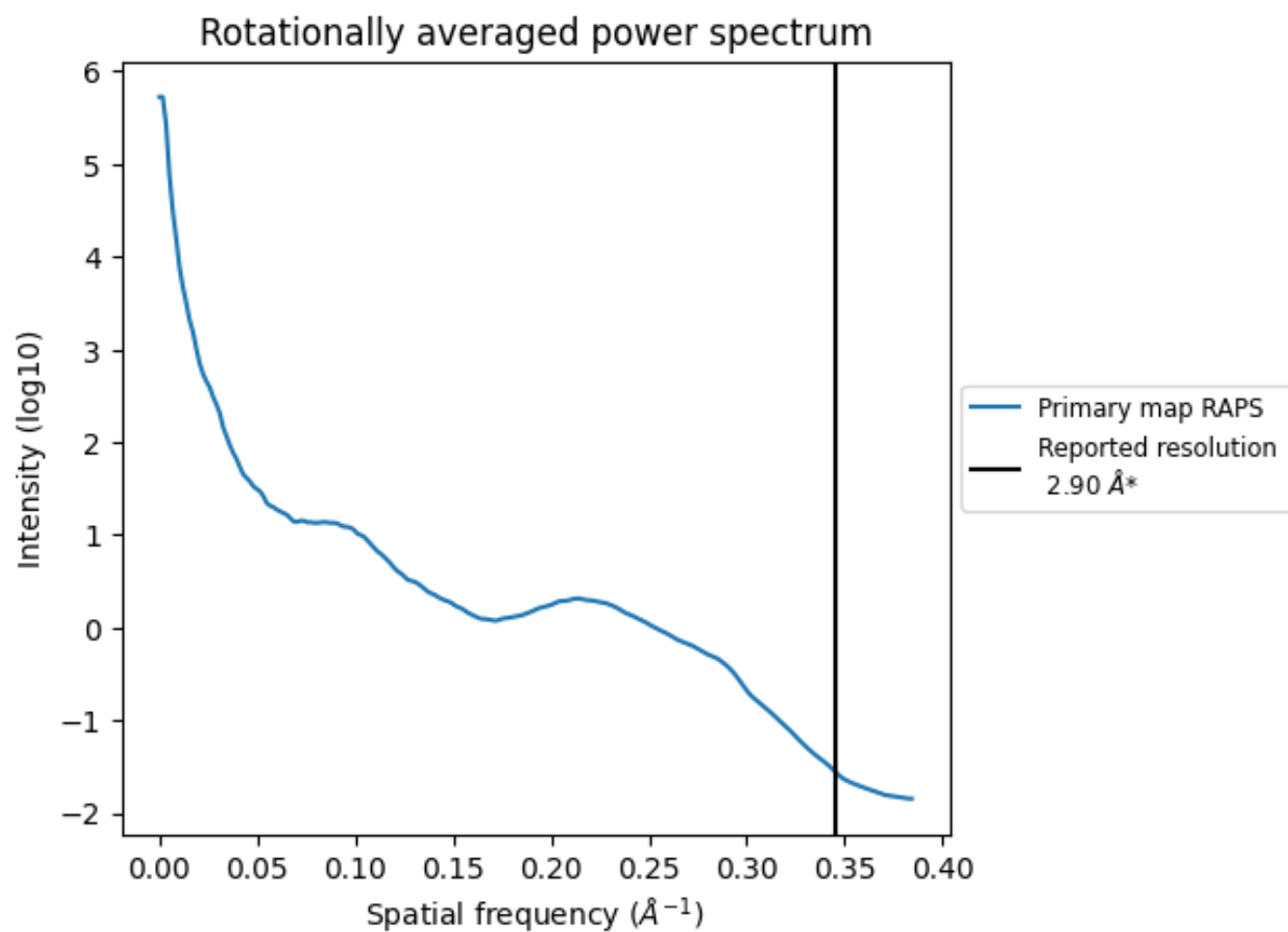
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1151 nm^3 ; this corresponds to an approximate mass of 1040 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

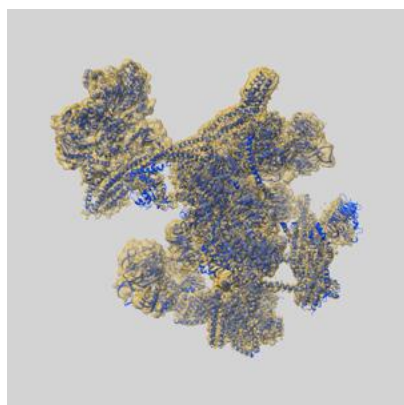
8 Fourier-Shell correlation ⓘ

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

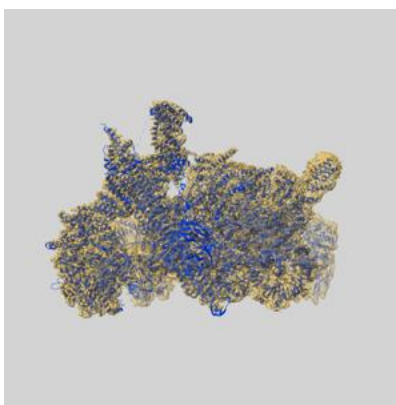
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19397 and PDB model 8RO0. Per-residue inclusion information can be found in section 3 on page 13.

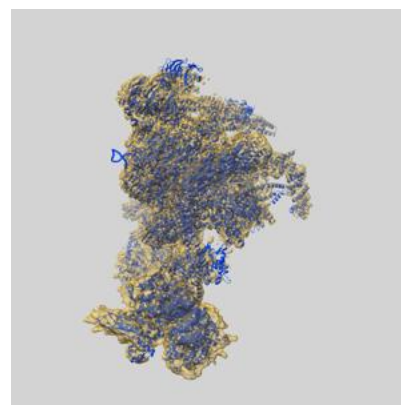
9.1 Map-model overlay [i](#)



X



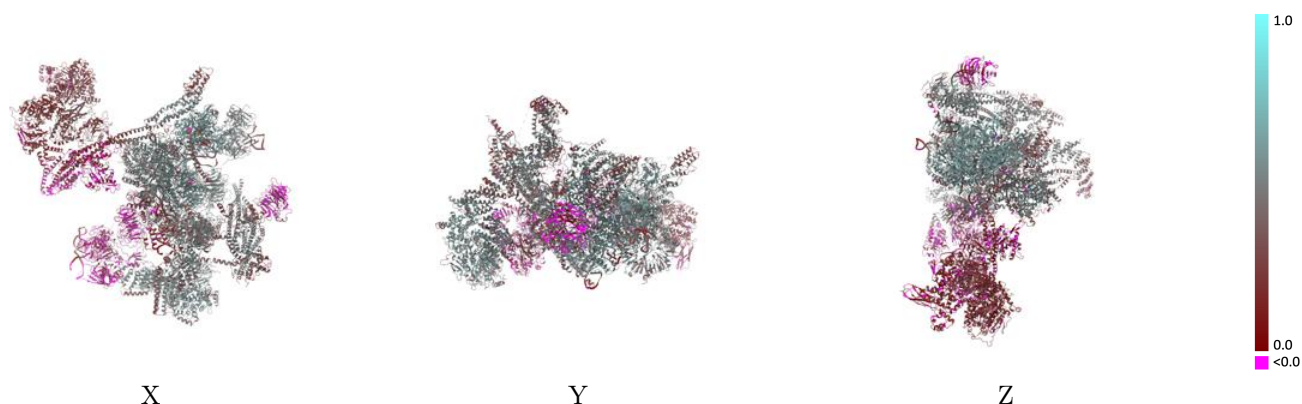
Y



Z

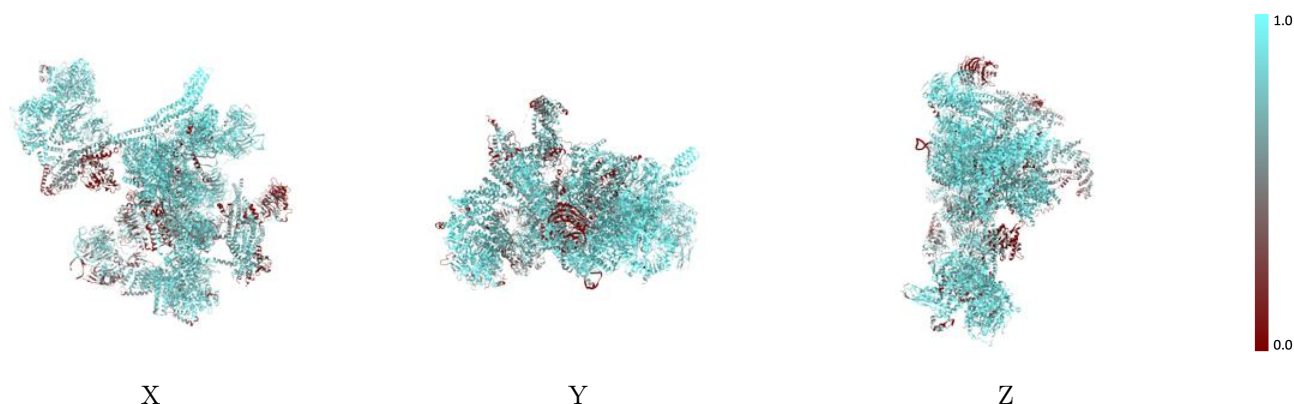
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



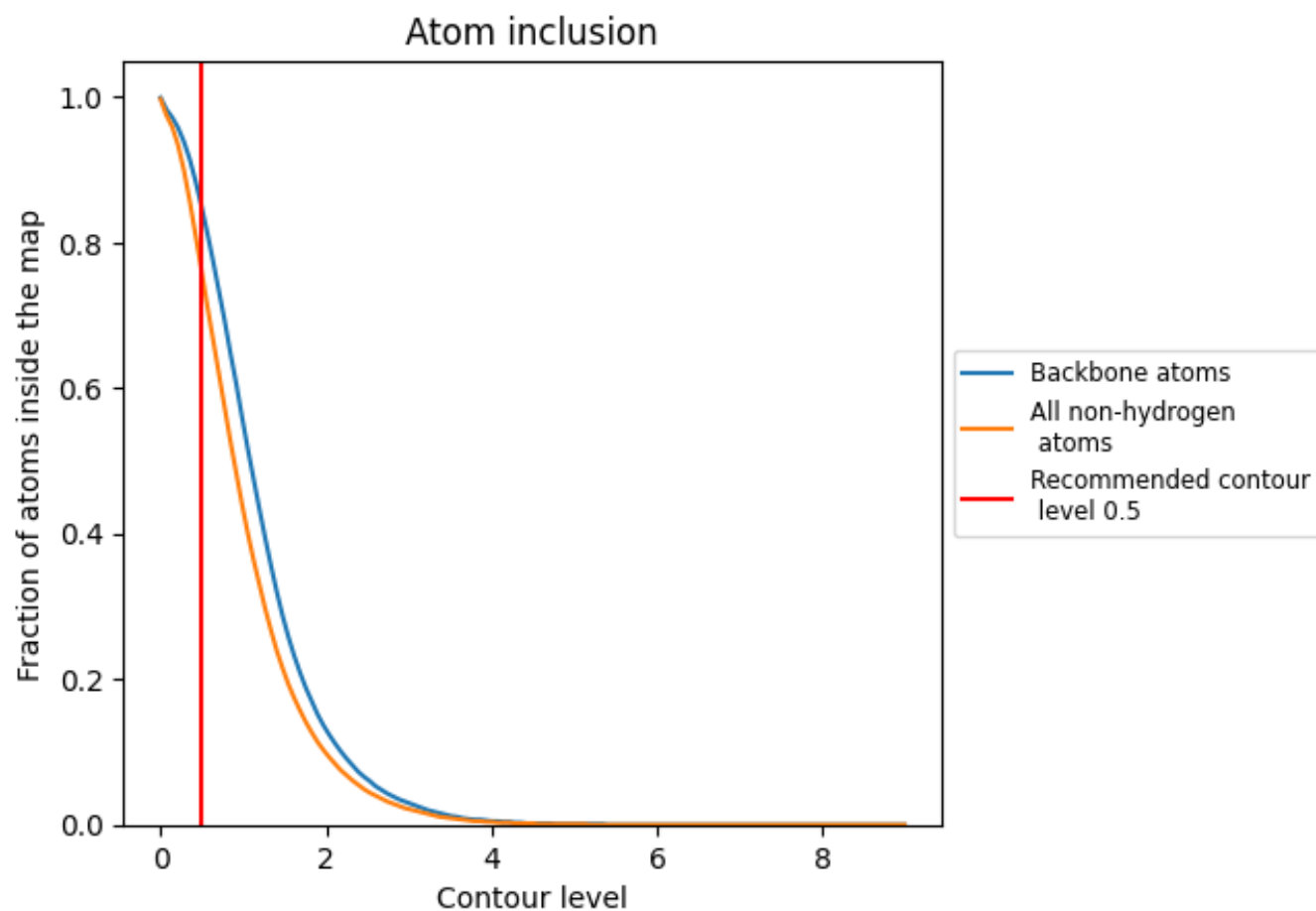
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 76% 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	 0.7580	 0.3720
2	 0.7730	 0.1980
5	 0.9440	 0.4570
6	 0.6260	 0.3220
A	 0.8000	 0.4350
B	 0.8460	 0.2000
C	 0.9420	 0.5700
D	 0.4670	 0.3640
E	 0.8940	 0.5330
I	 0.8460	 0.4750
In	 0.6220	 0.2310
J	 0.7620	 0.4580
K	 0.6820	 0.4230
L	 0.5830	 0.3790
M	 0.7150	 0.3100
N	 0.9410	 0.5520
O	 0.8020	 0.4680
P	 0.3610	 0.2980
PX	 0.4710	 0.0840
Q	 0.8220	 0.5150
R	 0.7750	 0.4450
S	 0.7380	 0.4350
T	 0.9210	 0.5490
TF	 0.8490	 0.3840
W	 0.6190	 0.1620
Z	 0.4980	 0.4050
a	 0.9130	 0.5030
b	 0.8860	 0.4550
c	 0.9100	 0.4790
d	 0.7980	 0.3850
e	 0.8640	 0.4680
f	 0.8600	 0.4670
g	 0.8250	 0.4430
h	 0.7500	 0.0960
i	 0.4880	 0.0510



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Chain	Atom inclusion	Q-score
j	 0.5000	 0.0490
k	 0.4860	 0.0630
l	 0.6030	 0.0520
m	 0.6560	 0.0740
n	 0.6890	 0.0690
o	 0.5080	 0.0310
p	 0.5550	 0.0610
q	 0.7370	 0.4590
r	 0.4870	 0.3880
s	 0.3600	 0.1630
t	 0.5380	 0.3930
y	 0.4010	 0.1490