



Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 02:03 pm BST

PDB ID : 9S2E / pdb_00009s2e
EMDB ID : EMD-54493
Title : Human intron-lariat spliceosome-Aquarius (ILSaqr)
Authors : Boreikaite, V.; Vorlaender, M.K.; Plaschka, C.
Deposited on : 2025-07-21
Resolution : 2.40 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:

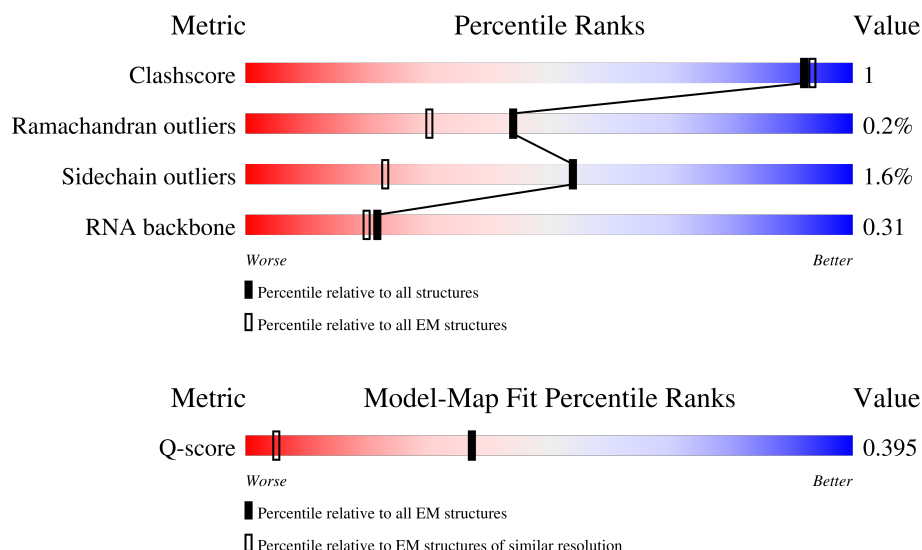
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

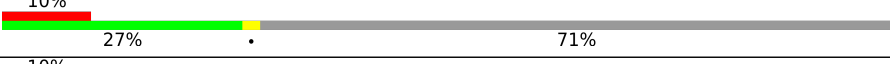
The reported resolution of this entry is 2.40 Å.

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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	187	
2	3	476	
3	5	116	

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Mol	Chain	Length	Quality of chain
4	6	106	
5	A	2335	
6	B	2136	
7	C	972	
8	D	285	
9	DX	795	
10	E	357	
11	GC	781	
12	I	855	
13	IN	61	
14	J	848	
15	K	225	
16	L	802	
17	L1	538	
18	L2	894	
19	M	243	
20	N	144	
21	O	420	
22	P	229	
23	Q	1485	
24	R	536	
25	S	166	
26	T	514	
27	TF	837	
28	W	579	

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Mol	Chain	Length	Quality of chain
29	YB	396	
30	Z	166	
31	a	126	
32	b	240	
33	c	119	
34	d	118	
35	e	92	
36	f	86	
37	g	76	
38	q	504	
38	r	504	
38	s	504	
38	t	504	
39	y	301	

2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 97335 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	41	Total	C	N	O	P	0	0
			863	386	142	294	41		

- Molecule 2 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	137	Total	C	N	O	S	0	0
			1159	732	198	226	3		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	92	Total	C	N	O	P	0	0
			1936	867	322	655	92		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1979	Total	C	N	O	S	0	0
			16460	10611	2881	2898	70		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	19	Total	C	N	O	0	0
			92	54	19	19		

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	908	Total	C	N	O	S	0	0
			7184	4598	1194	1357	35		

- Molecule 8 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	D	51	Total	C	N	O	0	0
			255	153	51	51		

- Molecule 9 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	DX	650	Total	C	N	O	0	0
			3294	1994	650	650		

- Molecule 10 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	299	Total	C	N	O	S	0	0
			2341	1470	411	447	13		

- Molecule 11 is a protein called Intron Large complex component GCFC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	GC	514	Total	C	N	O	0	0
			2590	1561	514	515		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	717	Total	C	N	O	S	0	0
			5972	3799	1064	1081	28		

- Molecule 13 is a RNA chain called Intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	IN	61	Total	C	N	O	P	0	0
			797	338	29	370	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	590	Total	C	N	O	S	0	0
			3699	2295	705	694	5		

- Molecule 15 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	209	Total	C	N	O	S	0	0
			1711	1068	305	329	9		

- Molecule 16 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	565	Total	C	N	O	S	0	0
			4346	2707	786	834	19		

- Molecule 17 is a protein called CWF19-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L1	268	Total	C	N	O		0	0
			1347	811	268	268			

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L2	366	Total	C	N	O	S	0	0
			3019	1911	522	563	23		

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	166	Total	C	N	O		0	0
			835	503	166	166			

- Molecule 20 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 21 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	288	Total	C	N	O	S	0	0
			2328	1463	412	433	20		

- Molecule 22 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	106	Total	C	N	O	S	0	0
			831	513	159	157	2		

- Molecule 23 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	1369	Total	C	N	O	S	0	0
			11219	7203	1933	2028	55		

- Molecule 24 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	R	303	Total	C	N	O	P	S	0	0
			2406	1510	432	449	2	13		

- Molecule 25 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 26 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	360	Total	C	N	O	S	0	0
			2854	1800	521	523	10		

- Molecule 27 is a protein called Tuftelin-interacting protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	TF	570	Total	C	N	O	0	0
			2878	1737	570	571		

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	173	Total	C	N	O	S	0	0
			1377	867	233	273	4		

- Molecule 29 is a protein called Probable splicing factor YJU2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	YB	147	Total	C	N	O	S	0	0
			1207	765	215	217	10		

- Molecule 30 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	37	Total	C	N	O	0	0
			186	112	37	37		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	83	Total	C	N	O	S	0	0
			651	408	114	122	7		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	95	Total	C	N	O	S	0	0
			725	455	136	127	7		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	81	Total	C	N	O	S	0	0
			641	409	112	116	4		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	97	Total	C	N	O	S	0	0
			784	490	148	141	5		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	79	Total	C	N	O	S	0	0
			653	412	116	120	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	76	Total	C	N	O	S	0	0
			593	383	97	107	6		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	137	Total	C	N	O	S	0	0
			1080	677	194	204	5		
38	r	137	Total	C	N	O	S	0	0
			1080	677	194	204	5		
38	s	137	Total	C	N	O	S	0	0
			1080	677	194	204	5		
38	t	137	Total	C	N	O	S	0	0
			1080	677	194	204	5		

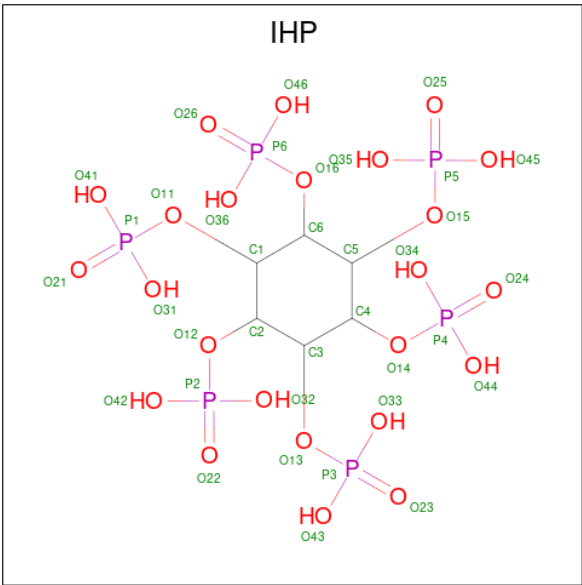
- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	80	Total	C	N	O	S	0	0
			630	401	103	124	2		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

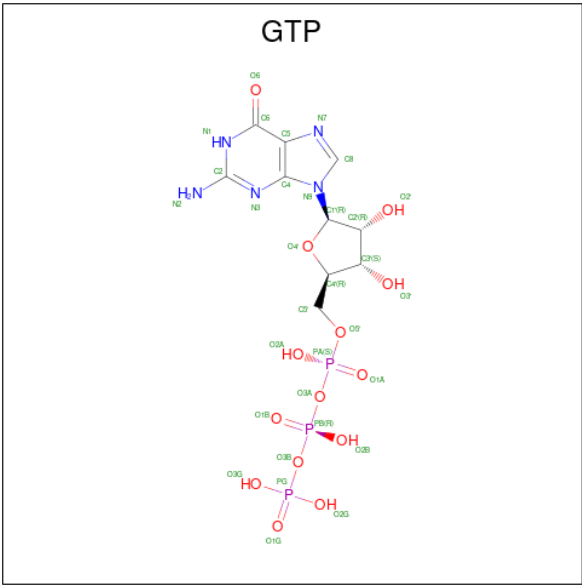
Mol	Chain	Residues	Atoms		AltConf
40	6	6	Total	Mg	0
			6	6	
40	C	1	Total	Mg	0
			1	1	

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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	

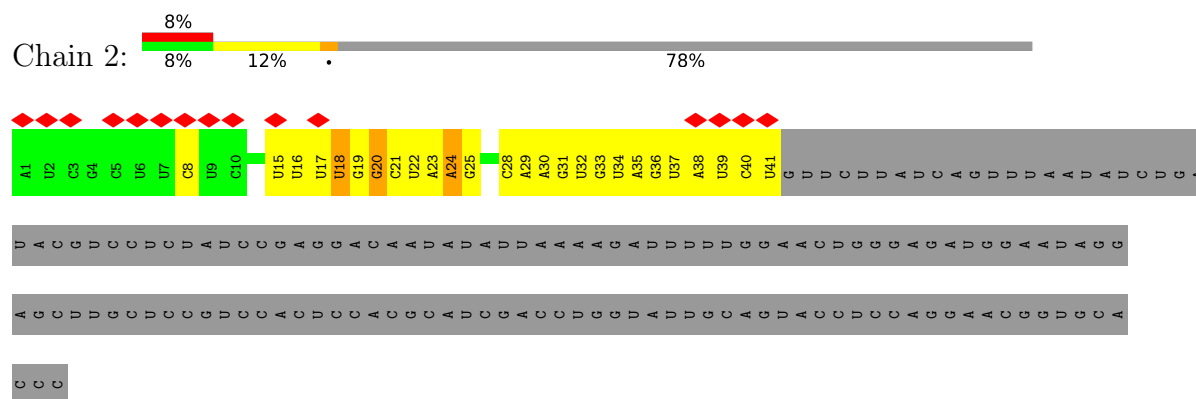
- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

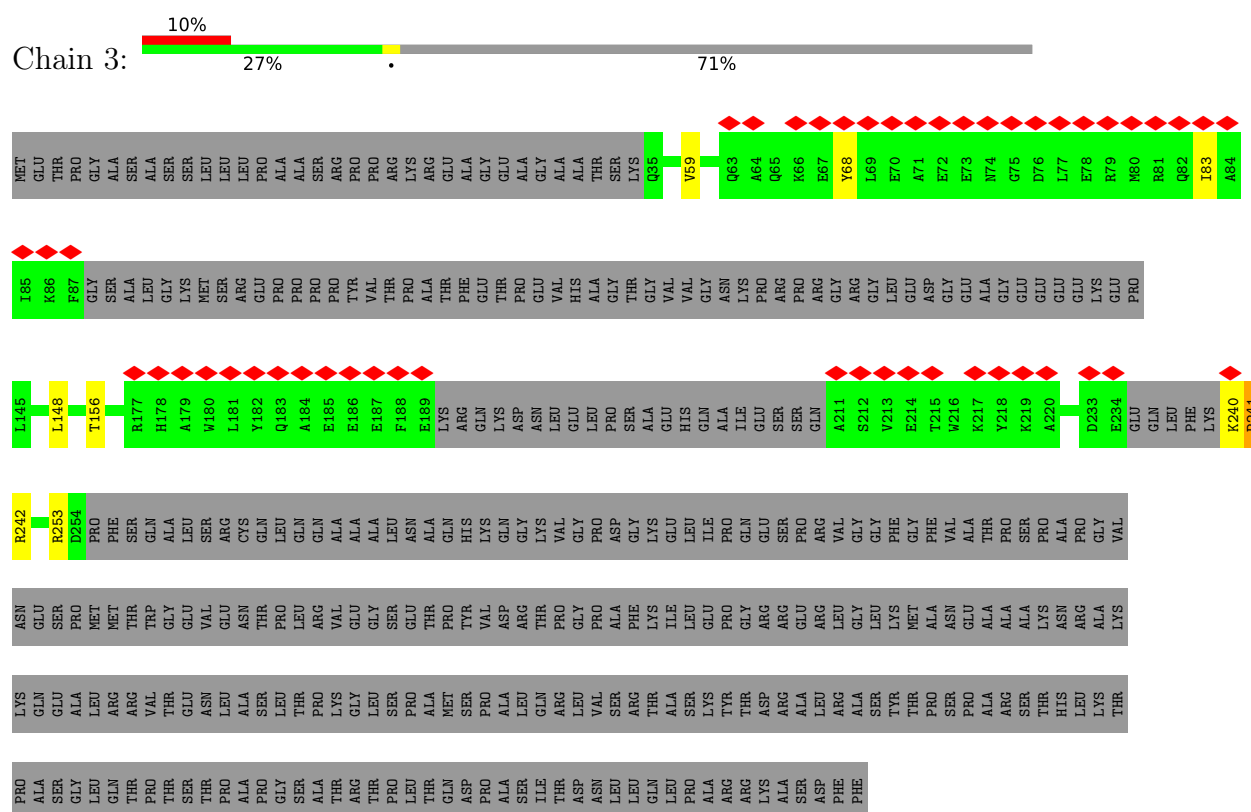
3 Residue-property plots [i](#)

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.

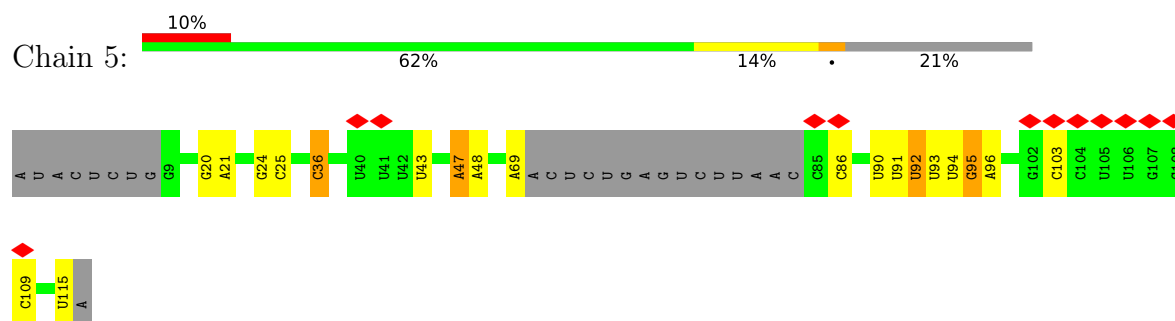
• Molecule 1: U2 snRNA



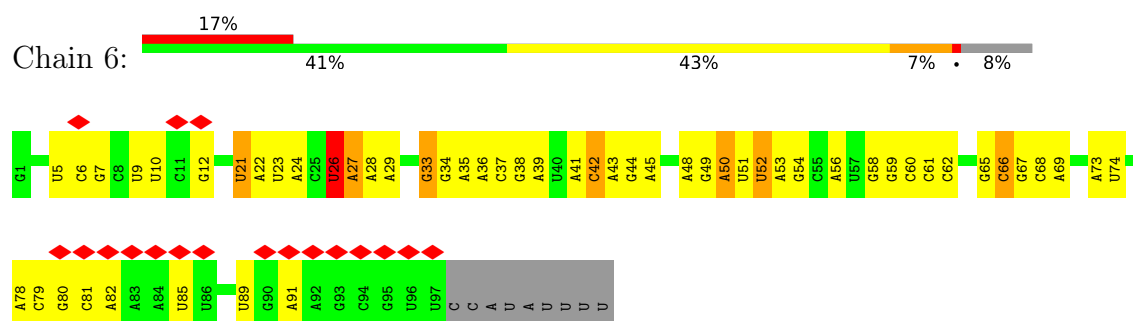
• Molecule 2: Splicing factor ESS-2 homolog



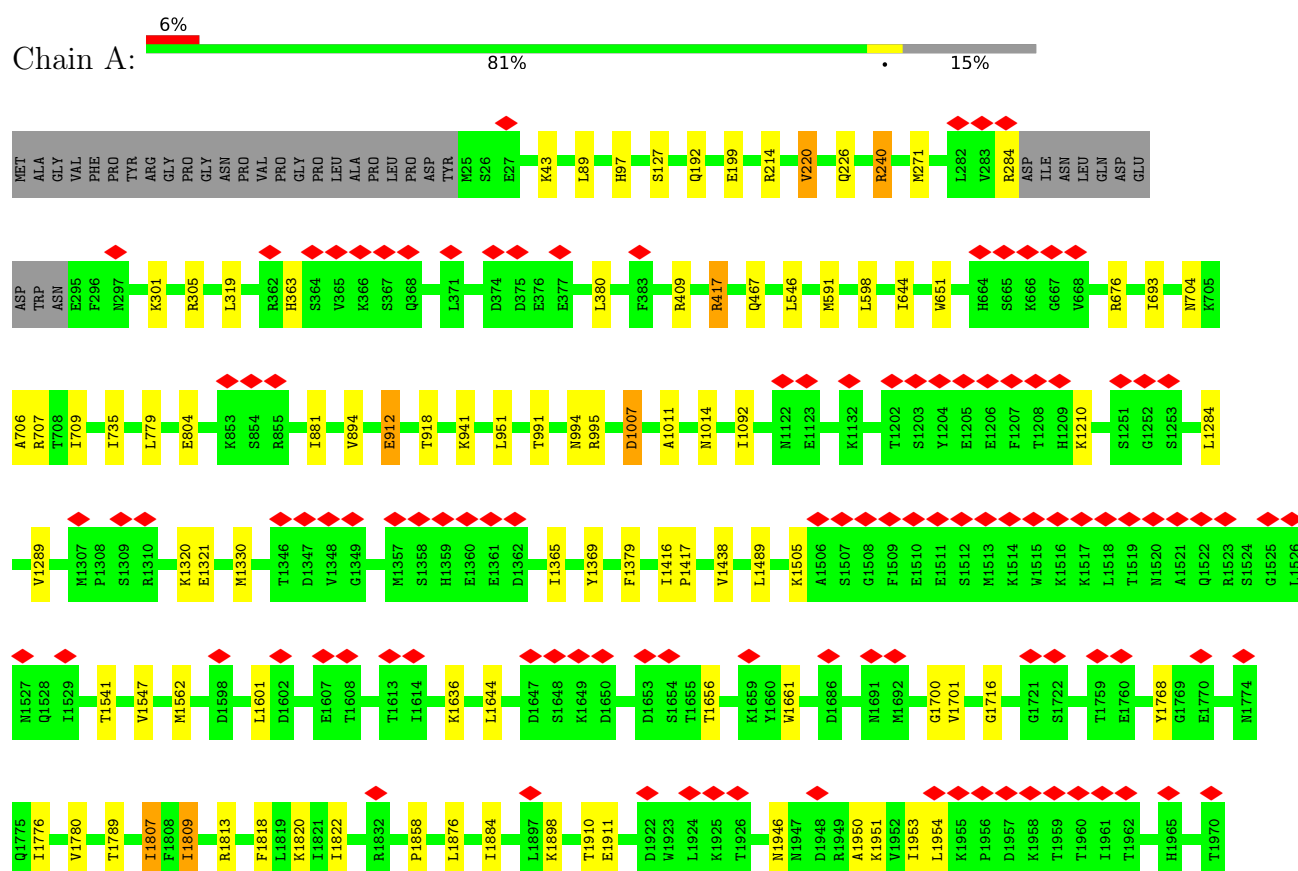
- Molecule 3: U5 snRNA



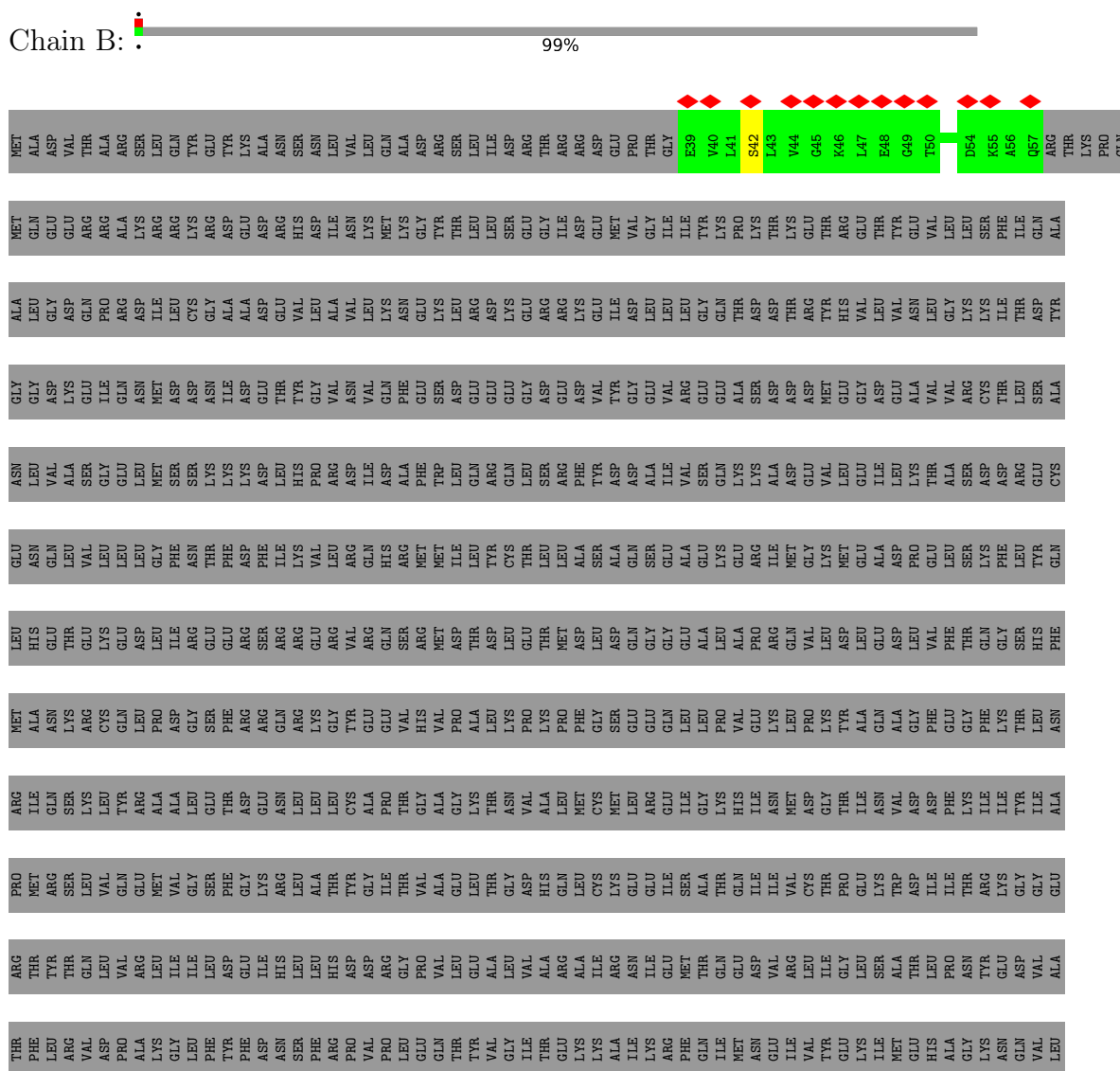
- Molecule 4: U6 snRNA



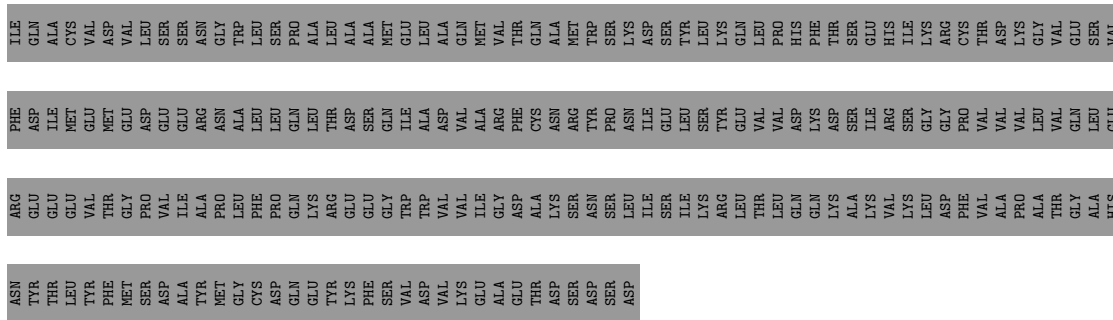
- Molecule 5: Pre-mRNA-processing-splicing factor 8



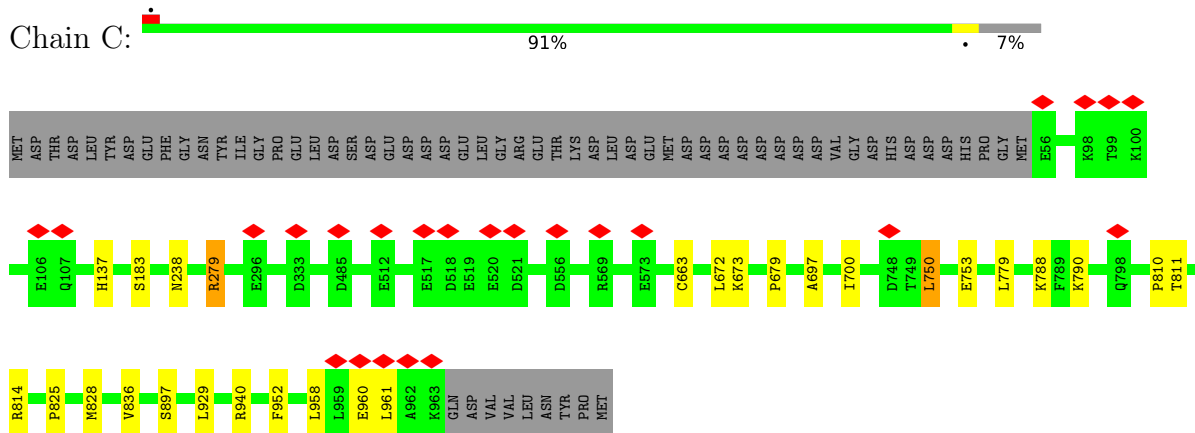
- Molecule 6: U5 small nuclear ribonucleoprotein 200 kDa helicase



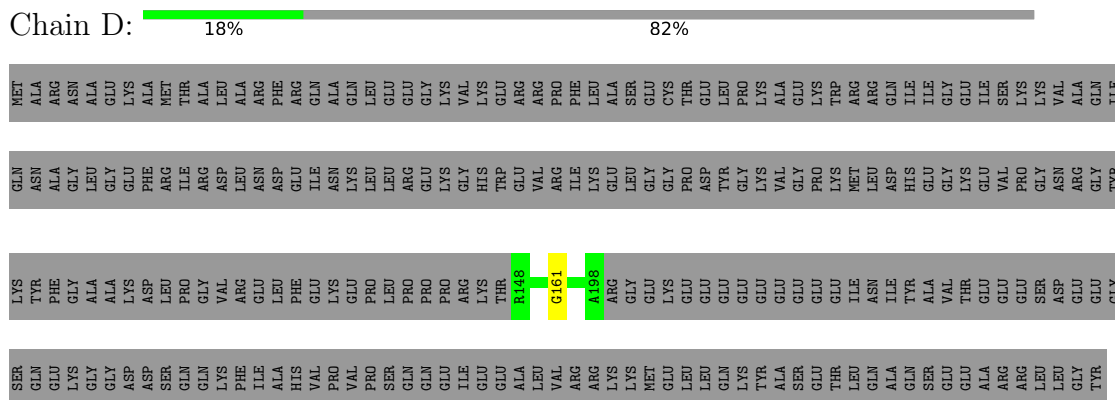




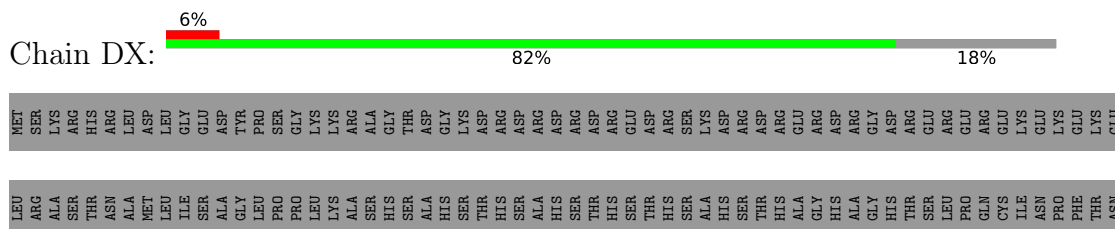
- Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component

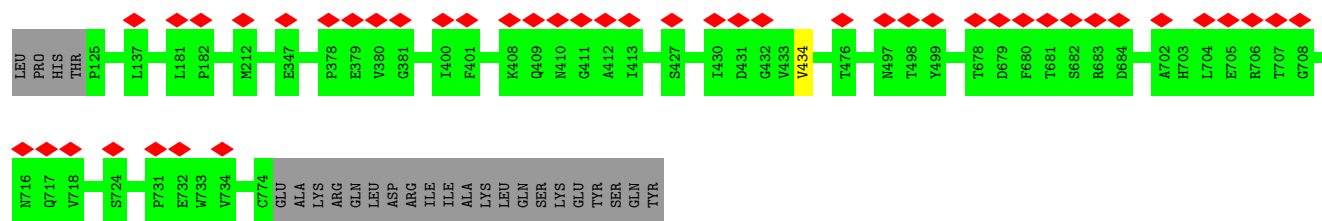


- Molecule 8: Pre-mRNA-splicing factor ISY1 homolog



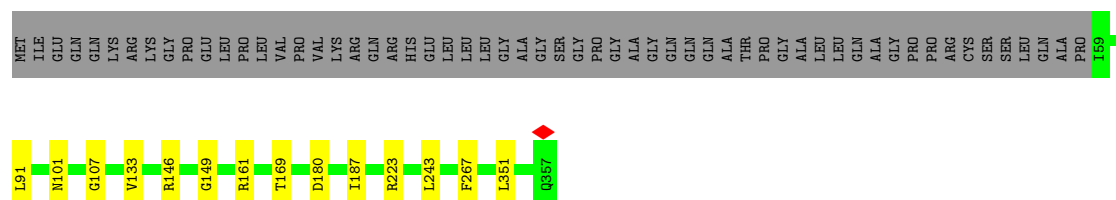
- Molecule 9: ATP-dependent RNA helicase DHX15





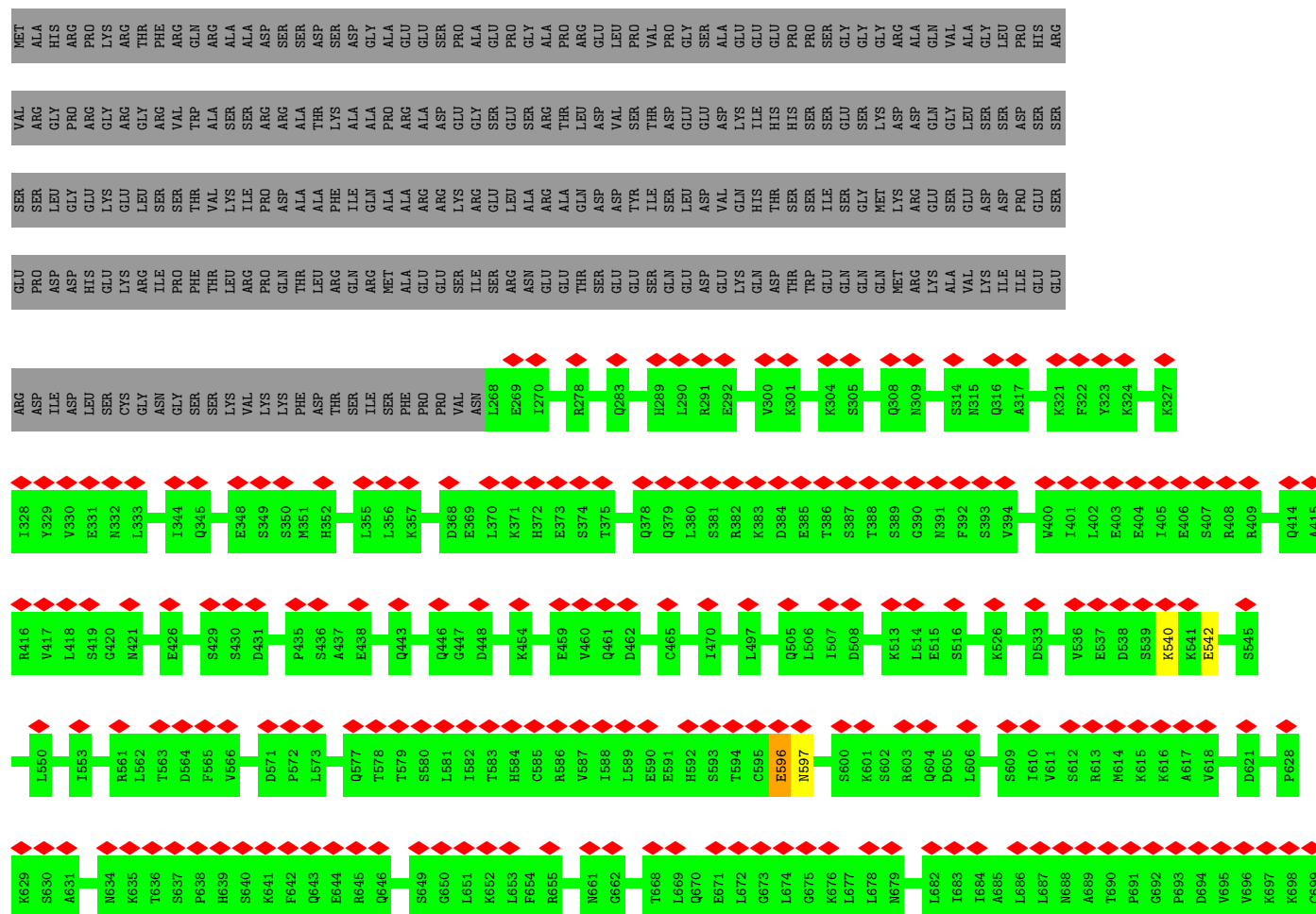
- Molecule 10: U5 small nuclear ribonucleoprotein 40 kDa protein

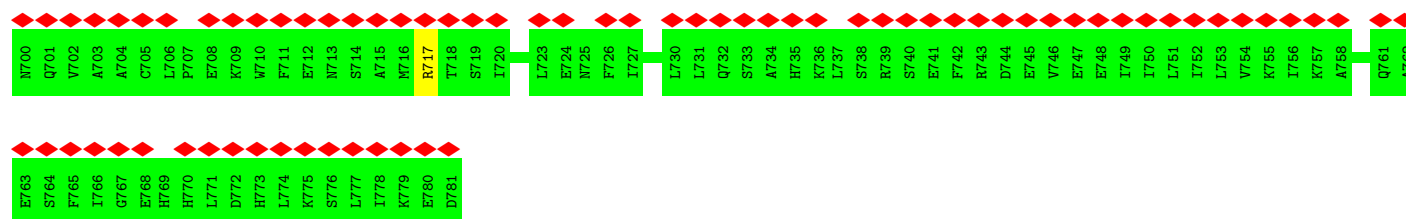
Chain E: 80% 16%



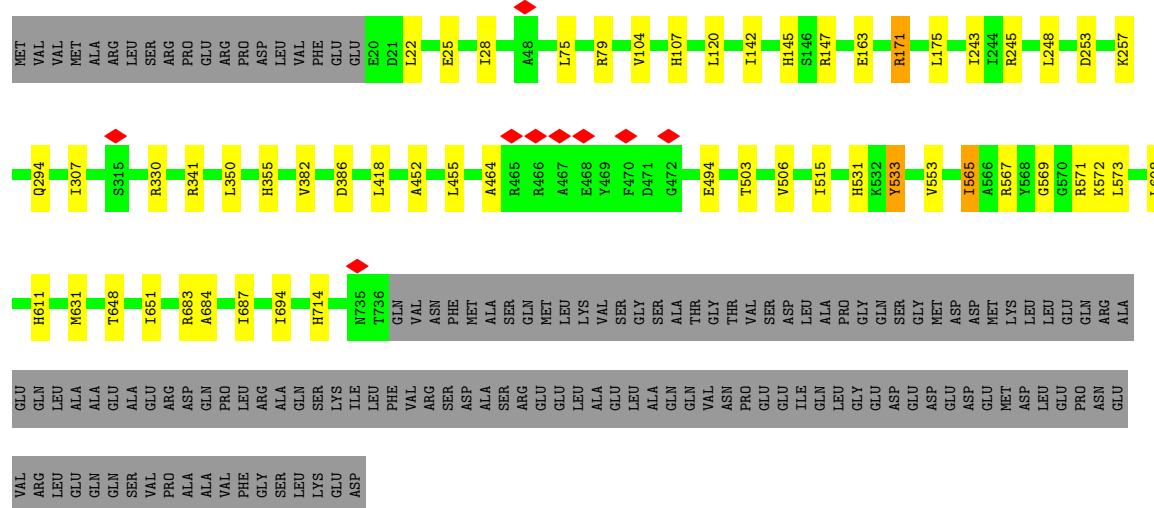
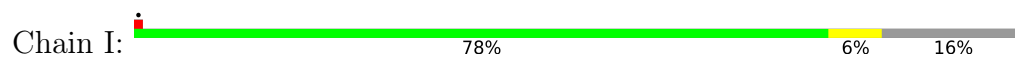
- Molecule 11: Intron Large complex component GCFC2

Chain GC: 36% 65% 34%





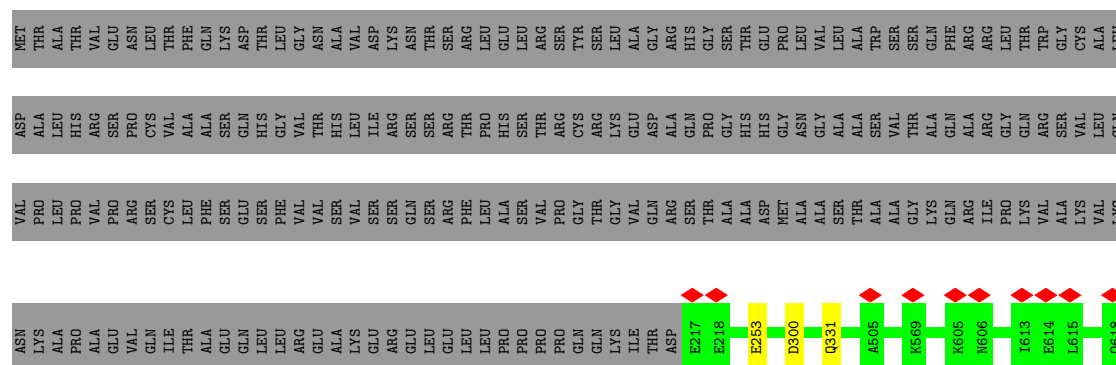
• Molecule 12: Pre-mRNA-splicing factor SYF1

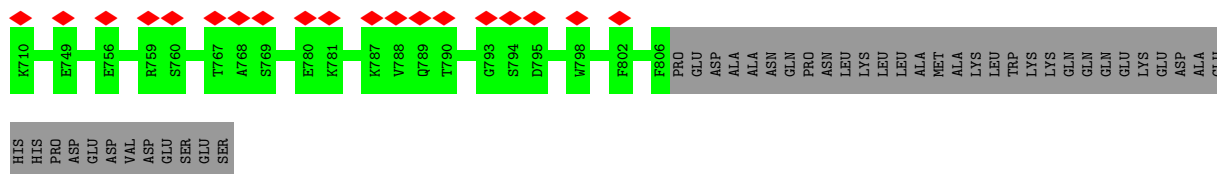


• Molecule 13: Intron



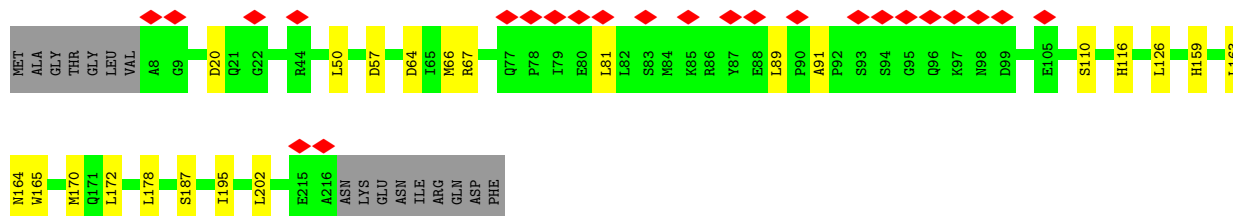
• Molecule 14: Crooked neck-like protein 1





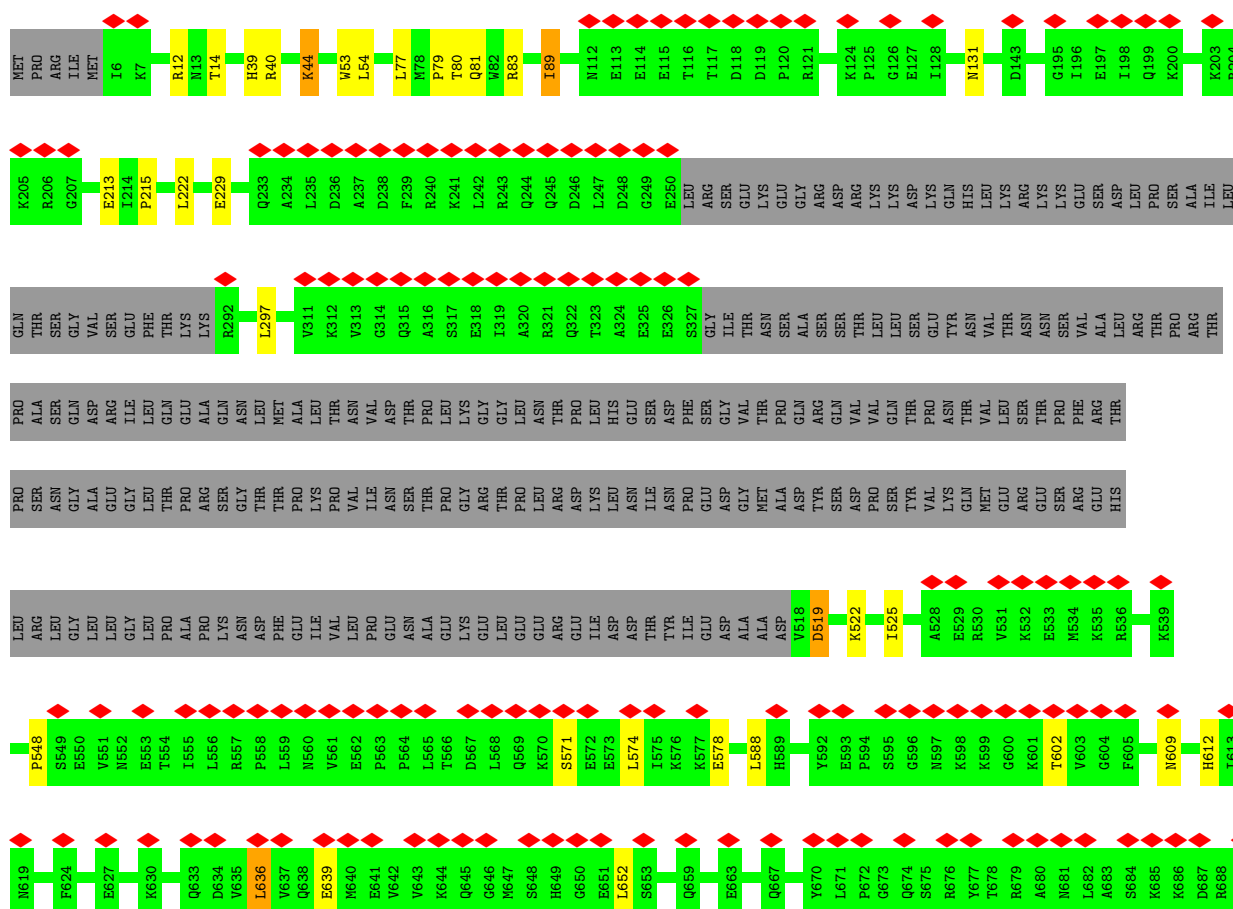
• Molecule 15: Pre-mRNA-splicing factor SPF27

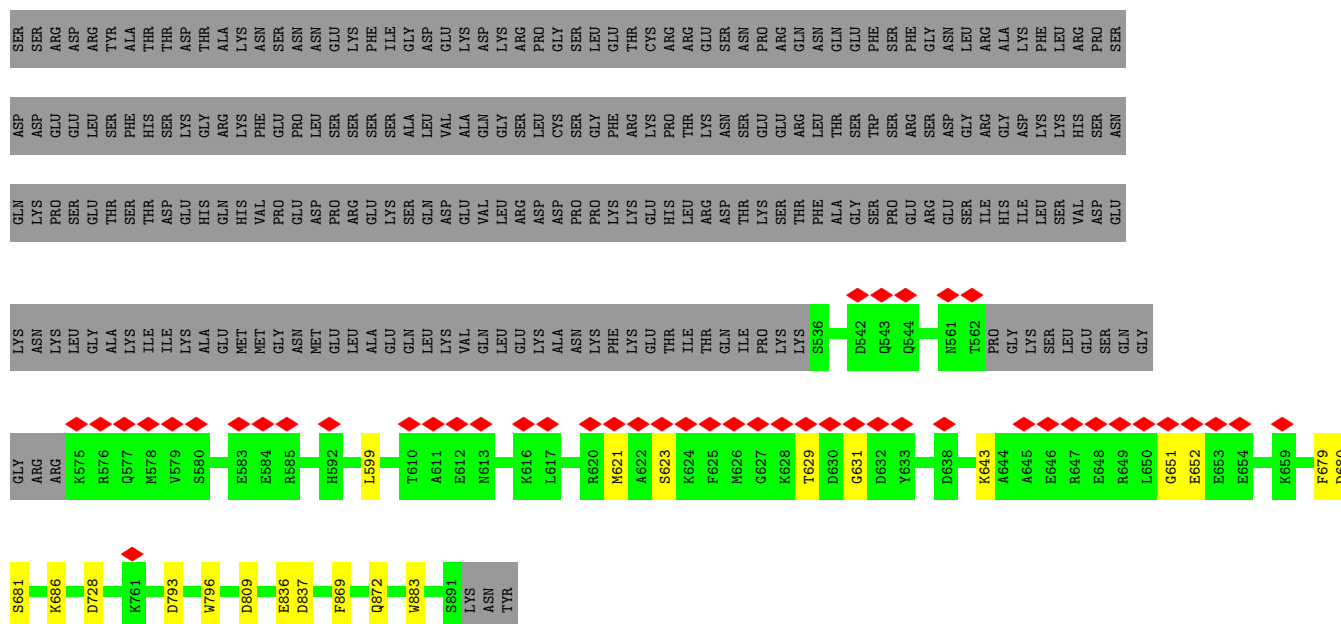
Chain K: 11% 83% 10% 7%



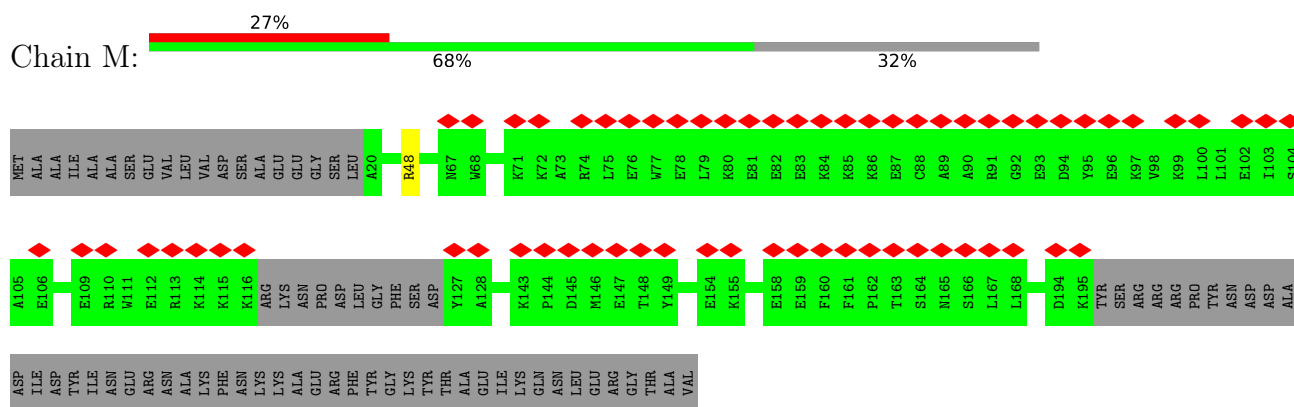
• Molecule 16: Cell division cycle 5-like protein

Chain L: 19% 65% 5% 30%

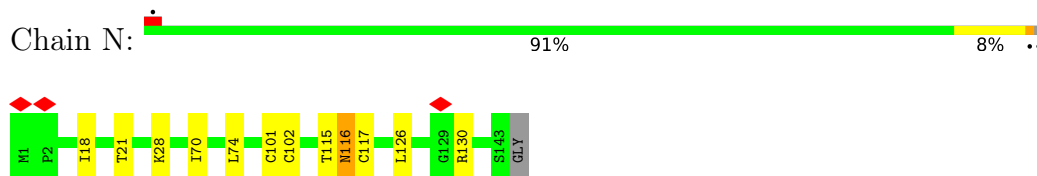




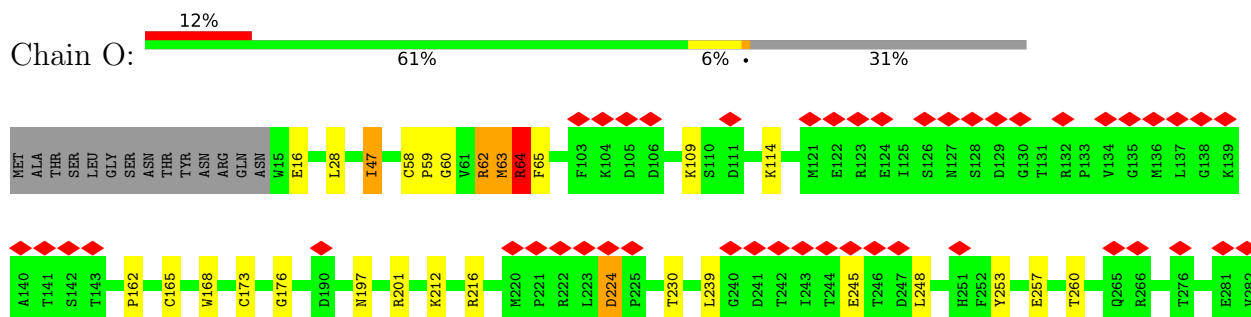
• Molecule 19: Pre-mRNA-splicing factor SYF2



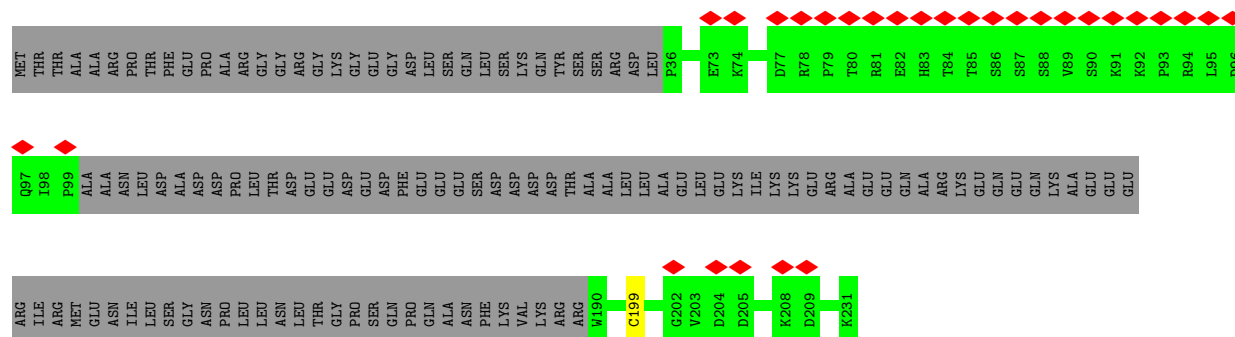
• Molecule 20: Protein BUD31 homolog



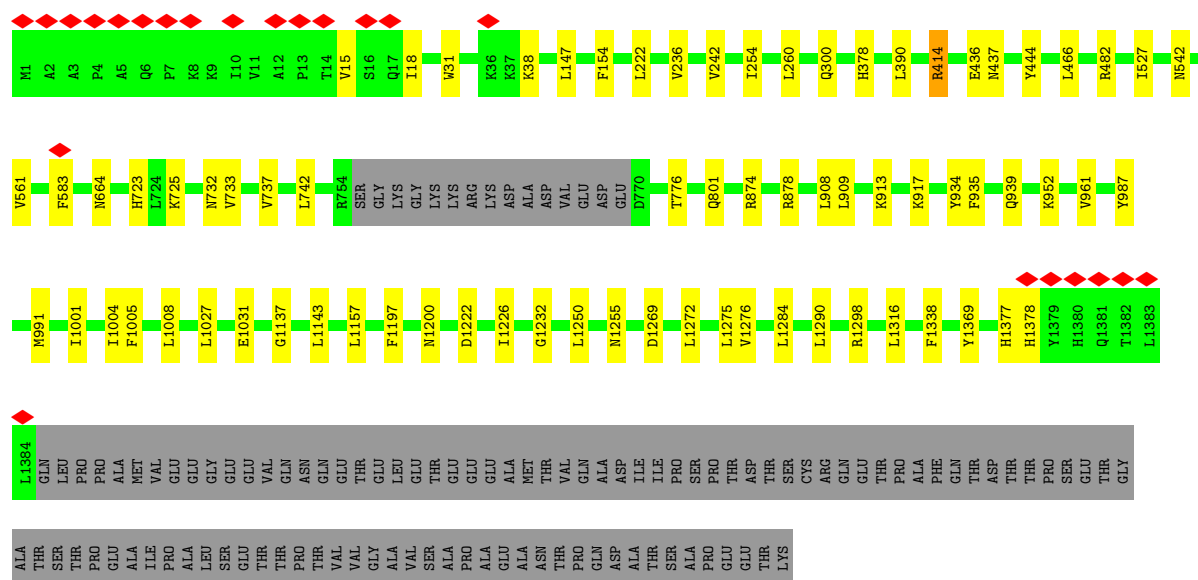
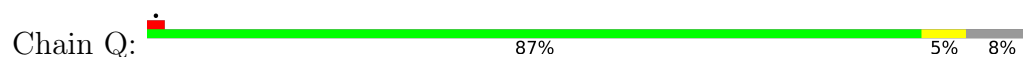
• Molecule 21: Pre-mRNA-splicing factor RBM22



- Molecule 22: Spliceosome-associated protein CWC15 homolog

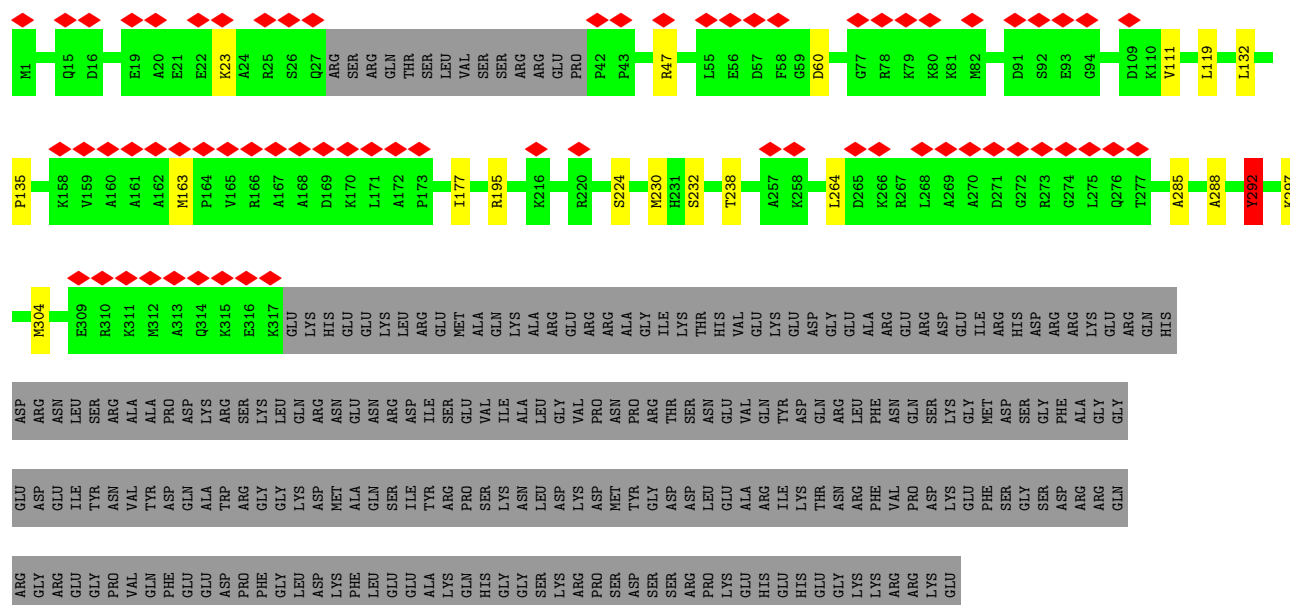


- Molecule 23: Intron-binding protein aquarius

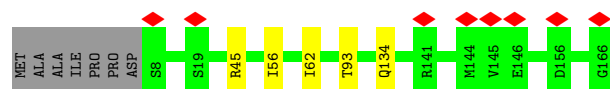


- Molecule 24: SNW domain-containing protein 1

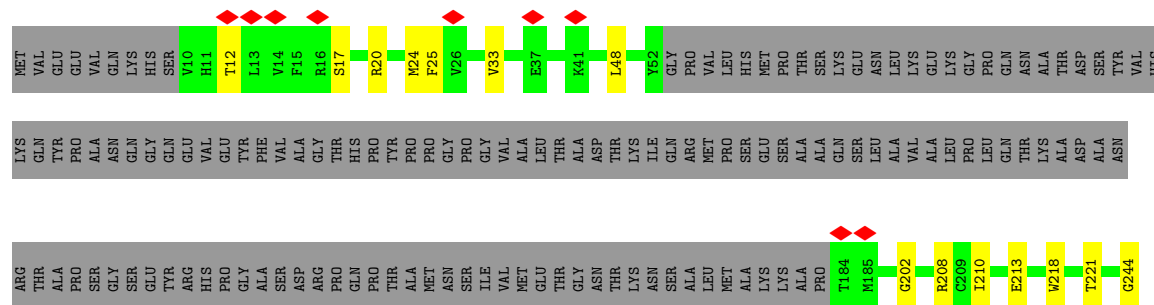




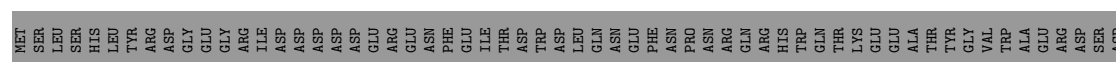
• Molecule 25: Peptidyl-prolyl cis-trans isomerase-like 1



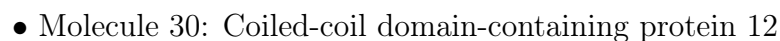
• Molecule 26: Pleiotropic regulator 1

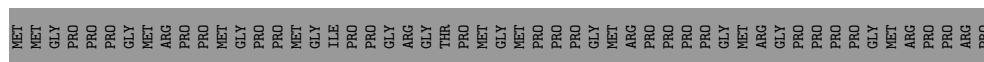


• Molecule 27: Tuftelin-interacting protein 11

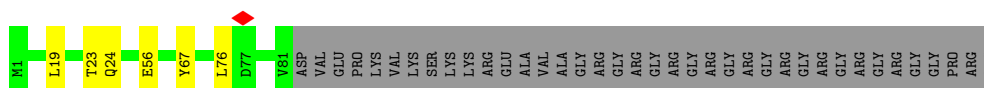


Chain YB:

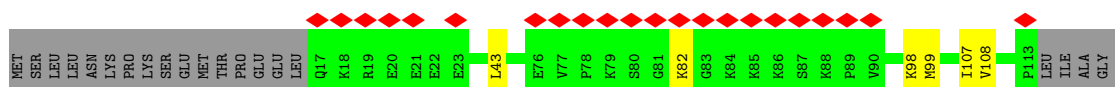




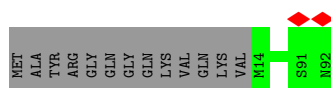
Chain c: 63% 5% 32%



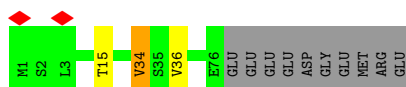
Chain d:



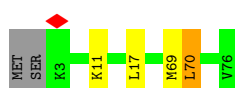
Chain e: 86% 14%



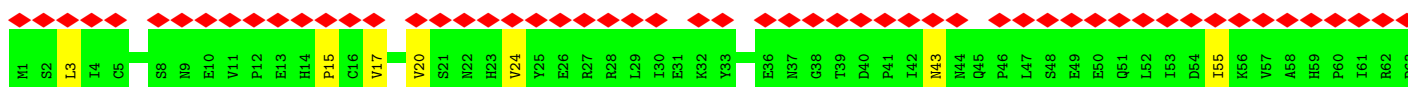
Chain f: 85% 12%

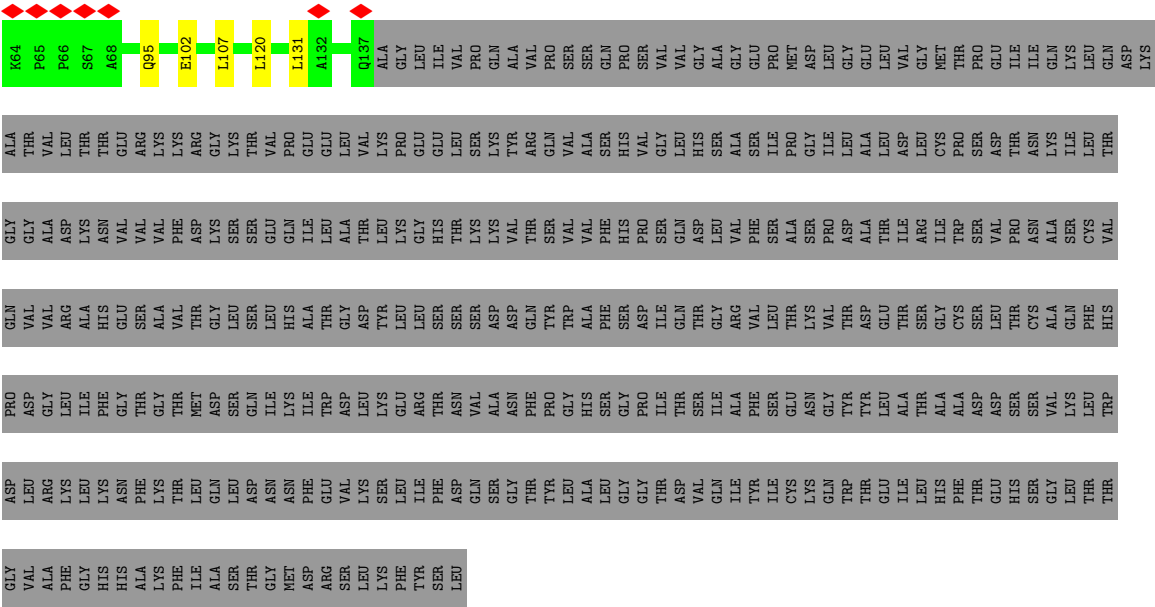


Chain g: 92% . . .

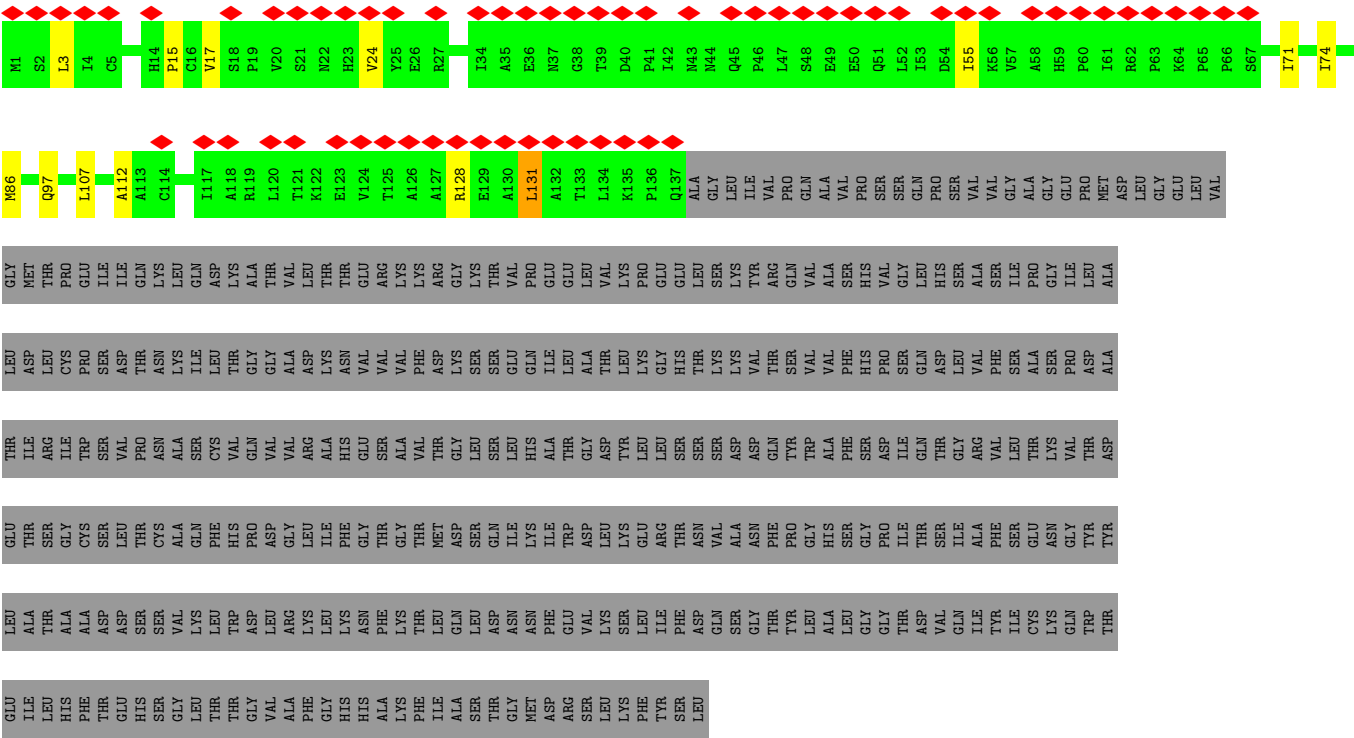


Chain q: 12% 25% 73%



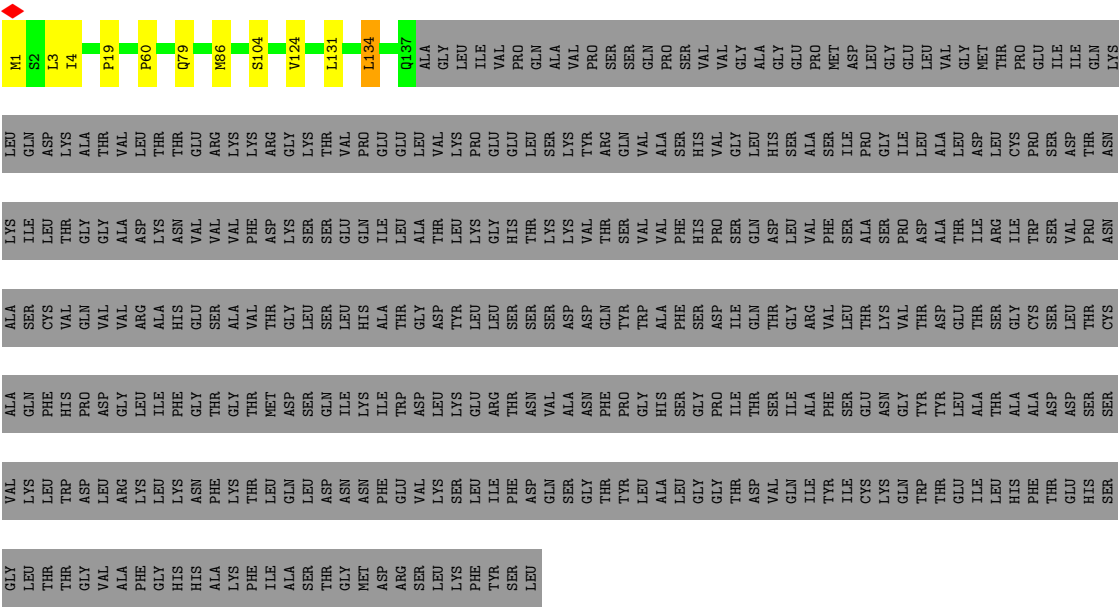


• Molecule 38: Pre-mRNA-processing factor 19

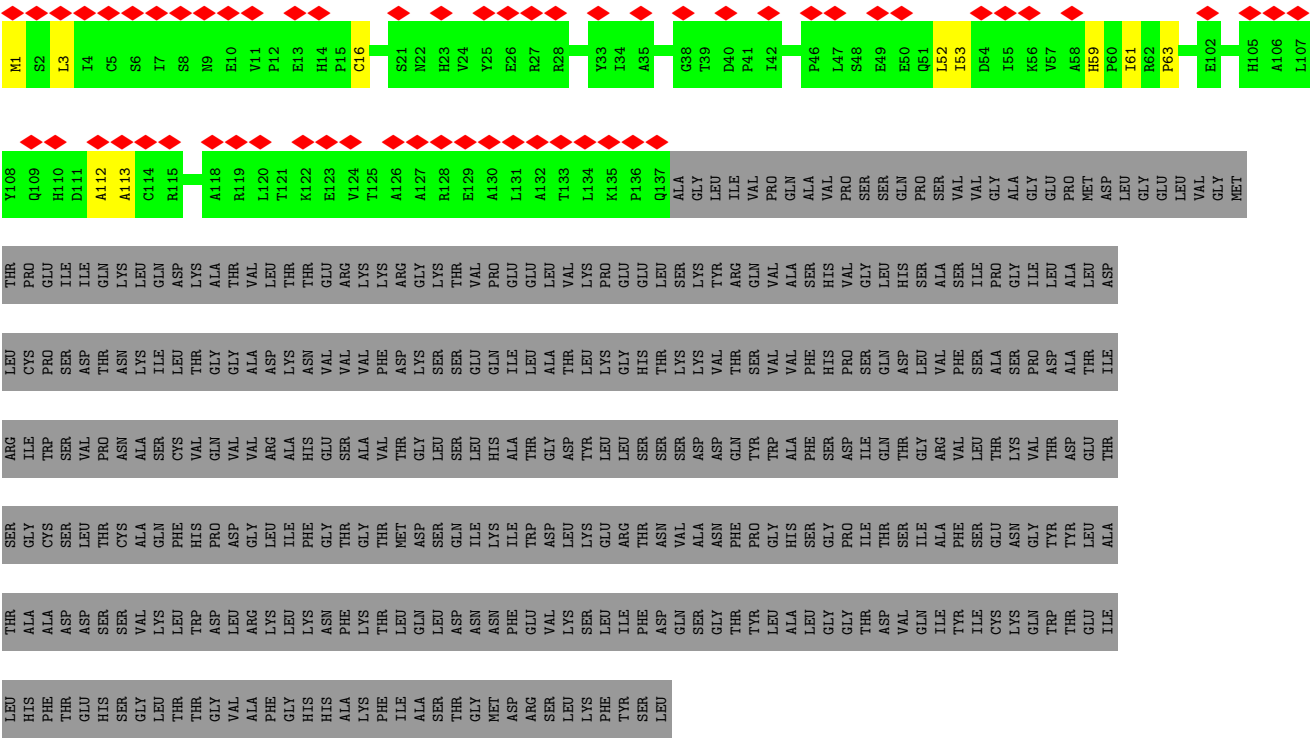


• Molecule 38: Pre-mRNA-processing factor 19



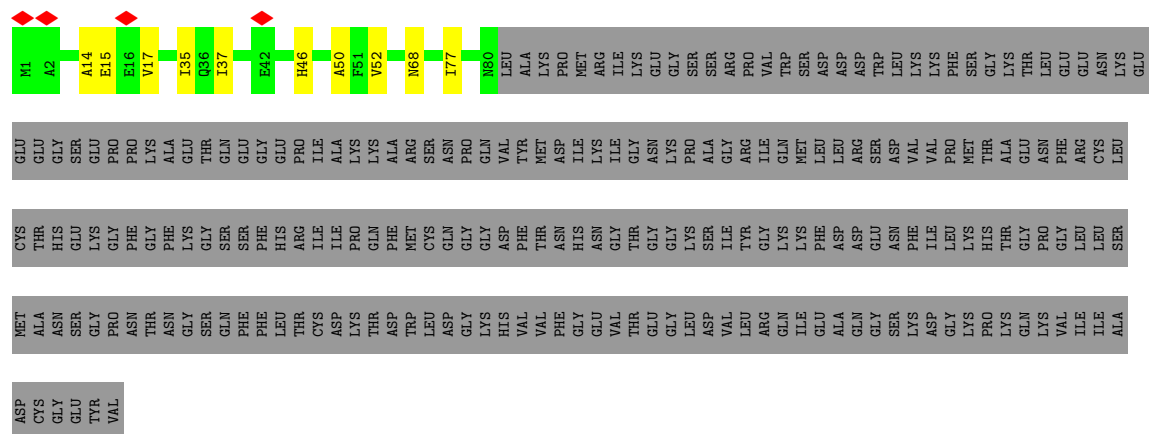


• Molecule 38: Pre-mRNA-processing factor 19



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	503031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	18.587	Depositor
Minimum map value	0.000	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	513.54236, 513.54236, 513.54236	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1463, 1.1463, 1.1463	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, MG, IHP, GTP, SEP

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	0.84	2/961 (0.2%)	1.08	5/1493 (0.3%)
2	3	0.33	0/1180	0.63	0/1584
3	5	0.63	0/2157	0.83	6/3351 (0.2%)
4	6	0.94	3/2323 (0.1%)	1.03	11/3619 (0.3%)
5	A	0.49	2/16909 (0.0%)	0.79	3/22925 (0.0%)
6	B	0.16	0/91	0.57	0/124
7	C	0.47	0/7346	0.73	1/9980 (0.0%)
8	D	0.32	0/255	0.81	0/355
9	DX	0.20	0/3330	0.58	1/4671 (0.0%)
10	E	0.45	1/2394 (0.0%)	0.70	0/3243
11	GC	0.27	0/2604	0.73	2/3648 (0.1%)
12	I	1.13	7/6116 (0.1%)	0.78	4/8267 (0.0%)
13	IN	0.65	0/867	1.33	9/1331 (0.7%)
14	J	0.34	0/3757	0.68	0/5172
15	K	0.58	0/1744	0.72	0/2357
16	L	1.51	2/4419 (0.0%)	0.88	6/5961 (0.1%)
17	L1	0.17	0/1360	0.50	0/1901
18	L2	0.46	0/3086	0.77	0/4143
19	M	0.21	0/837	0.60	0/1170
20	N	0.61	0/1210	0.93	1/1622 (0.1%)
21	O	0.48	0/2378	0.88	3/3211 (0.1%)
22	P	0.53	0/845	0.90	0/1132
23	Q	0.57	0/11495	0.75	0/15578
24	R	0.40	0/2433	0.83	2/3272 (0.1%)
25	S	0.25	0/1268	0.57	0/1714
26	T	0.57	0/2927	0.80	0/3980
27	TF	0.40	1/2900 (0.0%)	0.87	1/4056 (0.0%)
28	W	0.38	0/1407	0.73	0/1898
29	YB	0.40	0/1230	0.71	0/1653
30	Z	0.16	0/186	0.61	0/258
31	a	1.06	0/659	1.11	0/888
32	b	0.85	0/734	0.98	2/977 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.79	0/649	0.95	0/877
34	d	0.64	0/794	0.85	0/1061
35	e	0.75	0/661	0.85	0/886
36	f	0.82	0/605	0.89	0/817
37	g	0.92	0/584	1.07	1/779 (0.1%)
38	q	0.50	0/1102	0.72	1/1502 (0.1%)
38	r	0.30	0/1102	0.65	0/1502
38	s	0.51	0/1102	0.72	0/1502
38	t	0.34	0/1102	0.69	2/1502 (0.1%)
39	y	0.43	0/641	0.70	0/867
All	All	0.65	18/99750 (0.0%)	0.79	61/136829 (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
4	6	0	1
5	A	0	2
7	C	0	1
10	E	0	1
12	I	0	3
18	L2	0	1
21	O	0	1
23	Q	0	3
24	R	0	2
26	T	0	3
28	W	0	1
29	YB	0	1
36	f	0	1
All	All	0	21

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	519	ASP	CB-CG	88.33	3.72	1.52
12	I	533	TYR	CD1-CE1	43.19	2.68	1.38
12	I	533	TYR	CD2-CE2	40.02	2.58	1.38
12	I	533	TYR	CE2-CZ	28.84	2.07	1.38
12	I	533	TYR	CE1-CZ	27.74	2.04	1.38
12	I	533	TYR	CG-CD2	25.19	1.92	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	533	TYR	CG-CD1	23.54	1.88	1.39
4	6	24	A	P-OP1	-6.54	1.35	1.49
5	A	1007	ASP	CB-CG	-6.18	1.36	1.52
16	L	83	ARG	CG-CD	-6.08	1.34	1.52
10	E	267	PHE	CB-CG	-6.05	1.36	1.50
12	I	533	TYR	CB-CG	-5.63	1.39	1.51
4	6	23	U	P-OP1	-5.56	1.37	1.49
27	TF	496	TRP	C-N	-5.53	1.22	1.33
5	A	1014	ASN	CG-OD1	-5.50	1.13	1.23
1	2	23	A	P-OP1	-5.30	1.38	1.49
1	2	21	C	P-OP1	-5.27	1.38	1.49
4	6	22	A	P-OP1	-5.01	1.39	1.49

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	519	ASP	CA-CB-CG	11.54	124.14	112.60
5	A	941	LYS	N-CA-C	9.14	130.01	109.81
1	2	22	U	P-O3'-C3'	8.95	133.62	120.20
16	L	519	ASP	OD1-CG-OD2	-7.73	104.35	122.90
1	2	20	G	OP1-P-O3'	7.60	130.79	108.00
12	I	571	ARG	CA-C-N	7.33	135.54	121.54
12	I	571	ARG	C-N-CA	7.33	135.54	121.54
4	6	50	A	C2'-C3'-O3'	7.10	124.35	113.70
4	6	22	A	C4'-C3'-O3'	-6.71	99.33	109.40
1	2	22	U	OP1-P-O3'	-6.71	87.88	108.00
13	IN	146	U	O5'-C5'-C4'	6.62	121.43	111.50
3	5	90	U	N1-C1'-C2'	6.32	123.48	114.00
21	O	63	MET	CB-CG-SD	6.31	131.62	112.70
13	IN	145	U	P-O3'-C3'	6.29	129.63	120.20
3	5	92	U	O4'-C1'-N1	6.23	117.54	108.20
24	R	292	TYR	CA-CB-CG	6.22	125.09	113.90
1	2	22	U	OP2-P-O3'	6.13	126.40	108.00
4	6	66	C	N1-C1'-C2'	6.11	121.16	112.00
16	L	787	ARG	CB-CG-CD	-6.09	97.30	111.30
13	IN	3	A	C4'-C3'-C2'	-6.01	96.59	102.60
13	IN	146	U	O5'-P-OP2	6.00	126.01	108.00
13	IN	145	U	C2'-C3'-O3'	5.85	122.47	113.70
5	A	192	GLN	N-CA-C	5.82	118.91	110.42
3	5	91	U	N1-C1'-C2'	5.80	122.69	114.00
4	6	52	U	P-O3'-C3'	5.79	128.89	120.20
13	IN	151	U	C2'-C3'-O3'	-5.74	105.09	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	533	TYR	CD1-CG-CD2	5.73	126.69	118.10
3	5	95	G	C2'-C3'-O3'	5.72	118.08	109.50
9	DX	434	VAL	N-CA-C	-5.71	107.93	113.53
4	6	22	A	OP1-P-O3'	5.70	125.09	108.00
13	IN	144	A	C2'-C3'-O3'	5.66	117.99	109.50
4	6	21	U	C4'-C3'-O3'	-5.64	100.94	109.40
32	b	13	ILE	CA-C-N	5.56	132.17	121.54
32	b	13	ILE	C-N-CA	5.56	132.17	121.54
3	5	95	G	P-O3'-C3'	5.53	128.50	120.20
1	2	18	U	C2'-C3'-O3'	-5.52	101.22	109.50
13	IN	151	U	C5'-C4'-O4'	-5.51	101.54	109.80
24	R	292	TYR	N-CA-CB	-5.49	102.03	110.16
21	O	62	ARG	CA-CB-CG	5.47	125.03	114.10
38	q	102	GLU	CA-CB-CG	-5.46	103.19	114.10
13	IN	146	U	P-O5'-C5'	5.43	129.05	120.90
21	O	64	ARG	CA-CB-CG	5.43	124.95	114.10
11	GC	596	GLU	CA-C-N	5.41	131.87	121.54
11	GC	596	GLU	C-N-CA	5.41	131.87	121.54
12	I	171	ARG	CB-CG-CD	-5.33	99.05	111.30
27	TF	777	ILE	N-CA-C	5.31	119.53	111.89
5	A	1417	PRO	N-CA-C	-5.24	101.68	112.47
4	6	33	G	C2'-C3'-O3'	5.23	121.54	113.70
16	L	44	LYS	CD-CE-NZ	5.21	128.57	111.90
16	L	79	PRO	CA-C-N	5.18	132.97	124.31
16	L	79	PRO	C-N-CA	5.18	132.97	124.31
4	6	26	U	C2'-C3'-O3'	5.15	121.43	113.70
37	g	70	LEU	CA-CB-CG	5.10	134.16	116.30
4	6	42	C	P-O3'-C3'	5.06	127.80	120.20
7	C	750	LEU	CB-CG-CD2	-5.06	95.52	110.70
20	N	116	ASN	N-CA-CB	5.05	117.12	110.25
3	5	92	U	P-O3'-C3'	5.04	127.75	120.20
4	6	52	U	C2'-C3'-O3'	-5.04	101.95	109.50
4	6	33	G	P-O3'-C3'	5.01	127.71	120.20
38	t	61	ILE	CA-C-N	5.01	134.02	121.80
38	t	61	ILE	C-N-CA	5.01	134.02	121.80

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	6	26	U	Sidechain
5	A	409	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	A	995	ARG	Sidechain
7	C	279	ARG	Sidechain
10	E	146	ARG	Sidechain
12	I	531	HIS	Peptide
12	I	567	ARG	Sidechain
12	I	714	HIS	Peptide
18	L2	623	SER	Peptide
21	O	224	ASP	Peptide
23	Q	414	ARG	Sidechain
23	Q	874	ARG	Sidechain
23	Q	878	ARG	Sidechain
24	R	195	ARG	Sidechain
24	R	292	TYR	Sidechain
26	T	208	ARG	Sidechain
26	T	25	PHE	Peptide
26	T	308	ARG	Sidechain
28	W	129	ARG	Sidechain
29	YB	187	ARG	Sidechain
36	f	34	VAL	Peptide

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	863	0	435	3	0
2	3	1159	0	1111	6	0
3	5	1936	0	981	5	0
4	6	2075	0	1036	6	0
5	A	16460	0	16447	41	0
6	B	92	0	43	1	0
7	C	7184	0	7205	20	0
8	D	255	0	126	1	0
9	DX	3294	0	1638	0	0
10	E	2341	0	2275	5	0
11	GC	2590	0	1164	0	0
12	I	5972	0	5876	44	0
13	IN	797	0	403	1	0
14	J	3699	0	2575	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	1711	0	1665	17	0
16	L	4346	0	4129	31	0
17	L1	1347	0	686	0	0
18	L2	3019	0	2945	7	0
19	M	835	0	404	1	0
20	N	1184	0	1189	6	0
21	O	2328	0	2317	15	0
22	P	831	0	752	1	0
23	Q	11219	0	11197	41	0
24	R	2406	0	2451	8	0
25	S	1236	0	1210	4	0
26	T	2854	0	2812	13	0
27	TF	2878	0	1363	12	0
28	W	1377	0	1327	8	0
29	YB	1207	0	1212	1	0
30	Z	186	0	89	0	0
31	a	651	0	669	0	0
32	b	725	0	747	3	0
33	c	641	0	689	3	0
34	d	784	0	826	4	0
35	e	653	0	668	0	0
36	f	593	0	607	1	0
37	g	577	0	603	1	0
38	q	1080	0	1096	6	0
38	r	1080	0	1096	10	0
38	s	1080	0	1096	10	0
38	t	1080	0	1096	8	0
39	y	630	0	610	6	0
40	6	6	0	0	0	0
40	C	1	0	0	0	0
41	A	36	0	6	0	0
42	C	32	0	12	0	0
43	L2	1	0	0	0	0
43	N	3	0	0	0	0
43	YB	1	0	0	0	0
All	All	97335	0	86884	271	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 (271) 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)
12:I:533:TYR:CG	12:I:533:TYR:CD1	1.88	1.61
12:I:533:TYR:CG	12:I:533:TYR:CD2	1.92	1.57
12:I:533:TYR:CZ	12:I:533:TYR:CE1	2.04	1.45
12:I:533:TYR:CZ	12:I:533:TYR:CE2	2.07	1.42
12:I:533:TYR:CD2	12:I:533:TYR:CE2	2.58	0.92
12:I:533:TYR:CD1	12:I:533:TYR:CE1	2.68	0.82
3:5:103:C:H41	34:d:82:LYS:HG3	1.60	0.66
27:TF:795:ARG:HA	27:TF:801:LEU:H	1.60	0.65
5:A:1289:VAL:HG21	6:B:42:SER:HA	1.78	0.65
23:Q:725:LYS:HG2	23:Q:733:VAL:HG21	1.79	0.65
12:I:533:TYR:CD1	16:L:519:ASP:CG	2.75	0.64
15:K:126:LEU:HD22	26:T:48:LEU:HD13	1.80	0.64
5:A:1330:MET:HE1	5:A:1369:TYR:HB2	1.82	0.62
12:I:533:TYR:CE1	16:L:519:ASP:CG	2.78	0.62
38:s:131:LEU:HA	38:s:134:LEU:HD12	1.82	0.62
12:I:245:ARG:HA	12:I:248:LEU:HD12	1.81	0.61
38:q:120:LEU:HD22	38:s:124:VAL:HG21	1.83	0.61
7:C:810:PRO:HB2	7:C:814:ARG:HH21	1.65	0.60
5:A:1809:ILE:HD12	5:A:1818:PHE:HB2	1.84	0.60
12:I:25:GLU:HA	12:I:28:ILE:HD12	1.82	0.60
12:I:533:TYR:CZ	16:L:519:ASP:CG	2.80	0.60
12:I:257:LYS:HG2	12:I:294:GLN:HE22	1.66	0.60
12:I:533:TYR:CG	16:L:519:ASP:CG	2.79	0.59
5:A:199:GLU:HG3	5:A:240:ARG:HH22	1.67	0.59
12:I:533:TYR:CD2	16:L:519:ASP:CG	2.81	0.59
7:C:673:LYS:HD2	27:TF:730:ASN:HA	1.85	0.59
23:Q:732:ASN:HB2	23:Q:776:THR:HA	1.85	0.58
15:K:50:LEU:HD11	38:s:104:SER:HB2	1.83	0.58
27:TF:541:PRO:HG3	27:TF:573:LYS:HA	1.84	0.58
34:d:107:ILE:HG22	34:d:108:VAL:HG23	1.86	0.58
26:T:398:TRP:CD1	26:T:405:PHE:HA	2.39	0.58
38:s:60:PRO:HD3	38:t:1:MET:HG3	1.86	0.57
12:I:533:TYR:CE2	16:L:519:ASP:CG	2.82	0.57
7:C:679:PRO:HG3	27:TF:782:GLU:HA	1.87	0.57
38:r:17:VAL:HG22	38:r:24:VAL:HG22	1.85	0.57
23:Q:15:VAL:HA	23:Q:18:ILE:HD12	1.86	0.57
21:O:287:SER:HB3	21:O:300:VAL:HG21	1.85	0.56
12:I:565:ILE:HA	12:I:569:GLY:HA3	1.87	0.56
38:q:3:LEU:HD13	38:q:24:VAL:HG11	1.87	0.56
12:I:104:VAL:HG13	23:Q:934:TYR:HB3	1.87	0.56
27:TF:401:ALA:HB1	27:TF:459:LEU:HA	1.87	0.55
5:A:1776:ILE:HB	5:A:1858:PRO:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:300:GLN:HE22	23:Q:437:ASN:HB3	1.72	0.55
10:E:91:LEU:HD22	10:E:101:ASN:HD21	1.71	0.54
23:Q:436:GLU:HG2	23:Q:482:ARG:HH22	1.72	0.54
1:2:17:U:H4'	1:2:18:U:H4'	1.88	0.54
23:Q:1027:LEU:HG	23:Q:1031:GLU:HB3	1.90	0.54
23:Q:737:VAL:HG11	23:Q:742:LEU:HB2	1.90	0.54
23:Q:236:VAL:HG13	23:Q:242:VAL:HG21	1.90	0.54
12:I:684:ALA:HA	12:I:687:ILE:HD12	1.91	0.53
7:C:679:PRO:HB3	27:TF:782:GLU:O	2.09	0.53
10:E:133:VAL:HG21	10:E:169:THR:HG21	1.91	0.53
12:I:683:ARG:HB3	16:L:297:LEU:HD22	1.91	0.52
5:A:43:LYS:HE3	28:W:168:PHE:HB3	1.90	0.52
38:q:17:VAL:HG22	38:q:24:VAL:HG22	1.89	0.52
5:A:1974:GLU:HA	5:A:1977:ILE:HD12	1.92	0.52
15:K:66:MET:HG2	38:s:86:MET:HE1	1.92	0.52
27:TF:795:ARG:HA	27:TF:801:LEU:N	2.24	0.52
21:O:253:TYR:HE1	25:S:93:THR:HG22	1.75	0.52
26:T:314:ILE:HD12	26:T:324:HIS:HB2	1.92	0.52
15:K:57:ASP:H	38:q:95:GLN:HE22	1.59	0.51
5:A:1379:PHE:HD1	5:A:1416:ILE:HD11	1.74	0.51
5:A:1636:LYS:HB3	5:A:1656:THR:HB	1.92	0.51
12:I:307:ILE:HG12	12:I:330:ARG:HB3	1.92	0.51
16:L:548:PRO:HG3	26:T:24:MET:HE3	1.92	0.51
7:C:697:ALA:HA	7:C:700:ILE:HD12	1.93	0.51
5:A:1975:GLU:HA	5:A:1978:LYS:HD2	1.93	0.51
5:A:881:ILE:HG23	5:A:918:THR:HG23	1.93	0.50
12:I:452:ALA:HA	12:I:455:LEU:HD12	1.93	0.50
12:I:533:TYR:CD1	12:I:533:TYR:CB	2.80	0.50
21:O:64:ARG:HB3	21:O:162:PRO:HA	1.93	0.50
15:K:89:LEU:HD22	15:K:110:SER:HA	1.94	0.50
5:A:1951:LYS:HA	5:A:1954:LEU:HD12	1.94	0.50
7:C:663:CYS:HB2	7:C:828:MET:HB2	1.93	0.50
24:R:288:ALA:O	24:R:292:TYR:HB2	2.11	0.50
12:I:147:ARG:HH22	39:y:68:ASN:HB3	1.77	0.50
12:I:533:TYR:CD2	16:L:519:ASP:CB	2.95	0.50
5:A:912:GLU:HG3	16:L:44:LYS:HE2	1.94	0.50
27:TF:805:GLY:HA3	27:TF:836:ALA:HA	1.94	0.50
23:Q:1226:ILE:HG12	23:Q:1272:LEU:HD12	1.95	0.49
7:C:137:HIS:HD2	7:C:238:ASN:H	1.59	0.49
12:I:243:ILE:HG12	23:Q:527:ILE:HG22	1.93	0.49
38:q:20:VAL:HG12	38:q:43:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:223:ARG:HD2	16:L:793:LEU:HD21	1.94	0.49
12:I:464:ALA:HA	24:R:23:LYS:HD3	1.94	0.49
18:L2:629:THR:HG22	18:L2:631:GLY:H	1.76	0.49
2:3:68:TYR:HB2	2:3:83:ILE:HG21	1.94	0.49
23:Q:1137:GLY:HA3	23:Q:1157:LEU:HD12	1.94	0.49
27:TF:790:PRO:HA	27:TF:802:TYR:HA	1.93	0.49
5:A:991:THR:HG22	16:L:81:GLN:HE22	1.78	0.49
16:L:571:SER:HA	16:L:574:LEU:HD12	1.93	0.49
21:O:230:THR:H	23:Q:542:ASN:HD22	1.61	0.49
28:W:209:SER:HB2	28:W:212:GLU:HB2	1.95	0.49
12:I:22:LEU:HA	12:I:25:GLU:HB2	1.94	0.48
23:Q:31:TRP:HA	23:Q:38:LYS:HD3	1.95	0.48
1:2:24:A:H5'	1:2:25:G:H5''	1.95	0.48
26:T:345:ILE:HD11	26:T:359:LEU:HD13	1.96	0.48
26:T:398:TRP:HD1	26:T:405:PHE:HA	1.76	0.48
7:C:814:ARG:HG2	7:C:952:PHE:HB3	1.95	0.48
16:L:636:LEU:HD21	38:t:113:ALA:HB2	1.94	0.48
12:I:533:TYR:CE2	16:L:519:ASP:CB	2.97	0.48
38:r:15:PRO:HB2	38:r:55:ILE:HD12	1.94	0.48
26:T:210:ILE:HG12	26:T:221:THR:HG22	1.96	0.48
26:T:346:ILE:HD13	26:T:380:LEU:HD11	1.96	0.48
13:IN:144:A:H5''	13:IN:144:A:N3	2.29	0.47
7:C:779:LEU:HD11	7:C:825:PRO:HB2	1.95	0.47
5:A:1807:ILE:HD11	5:A:1822:ILE:HD11	1.96	0.47
12:I:533:TYR:CD1	16:L:519:ASP:CB	2.98	0.47
12:I:494:GLU:HG3	12:I:506:VAL:HG21	1.97	0.47
16:L:522:LYS:HA	16:L:525:ILE:HD12	1.97	0.47
20:N:115:THR:HG23	20:N:116:ASN:O	2.15	0.47
23:Q:1290:LEU:HD13	23:Q:1316:LEU:HD22	1.95	0.47
5:A:226:GLN:HB3	5:A:417:ARG:HH21	1.80	0.47
5:A:1661:TRP:CE2	5:A:1700:GLY:HA3	2.51	0.46
7:C:750:LEU:HD11	27:TF:740:ARG:HA	1.97	0.46
38:r:128:ARG:HA	38:r:131:LEU:HB2	1.97	0.46
39:y:35:ILE:HG23	39:y:52:VAL:HG22	1.97	0.46
15:K:164:ASN:ND2	28:W:58:PRO:HG2	2.30	0.46
16:L:639:GLU:HB3	38:t:112:ALA:HB1	1.97	0.46
23:Q:961:VAL:HG22	23:Q:987:TYR:HB2	1.98	0.46
5:A:1807:ILE:HD12	5:A:1820:LYS:HB3	1.96	0.46
21:O:58:CYS:HA	21:O:65:PHE:HA	1.96	0.46
7:C:836:VAL:HG22	7:C:897:SER:HB3	1.98	0.45
12:I:533:TYR:CZ	16:L:519:ASP:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:952:LYS:HE3	23:Q:991:MET:HE2	1.98	0.45
20:N:126:LEU:HB3	20:N:130:ARG:HD3	1.98	0.45
5:A:591:MET:HE2	5:A:598:LEU:HD11	1.98	0.45
26:T:213:GLU:HG3	26:T:218:TRP:CE2	2.52	0.45
38:q:15:PRO:HG2	38:q:55:ILE:HB	1.98	0.45
23:Q:378:HIS:CD2	23:Q:390:LEU:HB2	2.51	0.45
24:R:132:LEU:HD23	26:T:399:LYS:HE2	1.97	0.45
3:5:43:U:H4'	4:6:67:G:H22	1.82	0.45
12:I:533:TYR:CD2	12:I:533:TYR:CB	2.82	0.45
16:L:792:LEU:HD23	16:L:792:LEU:HA	1.76	0.45
5:A:1505:LYS:HG3	18:L2:836:GLU:HB3	1.99	0.45
18:L2:621:MET:HA	18:L2:643:LYS:HD3	1.98	0.45
29:YB:222:GLU:HG3	29:YB:226:LYS:HE3	1.99	0.45
24:R:297:LYS:HD3	24:R:297:LYS:HA	1.73	0.45
23:Q:913:LYS:HE2	23:Q:917:LYS:HE3	1.99	0.44
39:y:37:ILE:HG23	39:y:50:ALA:HB2	1.99	0.44
7:C:750:LEU:HD12	7:C:753:GLU:HG3	1.99	0.44
12:I:533:TYR:CE1	16:L:519:ASP:CB	3.01	0.44
15:K:195:ILE:HG21	16:L:784:LEU:HB3	1.98	0.44
23:Q:1222:ASP:HA	23:Q:1255:ASN:HB2	1.99	0.44
23:Q:1269:ASP:HA	23:Q:1298:ARG:HB2	1.98	0.44
4:6:27:A:N1	21:O:165:CYS:HA	2.33	0.44
8:D:161:GLY:HA3	12:I:171:ARG:NH2	2.33	0.44
16:L:578:GLU:HB3	38:r:112:ALA:HB1	1.99	0.44
23:Q:1250:LEU:HD12	23:Q:1369:TYR:HE1	1.82	0.44
5:A:1950:ALA:HA	5:A:1953:ILE:HD12	1.99	0.44
15:K:81:LEU:HA	38:s:79:GLN:HE22	1.82	0.44
38:s:19:PRO:HB3	38:t:53:ILE:HD13	1.99	0.44
5:A:214:ARG:HA	5:A:220:VAL:HG21	2.00	0.44
15:K:64:ASP:HA	15:K:67:ARG:HD2	1.99	0.44
21:O:212:LYS:HE2	21:O:216:ARG:HH22	1.81	0.44
25:S:56:ILE:HG23	25:S:62:ILE:HG22	2.00	0.44
12:I:142:ILE:HA	12:I:145:HIS:CE1	2.53	0.44
15:K:91:ALA:HB2	16:L:700:ARG:HH22	1.82	0.44
15:K:116:HIS:CE1	38:r:86:MET:HG3	2.53	0.44
15:K:172:LEU:HD23	15:K:172:LEU:HA	1.86	0.44
2:3:148:LEU:HD23	5:A:804:GLU:HA	1.99	0.44
5:A:1701:VAL:HA	5:A:1716:GLY:HA3	2.00	0.44
15:K:178:LEU:HD23	15:K:178:LEU:HA	1.86	0.44
12:I:355:HIS:CE1	12:I:386:ASP:H	2.36	0.44
21:O:59:PRO:HB2	21:O:63:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:168:TRP:HA	21:O:173:CYS:HB2	2.00	0.44
12:I:350:LEU:HA	12:I:350:LEU:HD23	1.84	0.43
2:3:59:VAL:HG13	24:R:304:MET:HE1	2.01	0.43
5:A:363:HIS:HB3	7:C:279:ARG:HH21	1.83	0.43
21:O:114:LYS:HB3	21:O:114:LYS:HE2	1.78	0.43
26:T:213:GLU:HG3	26:T:218:TRP:CZ2	2.53	0.43
21:O:239:LEU:HD21	21:O:248:LEU:HD11	2.01	0.43
7:C:788:LYS:HE2	7:C:790:LYS:HE3	1.99	0.43
25:S:45:ARG:HH12	28:W:62:VAL:HG11	1.82	0.43
2:3:242:ARG:HG2	22:P:199:CYS:HA	2.00	0.43
5:A:301:LYS:HE3	7:C:940:ARG:HA	2.01	0.43
5:A:1789:THR:HG21	18:L2:74:HIS:CE1	2.53	0.43
38:s:1:MET:HE1	38:t:59:HIS:HE1	1.84	0.43
38:s:3:LEU:HG	38:t:3:LEU:HG	1.99	0.43
38:s:4:ILE:HG12	38:t:63:PRO:HB3	2.01	0.43
5:A:1910:THR:HG23	5:A:1911:GLU:HG3	2.01	0.43
12:I:533:TYR:CG	16:L:519:ASP:CB	3.01	0.43
39:y:15:GLU:HA	39:y:46:HIS:HE2	1.84	0.43
16:L:39:HIS:CE1	16:L:40:ARG:HH11	2.37	0.43
23:Q:466:LEU:HA	23:Q:466:LEU:HD23	1.84	0.43
24:R:60:ASP:HB3	25:S:134:GLN:HA	2.00	0.43
33:c:76:LEU:HD13	34:d:98:LYS:HD3	2.00	0.43
4:6:21:U:H5''	20:N:116:ASN:ND2	2.34	0.42
21:O:197:ASN:O	21:O:201:ARG:HG3	2.19	0.42
18:L2:686:LYS:H	18:L2:686:LYS:HG3	1.70	0.42
20:N:28:LYS:HD2	28:W:189:ILE:HG23	2.01	0.42
32:b:50:LYS:HE3	32:b:60:GLU:HG2	2.01	0.42
33:c:19:LEU:HD12	33:c:23:THR:HB	2.01	0.42
3:5:36:C:H4'	5:A:284:ARG:HH21	1.84	0.42
37:g:17:LEU:HD13	37:g:70:LEU:HG	2.01	0.42
5:A:1011:ALA:HB2	16:L:80:THR:HB	2.02	0.42
15:K:163:LEU:HD12	15:K:163:LEU:HA	1.85	0.42
20:N:70:ILE:HG23	20:N:74:LEU:HB3	2.01	0.42
26:T:33:VAL:HB	38:r:97:GLN:HE22	1.84	0.42
39:y:35:ILE:HG12	39:y:52:VAL:HG13	2.01	0.42
2:3:240:LYS:HA	2:3:241:PRO:HD2	1.83	0.42
7:C:672:LEU:HD13	7:C:960:GLU:HG2	2.01	0.42
23:Q:908:LEU:HD22	23:Q:1004:ILE:HG23	2.01	0.42
23:Q:935:PHE:CE2	23:Q:939:GLN:HG3	2.54	0.42
23:Q:1001:ILE:HA	23:Q:1004:ILE:HD12	2.02	0.42
23:Q:1197:PHE:CZ	23:Q:1232:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:180:ASP:HB2	10:E:187:ILE:HD11	2.02	0.42
12:I:341:ARG:HH22	19:M:48:ARG:HA	1.85	0.42
15:K:170:MET:HE2	15:K:170:MET:HB3	1.95	0.42
5:A:305:ARG:HH11	7:C:929:LEU:HD21	1.85	0.42
5:A:994:ASN:HD21	5:A:1007:ASP:HA	1.85	0.42
5:A:1876:LEU:HD12	5:A:1884:ILE:HD11	2.02	0.42
10:E:161:ARG:HE	10:E:243:LEU:HD23	1.84	0.42
5:A:1320:LYS:NZ	18:L:796:TRP:HB3	2.35	0.41
5:A:1780:VAL:HG22	5:A:1809:ILE:HG23	2.01	0.41
16:L:721:LEU:HA	16:L:724:TYR:HD2	1.85	0.41
23:Q:154:PHE:CG	23:Q:260:LEU:HD21	2.55	0.41
38:r:17:VAL:HG23	38:r:55:ILE:HD11	2.00	0.41
16:L:77:LEU:HD22	24:R:285:ALA:HA	2.02	0.41
23:Q:1275:LEU:HD22	23:Q:1284:LEU:HD11	2.03	0.41
12:I:75:LEU:C	12:I:79:ARG:HE	2.28	0.41
23:Q:222:LEU:HD23	23:Q:222:LEU:HA	1.88	0.41
23:Q:909:LEU:HD23	23:Q:909:LEU:HA	1.93	0.41
23:Q:1005:PHE:HA	23:Q:1008:LEU:HD12	2.02	0.41
23:Q:1200:ASN:HB2	23:Q:1276:VAL:HG13	2.02	0.41
7:C:960:GLU:HG3	27:TF:727:ALA:HB2	2.01	0.41
23:Q:1143:LEU:HD23	23:Q:1143:LEU:HA	1.89	0.41
24:R:119:LEU:HD21	24:R:230:MET:HB3	2.03	0.41
4:6:38:G:H2'	4:6:39:A:H8	1.85	0.41
4:6:66:C:H1'	5:A:651:TRP:CD1	2.56	0.41
5:A:1974:GLU:HG3	5:A:1978:LYS:HE3	2.03	0.41
21:O:28:LEU:HD12	21:O:28:LEU:HA	1.85	0.41
23:Q:1157:LEU:HD23	23:Q:1157:LEU:HA	1.88	0.41
33:c:67:TYR:CG	34:d:99:MET:HE3	2.55	0.41
39:y:14:ALA:HB3	39:y:17:VAL:HG23	2.01	0.41
3:5:109:C:H4'	32:b:51:ILE:HA	2.02	0.41
7:C:958:LEU:HD23	7:C:961:LEU:HD12	2.03	0.41
12:I:608:LEU:HB2	12:I:611:HIS:CD2	2.55	0.41
38:r:71:ILE:HA	38:r:74:ILE:HD12	2.01	0.41
1:2:19:G:H5'	5:A:707:ARG:HD2	2.02	0.41
2:3:242:ARG:HE	2:3:242:ARG:HB3	1.61	0.41
3:5:47:A:O2'	3:5:48:A:H8	2.03	0.41
15:K:164:ASN:HD21	28:W:58:PRO:HG2	1.86	0.41
16:L:89:ILE:HD13	16:L:89:ILE:HG21	1.87	0.41
36:f:15:THR:HG23	36:f:34:VAL:HA	2.02	0.41
4:6:65:G:N2	4:6:67:G:H3'	2.36	0.41
23:Q:147:LEU:HD23	23:Q:147:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:TF:627:PRO:HB3	27:TF:679:ILE:HA	2.02	0.41
28:W:109:ASN:HB2	28:W:114:TYR:CD1	2.56	0.41
5:A:1562:MET:HE2	5:A:1562:MET:HB3	1.87	0.40
12:I:418:LEU:HD23	12:I:418:LEU:HA	1.78	0.40
15:K:165:TRP:CD1	28:W:60:VAL:HG11	2.55	0.40
23:Q:254:ILE:HD13	23:Q:254:ILE:HA	1.90	0.40
38:t:16:CYS:HB2	38:t:52:LEU:HB3	2.02	0.40
5:A:271:MET:HE2	5:A:271:MET:HB3	1.99	0.40
7:C:679:PRO:HD3	7:C:811:THR:OG1	2.20	0.40
23:Q:561:VAL:H	23:Q:664:ASN:ND2	2.19	0.40
16:L:609:ASN:HA	16:L:612:HIS:CD2	2.56	0.40
21:O:230:THR:H	23:Q:542:ASN:ND2	2.19	0.40
23:Q:723:HIS:CE1	23:Q:801:GLN:HG3	2.56	0.40
23:Q:1284:LEU:HD23	23:Q:1284:LEU:HA	1.86	0.40
26:T:17:SER:HA	26:T:20:ARG:HD3	2.02	0.40
18:L2:869:PHE:HA	18:L2:872:GLN:HG3	2.02	0.40
20:N:18:ILE:HG21	20:N:70:ILE:HD11	2.02	0.40
38:r:3:LEU:HD23	38:r:3:LEU:HA	1.84	0.40
38:r:107:LEU:HD23	38:r:107:LEU:HA	1.90	0.40
5:A:706:ALA:HA	5:A:709:ILE:HD12	2.03	0.40
12:I:120:LEU:HD23	12:I:120:LEU:HA	1.91	0.40
12:I:648:THR:HA	12:I:651:ILE:HD12	2.03	0.40
21:O:60:GLY:HA3	21:O:63:MET:HE2	2.02	0.40
32:b:25:ARG:HG2	32:b:49:ARG:HG2	2.04	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
2	3	129/476 (27%)	123 (95%)	5 (4%)	1 (1%)	16 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	1975/2335 (85%)	1885 (95%)	89 (4%)	1 (0%)	48	64
6	B	17/2136 (1%)	16 (94%)	1 (6%)	0	100	100
7	C	906/972 (93%)	884 (98%)	22 (2%)	0	100	100
8	D	49/285 (17%)	49 (100%)	0	0	100	100
9	DX	648/795 (82%)	634 (98%)	14 (2%)	0	100	100
10	E	297/357 (83%)	283 (95%)	12 (4%)	2 (1%)	18	28
11	GC	512/781 (66%)	496 (97%)	11 (2%)	5 (1%)	12	20
12	I	715/855 (84%)	698 (98%)	15 (2%)	2 (0%)	36	50
14	J	588/848 (69%)	572 (97%)	16 (3%)	0	100	100
15	K	207/225 (92%)	203 (98%)	3 (1%)	1 (0%)	24	37
16	L	559/802 (70%)	535 (96%)	22 (4%)	2 (0%)	30	43
17	L1	266/538 (49%)	262 (98%)	3 (1%)	1 (0%)	30	43
18	L2	360/894 (40%)	335 (93%)	24 (7%)	1 (0%)	36	50
19	M	162/243 (67%)	159 (98%)	3 (2%)	0	100	100
20	N	141/144 (98%)	131 (93%)	10 (7%)	0	100	100
21	O	286/420 (68%)	260 (91%)	22 (8%)	4 (1%)	9	13
22	P	102/229 (44%)	95 (93%)	7 (7%)	0	100	100
23	Q	1365/1485 (92%)	1340 (98%)	25 (2%)	0	100	100
24	R	297/536 (55%)	271 (91%)	25 (8%)	1 (0%)	36	50
25	S	157/166 (95%)	154 (98%)	3 (2%)	0	100	100
26	T	356/514 (69%)	342 (96%)	12 (3%)	2 (1%)	21	32
27	TF	560/837 (67%)	545 (97%)	13 (2%)	2 (0%)	30	43
28	W	169/579 (29%)	157 (93%)	10 (6%)	2 (1%)	10	16
29	YB	143/396 (36%)	140 (98%)	3 (2%)	0	100	100
30	Z	35/166 (21%)	35 (100%)	0	0	100	100
31	a	81/126 (64%)	77 (95%)	4 (5%)	0	100	100
32	b	89/240 (37%)	83 (93%)	5 (6%)	1 (1%)	11	18
33	c	79/119 (66%)	76 (96%)	3 (4%)	0	100	100
34	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
35	e	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
36	f	74/86 (86%)	72 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	72/76 (95%)	65 (90%)	7 (10%)	0	100	100
38	q	135/504 (27%)	134 (99%)	1 (1%)	0	100	100
38	r	135/504 (27%)	133 (98%)	2 (2%)	0	100	100
38	s	135/504 (27%)	133 (98%)	2 (2%)	0	100	100
38	t	135/504 (27%)	132 (98%)	3 (2%)	0	100	100
39	y	78/301 (26%)	78 (100%)	0	0	100	100
All	All	12186/21188 (58%)	11751 (96%)	407 (3%)	28 (0%)	44	58

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	GC	542	GLU
11	GC	596	GLU
11	GC	597	ASN
11	GC	717	ARG
12	I	107	HIS
21	O	224	ASP
24	R	135	PRO
5	A	1092	ILE
17	L1	197	LEU
21	O	176	GLY
27	TF	790	PRO
28	W	208	PRO
32	b	78	VAL
16	L	215	PRO
11	GC	540	LYS
12	I	572	LYS
15	K	20	ASP
27	TF	419	ASP
10	E	149	GLY
16	L	602	THR
21	O	289	ASN
2	3	241	PRO
26	T	202	GLY
18	L2	651	GLY
21	O	47	ILE
10	E	107	GLY
28	W	205	VAL
26	T	244	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	124/395 (31%)	122 (98%)	2 (2%)	55	76
5	A	1790/2108 (85%)	1755 (98%)	35 (2%)	48	70
7	C	807/866 (93%)	806 (100%)	1 (0%)	88	95
8	D	1/240 (0%)	1 (100%)	0	100	100
9	DX	37/704 (5%)	37 (100%)	0	100	100
10	E	256/300 (85%)	255 (100%)	1 (0%)	84	92
11	GC	15/715 (2%)	15 (100%)	0	100	100
12	I	631/749 (84%)	620 (98%)	11 (2%)	53	74
14	J	183/751 (24%)	180 (98%)	3 (2%)	55	76
15	K	183/196 (93%)	180 (98%)	3 (2%)	55	76
16	L	424/709 (60%)	408 (96%)	16 (4%)	29	49
17	L1	14/469 (3%)	14 (100%)	0	100	100
18	L2	331/806 (41%)	320 (97%)	11 (3%)	33	55
19	M	4/209 (2%)	4 (100%)	0	100	100
20	N	130/130 (100%)	126 (97%)	4 (3%)	35	57
21	O	258/361 (72%)	250 (97%)	8 (3%)	35	57
22	P	78/203 (38%)	78 (100%)	0	100	100
23	Q	1239/1336 (93%)	1233 (100%)	6 (0%)	81	91
24	R	253/457 (55%)	247 (98%)	6 (2%)	43	65
25	S	129/134 (96%)	129 (100%)	0	100	100
26	T	313/441 (71%)	311 (99%)	2 (1%)	78	89
27	TF	27/746 (4%)	27 (100%)	0	100	100
28	W	146/502 (29%)	142 (97%)	4 (3%)	39	62
29	YB	130/346 (38%)	127 (98%)	3 (2%)	44	66
30	Z	1/143 (1%)	1 (100%)	0	100	100
31	a	73/101 (72%)	65 (89%)	8 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	b	75/177 (42%)	70 (93%)	5 (7%)	15	26
33	c	76/101 (75%)	74 (97%)	2 (3%)	40	63
34	d	91/110 (83%)	90 (99%)	1 (1%)	65	82
35	e	74/84 (88%)	74 (100%)	0	100	100
36	f	65/74 (88%)	64 (98%)	1 (2%)	57	77
37	g	64/66 (97%)	62 (97%)	2 (3%)	35	57
38	q	122/435 (28%)	120 (98%)	2 (2%)	55	76
38	r	122/435 (28%)	121 (99%)	1 (1%)	73	86
38	s	122/435 (28%)	121 (99%)	1 (1%)	73	86
38	t	122/435 (28%)	122 (100%)	0	100	100
39	y	65/252 (26%)	64 (98%)	1 (2%)	57	77
All	All	8575/16721 (51%)	8435 (98%)	140 (2%)	54	76

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	156	THR
2	3	253	ARG
5	A	89	LEU
5	A	97	HIS
5	A	127	SER
5	A	220	VAL
5	A	240	ARG
5	A	319	LEU
5	A	380	LEU
5	A	417	ARG
5	A	467	GLN
5	A	546	LEU
5	A	644	ILE
5	A	676	ARG
5	A	693	ILE
5	A	704	ASN
5	A	735	ILE
5	A	779	LEU
5	A	894	VAL
5	A	912	GLU
5	A	951	LEU
5	A	1210	LYS

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Mol	Chain	Res	Type
5	A	1284	LEU
5	A	1321	GLU
5	A	1365	ILE
5	A	1438	VAL
5	A	1489	LEU
5	A	1541	THR
5	A	1547	VAL
5	A	1601	LEU
5	A	1644	LEU
5	A	1768	TYR
5	A	1807	ILE
5	A	1809	ILE
5	A	1813	ARG
5	A	1898	LYS
5	A	1946	ASN
7	C	183	SER
10	E	351	LEU
12	I	163	GLU
12	I	175	LEU
12	I	253	ASP
12	I	382	VAL
12	I	503	THR
12	I	515	ILE
12	I	553	VAL
12	I	565	ILE
12	I	573	LEU
12	I	631	MET
12	I	694	ILE
14	J	253	GLU
14	J	300	ASP
14	J	331	GLN
15	K	159	HIS
15	K	187	SER
15	K	202	LEU
16	L	12	ARG
16	L	14	THR
16	L	53	TRP
16	L	54	LEU
16	L	89	ILE
16	L	131	ASN
16	L	213	GLU
16	L	222	LEU

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Mol	Chain	Res	Type
16	L	229	GLU
16	L	588	LEU
16	L	614	THR
16	L	636	LEU
16	L	652	LEU
16	L	705	THR
16	L	747	LEU
16	L	770	LEU
18	L2	62	ASP
18	L2	599	LEU
18	L2	652	GLU
18	L2	679	PHE
18	L2	680	ASP
18	L2	681	SER
18	L2	728	ASP
18	L2	793	ASP
18	L2	809	ASP
18	L2	837	ASP
18	L2	883	TRP
20	N	21	THR
20	N	101	CYS
20	N	102	CYS
20	N	117	CYS
21	O	16	GLU
21	O	47	ILE
21	O	62	ARG
21	O	64	ARG
21	O	109	LYS
21	O	245	GLU
21	O	257	GLU
21	O	260	THR
23	Q	414	ARG
23	Q	444	TYR
23	Q	583	PHE
23	Q	1338	PHE
23	Q	1377	HIS
23	Q	1378	HIS
24	R	47	ARG
24	R	111	VAL
24	R	163	MET
24	R	177	ILE
24	R	238	THR

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Mol	Chain	Res	Type
24	R	264	LEU
26	T	12	THR
26	T	261	LEU
28	W	63	LYS
28	W	193	LEU
28	W	204	ASP
28	W	212	GLU
29	YB	192	GLU
29	YB	217	LEU
29	YB	221	THR
31	a	1	MET
31	a	33	ILE
31	a	46	ILE
31	a	60	GLN
31	a	61	VAL
31	a	66	SER
31	a	69	ARG
31	a	76	MET
32	b	32	LYS
32	b	70	VAL
32	b	71	LEU
32	b	78	VAL
32	b	83	GLU
33	c	24	GLN
33	c	56	GLU
34	d	43	LEU
36	f	36	VAL
37	g	11	LYS
37	g	69	MET
38	q	107	LEU
38	q	131	LEU
38	r	131	LEU
38	s	134	LEU
39	y	77	ILE

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

Mol	Chain	Res	Type
2	3	48	GLN
2	3	246	HIS
5	A	368	GLN
5	A	467	GLN

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Mol	Chain	Res	Type
5	A	517	HIS
5	A	704	ASN
5	A	755	HIS
5	A	793	ASN
5	A	994	ASN
5	A	1096	HIS
5	A	1217	GLN
5	A	1241	HIS
5	A	1367	ASN
5	A	1674	HIS
5	A	1811	ASN
5	A	1946	ASN
5	A	1965	HIS
7	C	60	HIS
7	C	125	ASN
7	C	139	HIS
7	C	201	ASN
7	C	245	HIS
7	C	280	HIS
7	C	306	ASN
7	C	451	HIS
7	C	890	HIS
10	E	101	ASN
10	E	215	ASN
12	I	294	GLN
12	I	346	ASN
12	I	352	GLN
12	I	425	ASN
12	I	519	GLN
12	I	523	ASN
12	I	611	HIS
12	I	663	HIS
12	I	714	HIS
14	J	331	GLN
14	J	340	GLN
16	L	81	GLN
16	L	538	HIS
16	L	597	ASN
18	L2	553	GLN
18	L2	718	HIS
20	N	53	HIS
20	N	87	ASN

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Mol	Chain	Res	Type
20	N	116	ASN
21	O	25	GLN
21	O	119	GLN
23	Q	34	HIS
23	Q	118	HIS
23	Q	165	GLN
23	Q	278	HIS
23	Q	300	GLN
23	Q	338	GLN
23	Q	483	GLN
23	Q	586	GLN
23	Q	835	GLN
23	Q	875	HIS
23	Q	1007	GLN
23	Q	1267	GLN
23	Q	1350	HIS
24	R	242	GLN
24	R	279	HIS
26	T	29	ASN
26	T	269	GLN
26	T	350	HIS
26	T	371	HIS
26	T	394	ASN
26	T	451	HIS
26	T	500	HIS
28	W	127	GLN
28	W	184	ASN
29	YB	78	ASN
34	d	34	GLN
34	d	41	GLN
34	d	69	ASN
35	e	83	ASN
38	q	95	GLN
38	q	137	GLN
38	r	97	GLN
38	s	22	ASN
38	s	79	GLN
38	s	105	HIS
38	t	59	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	40/187 (21%)	19 (47%)	0
13	IN	59/61 (96%)	37 (62%)	4 (6%)
3	5	90/116 (77%)	10 (11%)	6 (6%)
4	6	96/106 (90%)	43 (44%)	11 (11%)
All	All	285/470 (60%)	109 (38%)	21 (7%)

All (109) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	C
1	2	15	U
1	2	16	U
1	2	20	G
1	2	24	A
1	2	28	C
1	2	29	A
1	2	30	A
1	2	31	G
1	2	32	U
1	2	33	G
1	2	34	U
1	2	35	A
1	2	36	G
1	2	37	U
1	2	38	A
1	2	39	U
1	2	40	C
1	2	41	U
3	5	20	G
3	5	25	C
3	5	36	C
3	5	69	A
3	5	86	C
3	5	93	U
3	5	94	U
3	5	95	G
3	5	96	A
3	5	115	U
4	6	5	U
4	6	6	C
4	6	7	G
4	6	9	U
4	6	10	U

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Mol	Chain	Res	Type
4	6	12	G
4	6	26	U
4	6	27	A
4	6	28	A
4	6	29	A
4	6	33	G
4	6	34	G
4	6	35	A
4	6	36	A
4	6	37	C
4	6	41	A
4	6	42	C
4	6	43	A
4	6	44	G
4	6	45	A
4	6	48	A
4	6	49	G
4	6	51	U
4	6	53	A
4	6	54	G
4	6	56	A
4	6	58	G
4	6	59	G
4	6	60	C
4	6	61	C
4	6	62	C
4	6	68	C
4	6	69	A
4	6	73	A
4	6	74	U
4	6	78	A
4	6	79	C
4	6	80	G
4	6	81	C
4	6	82	A
4	6	85	U
4	6	89	U
4	6	91	A
13	IN	2	U
13	IN	3	A
13	IN	4	A
13	IN	6	U

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Mol	Chain	Res	Type
13	IN	8	U
13	IN	9	U
13	IN	11	U
13	IN	12	U
13	IN	17	U
13	IN	20	U
13	IN	21	U
13	IN	22	U
13	IN	23	U
13	IN	24	U
13	IN	137	U
13	IN	138	U
13	IN	139	U
13	IN	140	U
13	IN	141	U
13	IN	142	U
13	IN	143	U
13	IN	144	A
13	IN	145	U
13	IN	146	U
13	IN	147	U
13	IN	148	U
13	IN	150	U
13	IN	151	U
13	IN	152	U
13	IN	55	U
13	IN	56	U
13	IN	58	U
13	IN	59	U
13	IN	60	U
13	IN	61	U
13	IN	62	U
13	IN	65	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	20	G
3	5	21	A
3	5	24	G
3	5	47	A
3	5	92	U

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Mol	Chain	Res	Type
3	5	95	G
4	6	5	U
4	6	27	A
4	6	33	G
4	6	35	A
4	6	37	C
4	6	50	A
4	6	52	U
4	6	58	G
4	6	73	A
4	6	78	A
4	6	79	C
13	IN	1	G
13	IN	2	U
13	IN	3	A
13	IN	144	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	SEP	R	224	24	8,9,10	1.41	1 (12%)	8,12,14	1.27	0
24	SEP	R	232	24	8,9,10	1.32	1 (12%)	8,12,14	1.65	2 (25%)

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
24	SEP	R	224	24	-	0/5/8/10	-
24	SEP	R	232	24	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	224	SEP	P-O1P	3.07	1.60	1.50
24	R	232	SEP	P-O1P	2.88	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	232	SEP	P-OG-CB	-3.47	108.74	118.30
24	R	232	SEP	OG-CB-CA	2.55	110.63	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	GTP	C	1500	40	30,34,34	1.11	1 (3%)	46,54,54	1.81	10 (21%)
41	IHP	A	3000	-	36,36,36	2.02	9 (25%)	54,60,60	1.54	4 (7%)

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	1500	40	-	0/22/38/38	0/3/3/3
41	IHP	A	3000	-	-	5/30/54/54	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	A	3000	IHP	P1-O11	4.52	1.67	1.59
41	A	3000	IHP	P2-O12	4.32	1.67	1.59
41	A	3000	IHP	P6-O16	4.08	1.67	1.59
41	A	3000	IHP	P5-O15	4.00	1.66	1.59
41	A	3000	IHP	P3-O13	3.97	1.66	1.59
41	A	3000	IHP	P4-O14	3.86	1.66	1.59
41	A	3000	IHP	C3-C2	-3.32	1.45	1.52
41	A	3000	IHP	O13-C3	-2.75	1.34	1.44
42	C	1500	GTP	C5-N7	-2.51	1.34	1.39
41	A	3000	IHP	O12-C2	-2.29	1.35	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	A	3000	IHP	O11-C1-C2	5.67	122.04	108.69
42	C	1500	GTP	C5-C4-N3	-5.18	120.05	128.46
42	C	1500	GTP	C2-N3-C4	4.48	120.28	112.30
41	A	3000	IHP	O13-C3-C2	4.37	118.99	108.69
42	C	1500	GTP	PB-O3B-PG	-4.07	118.87	132.83
41	A	3000	IHP	O12-C2-C3	3.91	117.91	108.69
41	A	3000	IHP	O12-C2-C1	3.87	117.81	108.69
42	C	1500	GTP	C2-N1-C6	-3.40	118.89	125.10
42	C	1500	GTP	N9-C4-N3	3.40	132.77	125.94
42	C	1500	GTP	PA-O3A-PB	-3.01	122.51	132.83
42	C	1500	GTP	N9-C8-N7	-2.99	107.75	113.39
42	C	1500	GTP	C5-C6-N1	2.93	120.64	113.19
42	C	1500	GTP	C8-N7-C5	2.69	109.12	104.24
42	C	1500	GTP	O6-C6-C5	-2.41	120.22	126.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C2-C1-O11-P1
41	A	3000	IHP	C4-O14-P4-O34
41	A	3000	IHP	C6-O16-P6-O36

Continued on next page...

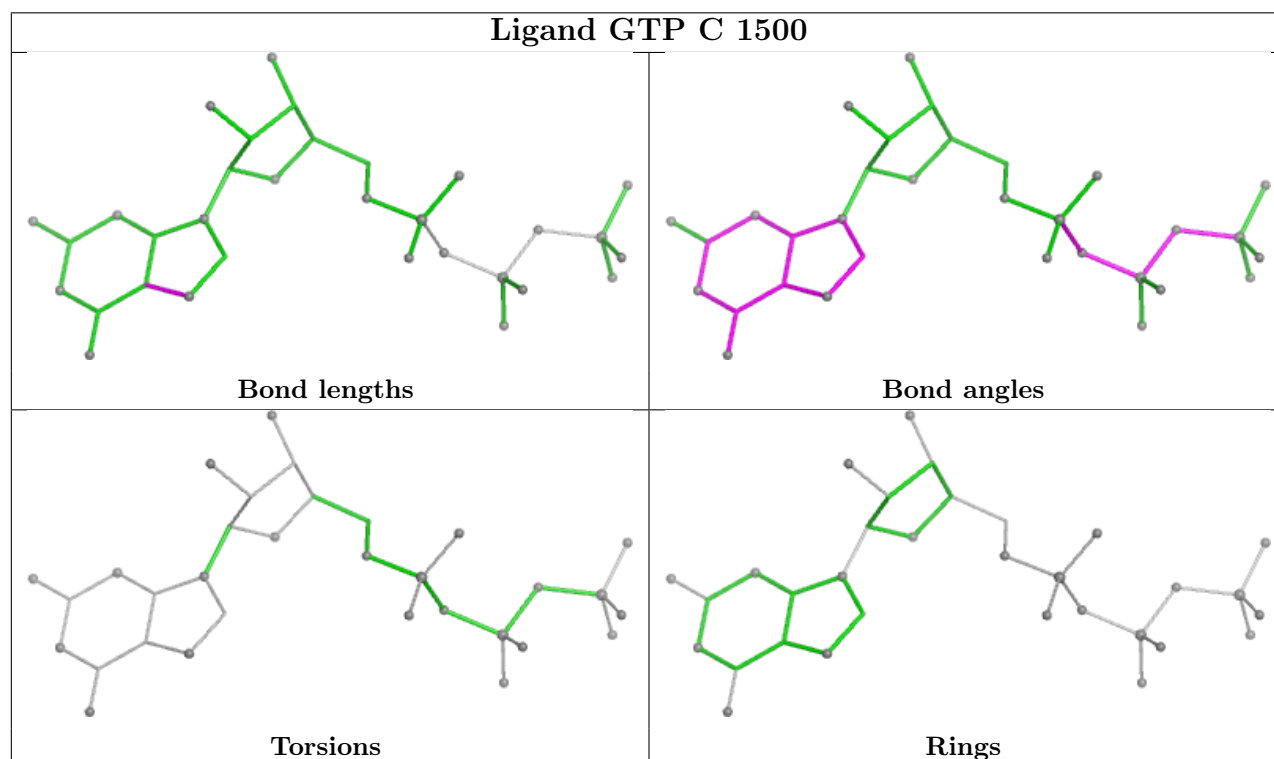
Continued from previous page...

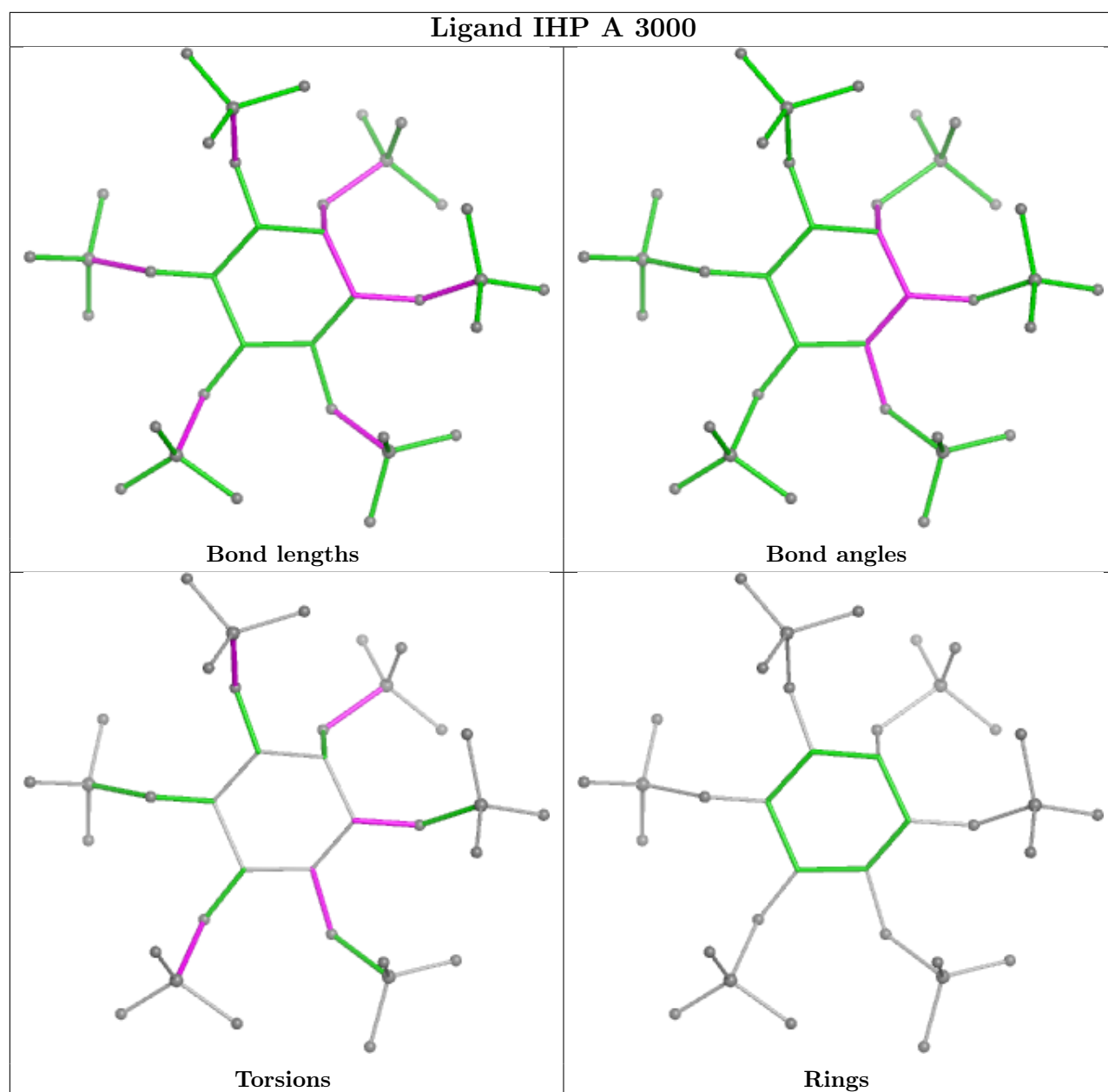
Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C3-C2-O12-P2
41	A	3000	IHP	C3-O13-P3-O33

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	IN	1
23	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	IN	154:U	O3'	50:U	P	168.10
1	Q	814:MET	C	815:GLN	N	1.16

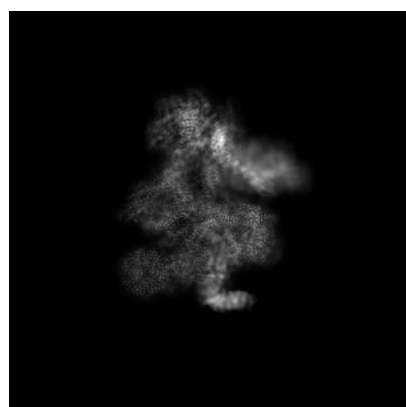
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54493. These allow visual inspection of the internal detail of the map and identification of artifacts.

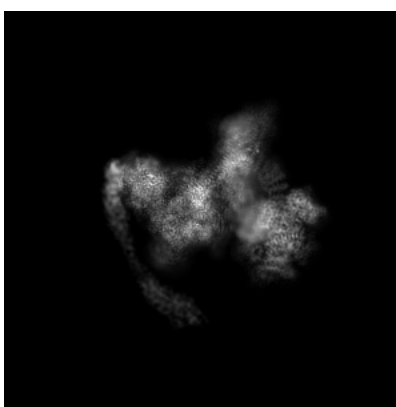
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

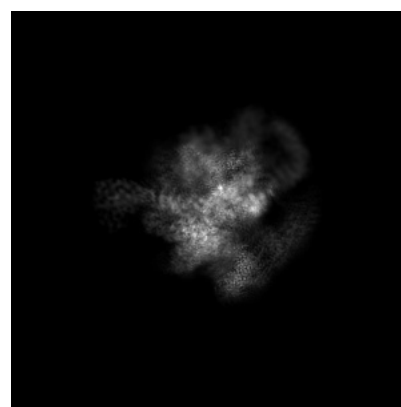
6.1.1 Primary map



X



Y

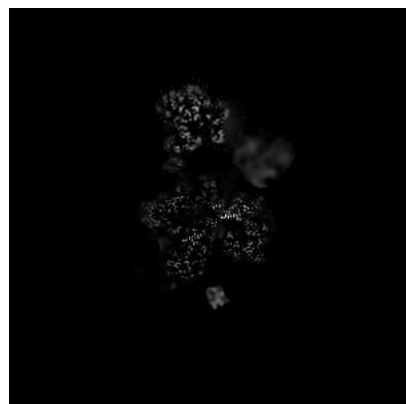


Z

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

6.2 Central slices [i](#)

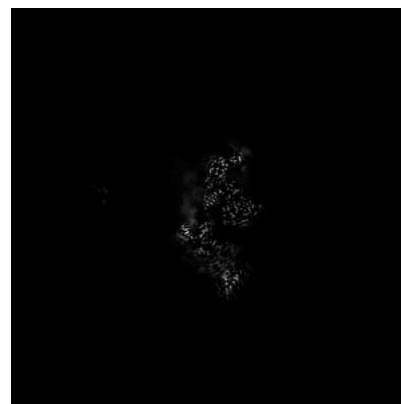
6.2.1 Primary map



X Index: 224



Y Index: 224

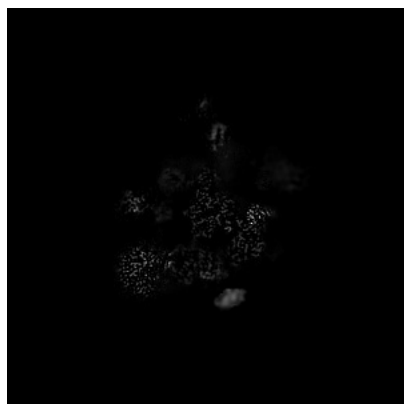


Z Index: 224

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: 250



Y Index: 237

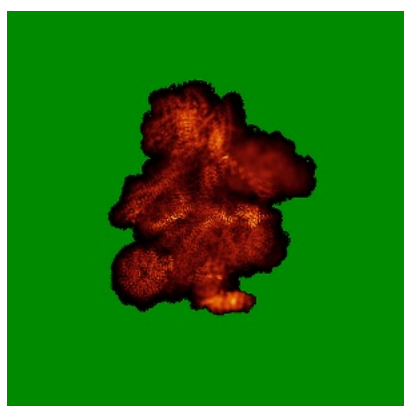


Z Index: 217

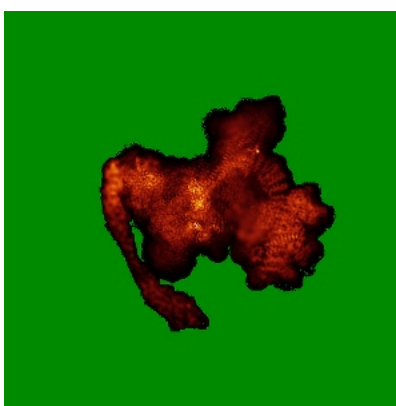
The images above show the largest variance slices of the map in three orthogonal directions.

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

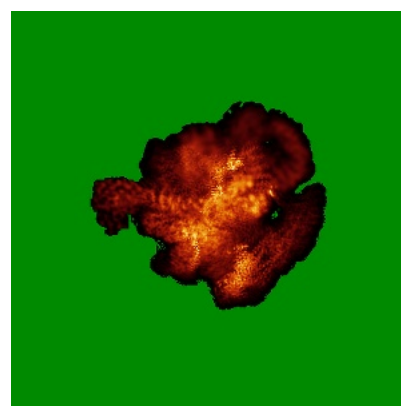
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

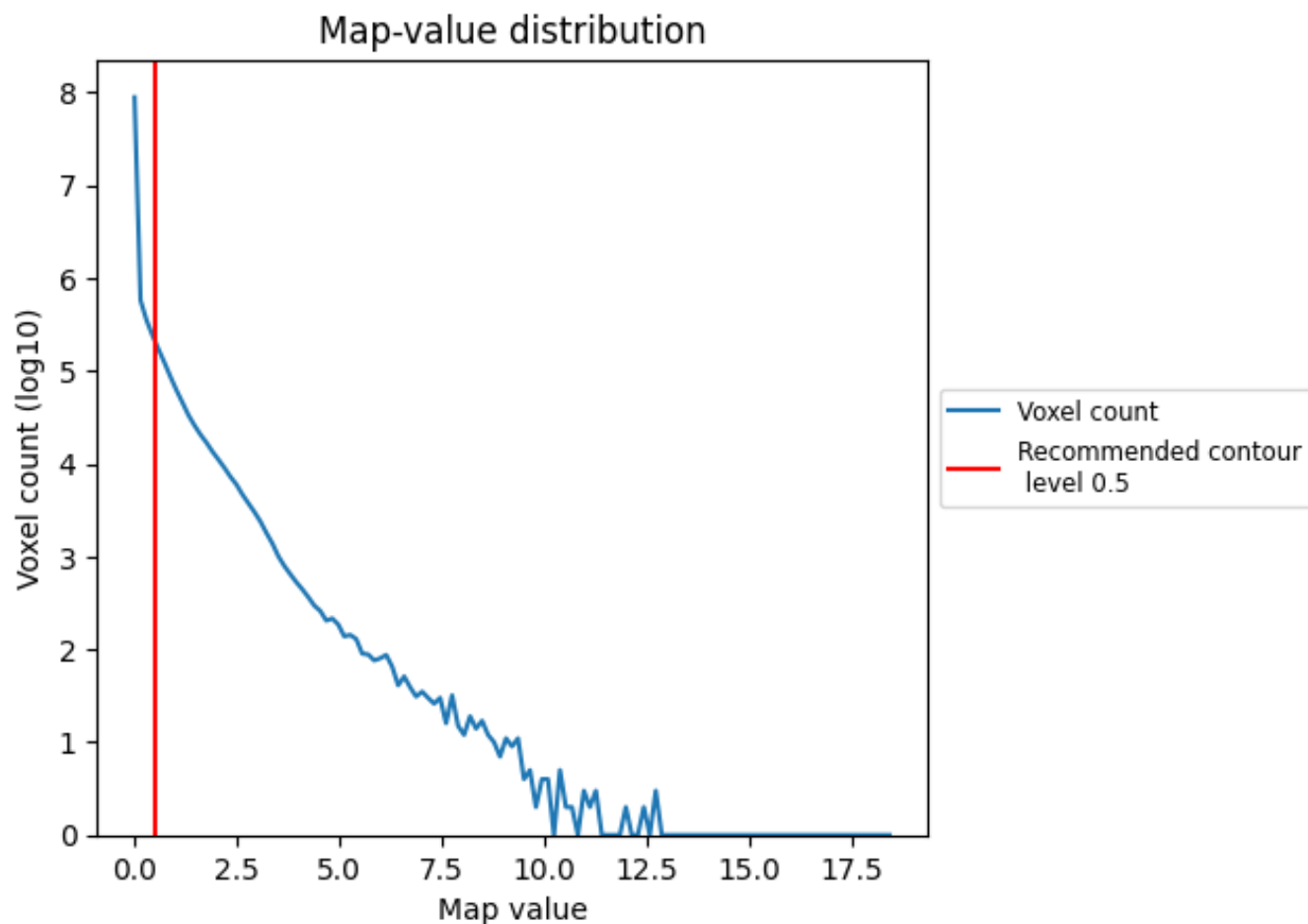
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

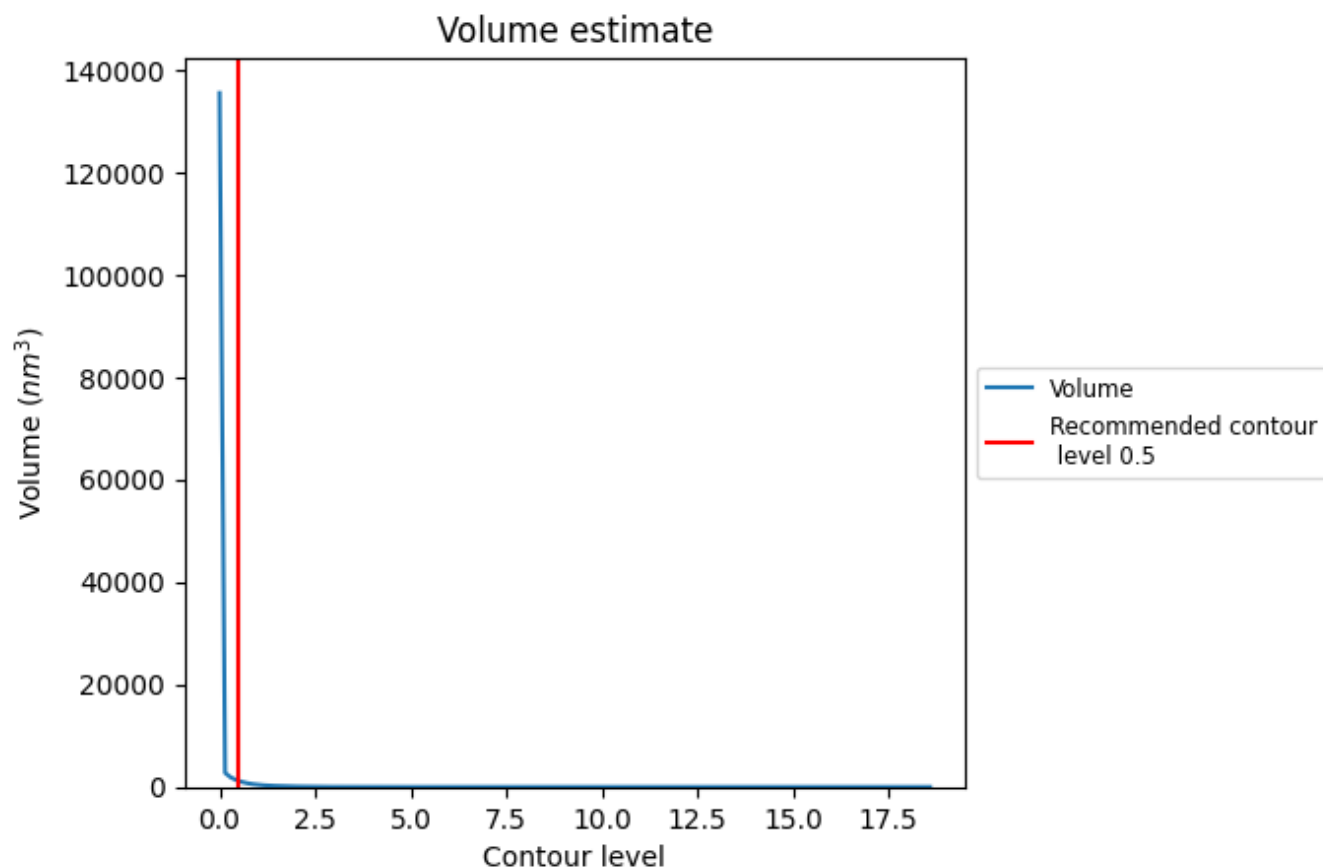
This section contains the results of statistical analysis of the map.

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.

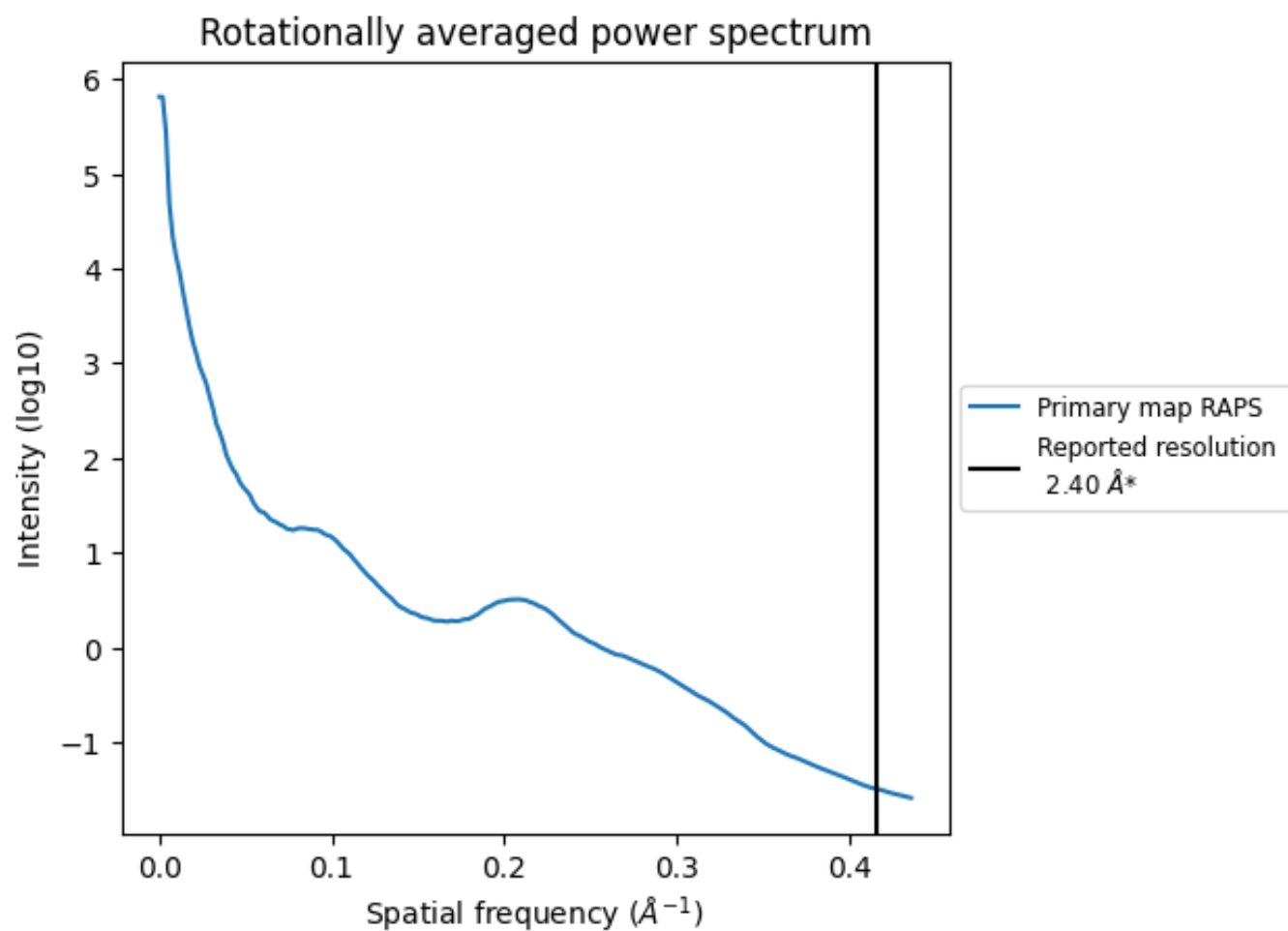
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192 nm^3 ; this corresponds to an approximate mass of 1076 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 0.417 Å⁻¹

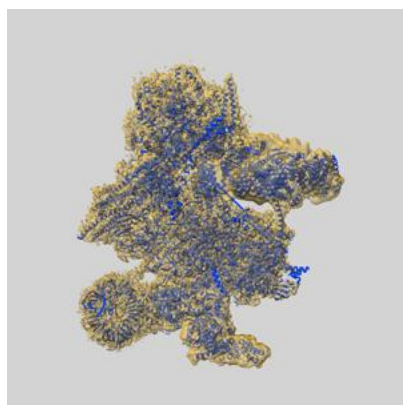
8 Fourier-Shell correlation ⓘ

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

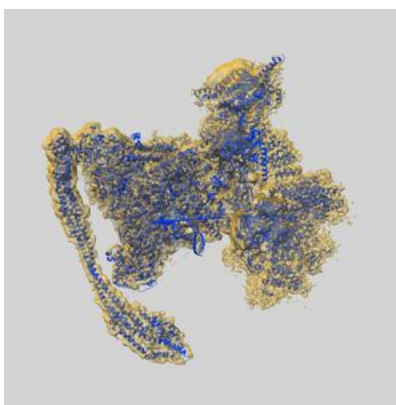
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54493 and PDB model 9S2E. Per-residue inclusion information can be found in section [3](#) on page [13](#).

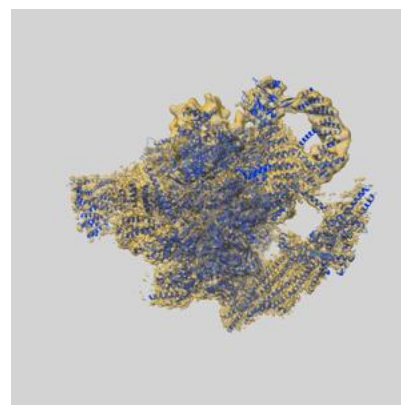
9.1 Map-model overlay [i](#)



X



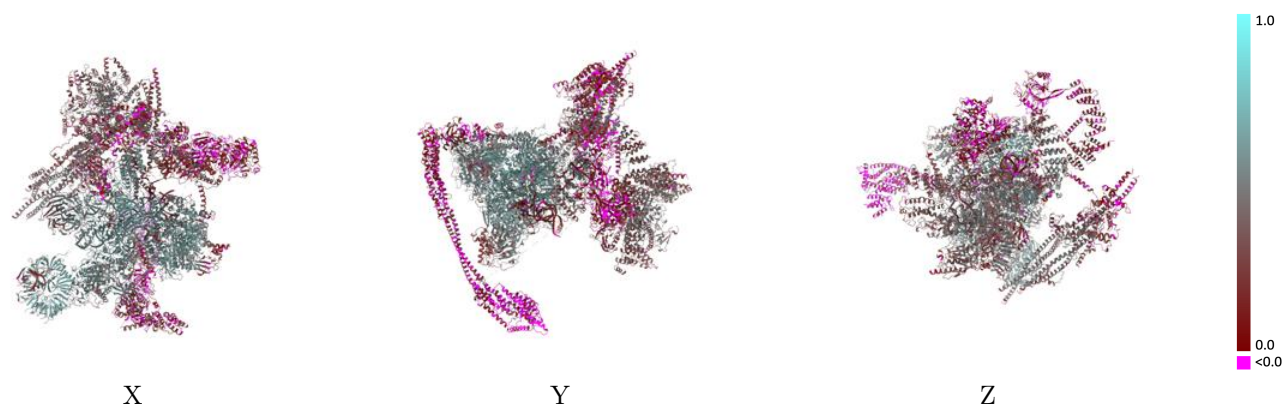
Y



Z

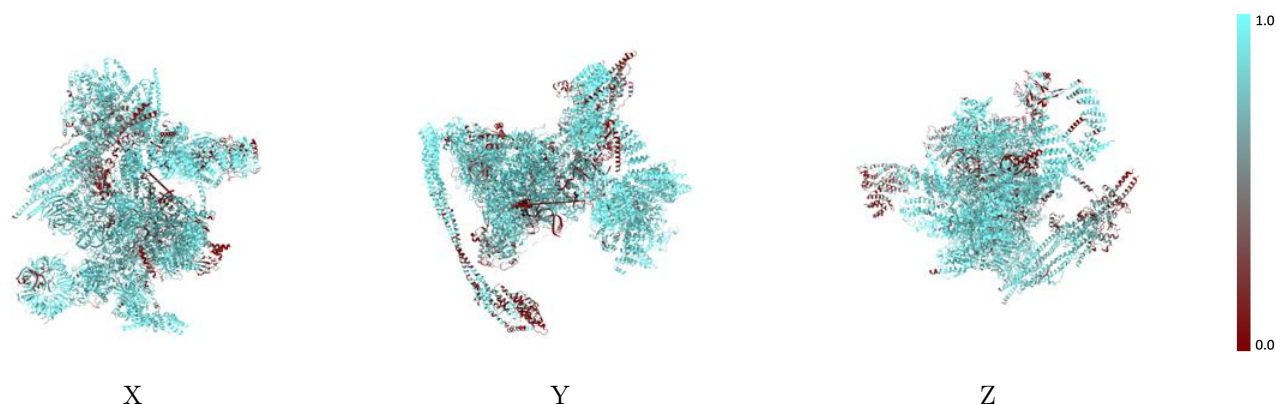
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



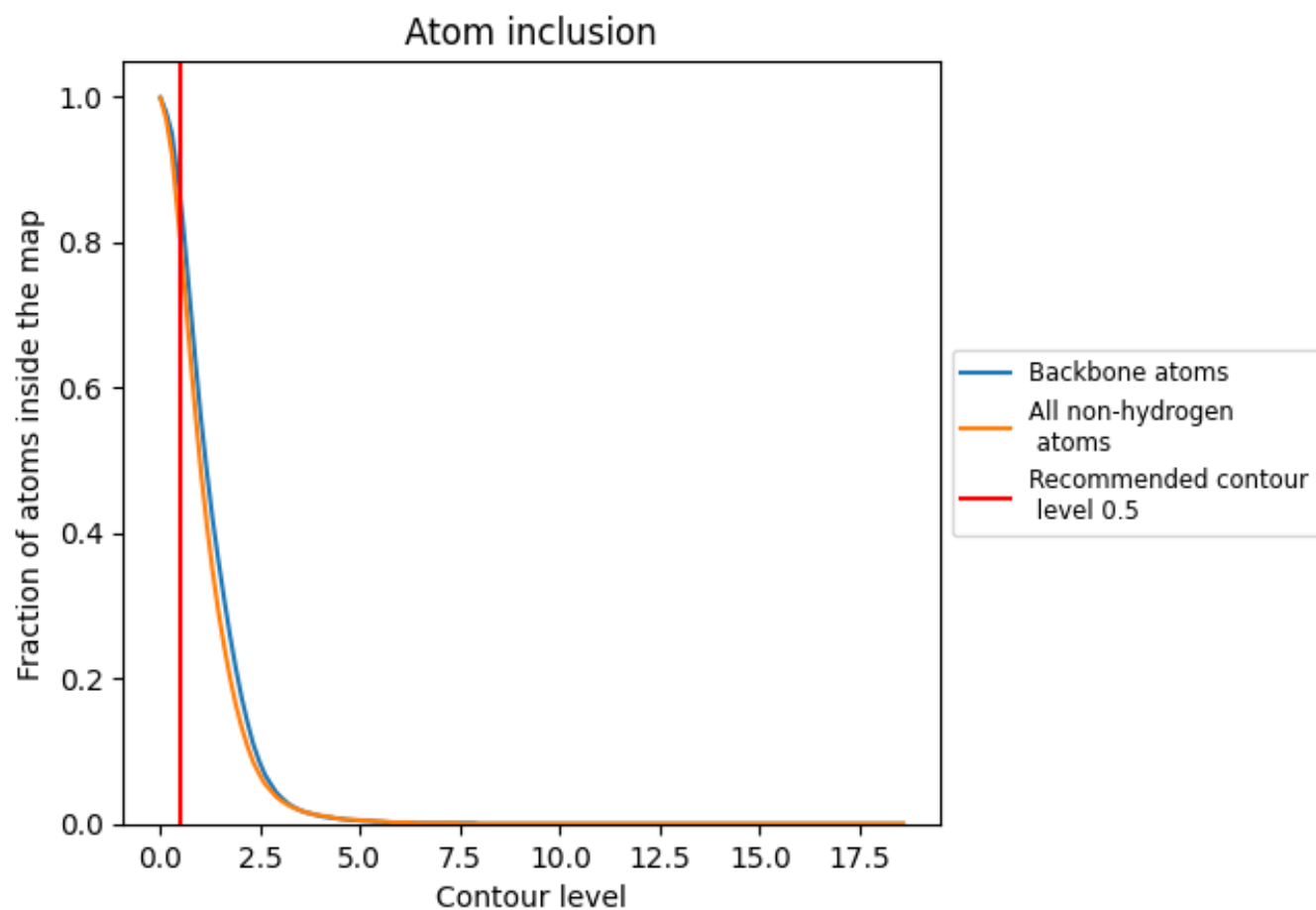
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 86% of all backbone atoms, 80% 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	 0.8020	 0.3950
2	 0.5630	 0.2660
3	 0.5380	 0.4030
5	 0.8480	 0.5340
6	 0.8030	 0.4220
A	 0.8350	 0.5420
B	 0.3040	 0.5060
C	 0.8790	 0.4650
D	 1.0000	 0.3820
DX	 0.9210	 0.0590
E	 0.9200	 0.4620
GC	 0.4460	 -0.0040
I	 0.9380	 0.3650
IN	 0.6210	 0.2400
J	 0.9000	 0.3530
K	 0.7450	 0.3650
L	 0.6610	 0.3380
L1	 0.4980	 0.0590
L2	 0.7280	 0.4880
M	 0.6000	 0.2670
N	 0.9040	 0.5650
O	 0.7280	 0.4280
P	 0.6940	 0.4430
Q	 0.9090	 0.3720
R	 0.6540	 0.4290
S	 0.7820	 0.2940
T	 0.9320	 0.5930
TF	 0.8500	 0.0880
W	 0.6520	 0.4200
YB	 0.6370	 0.3440
Z	 0.9140	 0.1620
a	 0.9550	 0.6080
b	 0.8480	 0.5350
c	 0.9240	 0.5820
d	 0.7100	 0.4780



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Chain	Atom inclusion	Q-score
e	 0.9140	 0.5860
f	 0.8730	 0.5710
g	 0.9050	 0.5820
q	 0.5070	 0.2720
r	 0.4570	 0.2470
s	 0.8390	 0.3930
t	 0.4820	 0.2270
y	 0.7930	 0.2600