



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 09:42 PM UTC

PDB ID : 6BK8 / pdb_00006bk8
EMDB ID : EMD-7109
Title : S. cerevisiae spliceosomal post-catalytic P complex
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2017-11-07
Resolution : 3.30 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.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

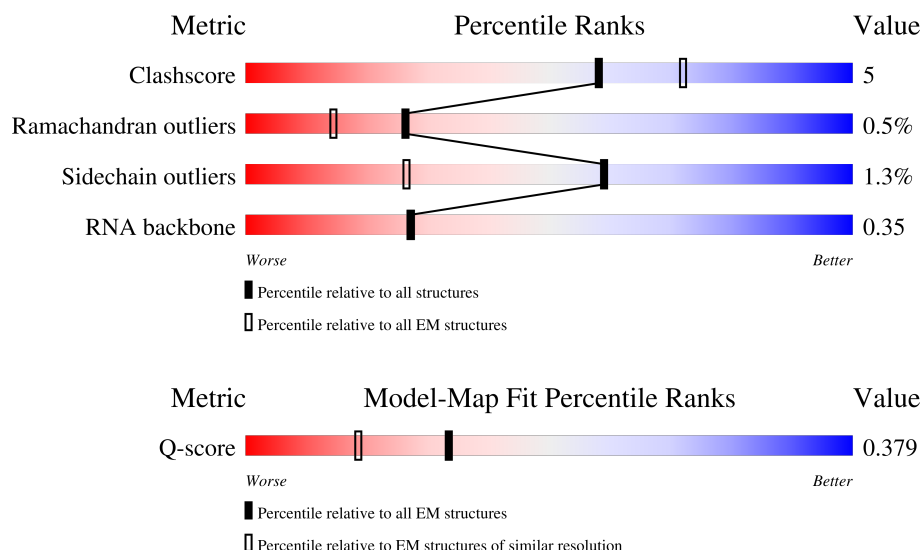
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	1175	9% 7% 89%
2	5	214	10% 32% 13% 52%
3	6	112	15% 53% 33% 5% 9%

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Mol	Chain	Length	Quality of chain
4	e	34	
5	i	59	
6	A	2413	
7	B	1008	
8	D	451	
9	E	379	
10	F	364	
11	G	339	
12	H	175	
13	I	157	
14	K	135	
15	L	577	
16	M	455	
17	N	251	
18	O	382	
19	P	1145	
20	R	215	
21	S	590	
22	T	687	
23	U	859	
24	X	219	
25	Y	16	
26	a	110	
26	q	110	
27	b	86	

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Mol	Chain	Length	Quality of chain
27	m	86	
28	c	94	
28	l	94	
29	d	77	
29	n	77	
30	f	196	
30	k	196	
31	g	101	
31	o	101	
32	h	146	
32	p	146	
33	r	111	
34	s	238	
35	u	503	
35	v	503	
35	w	503	
35	x	503	
36	y	175	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 82745 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	135	Total	C	N	O	P	0	0
			2848	1272	472	969	135		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	103	Total	C	N	O	P	0	0
			2173	973	367	730	103		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	102	Total	C	N	O	P	0	0
			2170	972	386	710	102		

- Molecule 4 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	34	Total	C	N	O	P	0	0
			707	319	107	247	34		

- Molecule 5 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	59	Total	C	N	O	P	0	0
			1239	558	202	420	59		

- Molecule 6 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1960	Total	C	N	O	S	0	0
			16159	10381	2786	2933	59		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	899	Total	C	N	O	S	0	0
			7179	4638	1191	1321	29		

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	359	Total	C	N	O	S	0	0
			2826	1786	497	533	10		

- Molecule 9 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1494	939	276	273	6		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	199	Total	C	N	O	S	0	0
			1576	991	277	293	15		

- Molecule 11 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	255	Total	C	N	O	S	0	0
			2048	1297	362	378	11		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	70	Total	C	N	O	S	0	0
			570	357	113	99	1		

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	156	Total	C	N	O	S	0	0
			1283	803	239	231	10		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	82	Total	C	N	O	S	0	0
			550	332	106	111	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	412	Total	C	N	O	S	0	0
			3353	2160	556	620	17		

- Molecule 16 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	326	Total	C	N	O	S	0	0
			2607	1649	465	485	8		

- Molecule 17 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	167	Total	C	N	O	S	0	0
			1326	856	233	233	4		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	229	Total	C	N	O	S	0	0
			1935	1211	347	368	9		

- Molecule 19 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	653	Total	C	N	O	S	0	0
			3872	2393	736	740	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	101	Total	C	N	O	S	0	0
			813	499	150	163	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	238	Total	C	N	O	S	0	0
			1948	1218	355	368	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	483	Total	C	N	O	S	0	0
			3370	2113	624	625	8		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	637	Total	C	N	O	S	0	0
			3625	2226	689	703	7		

- Molecule 24 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	219	Total	C	N	O	0	0
			1095	657	219	219		

- Molecule 25 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
26	q	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
27	m	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	l	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
29	n	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
30	k	78	Total	C	N	O	S	0	0
			610	389	109	109	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	o	78	Total	C	N	O	S	0	0
			600	384	104	110	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
32	p	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 33 is a protein called Lea1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 34 is a protein called Msl1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 35 is a protein called Pre-mRNA-processing factor Prp19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	u	435	Total	C	N	O	0	0
			2156	1286	435	435		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	438	Total	C	N	O	0	0
			2171	1295	438	438		
35	x	116	Total	C	N	O	0	0
			578	346	116	116		

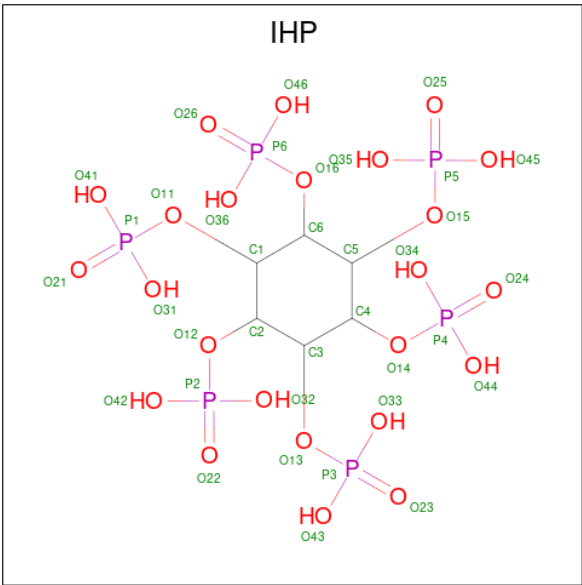
- Molecule 36 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	110	Total	C	N	O	0	0
			548	328	110	110		

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

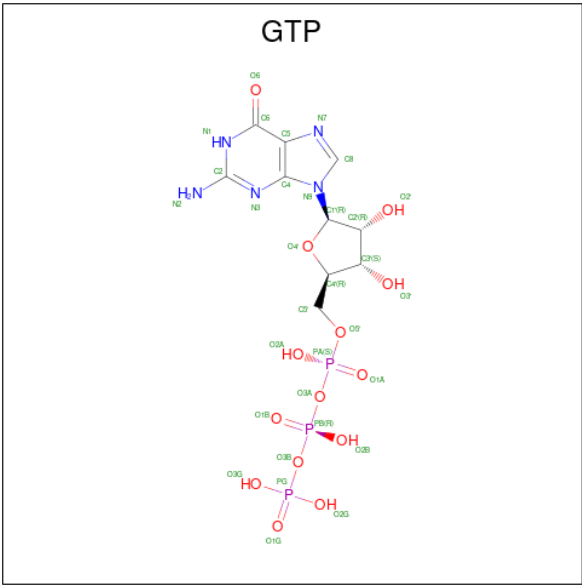
Mol	Chain	Residues	Atoms		AltConf
37	6	4	Total	Mg	0
			4	4	
37	B	1	Total	Mg	0
			1	1	

- 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	

- 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	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

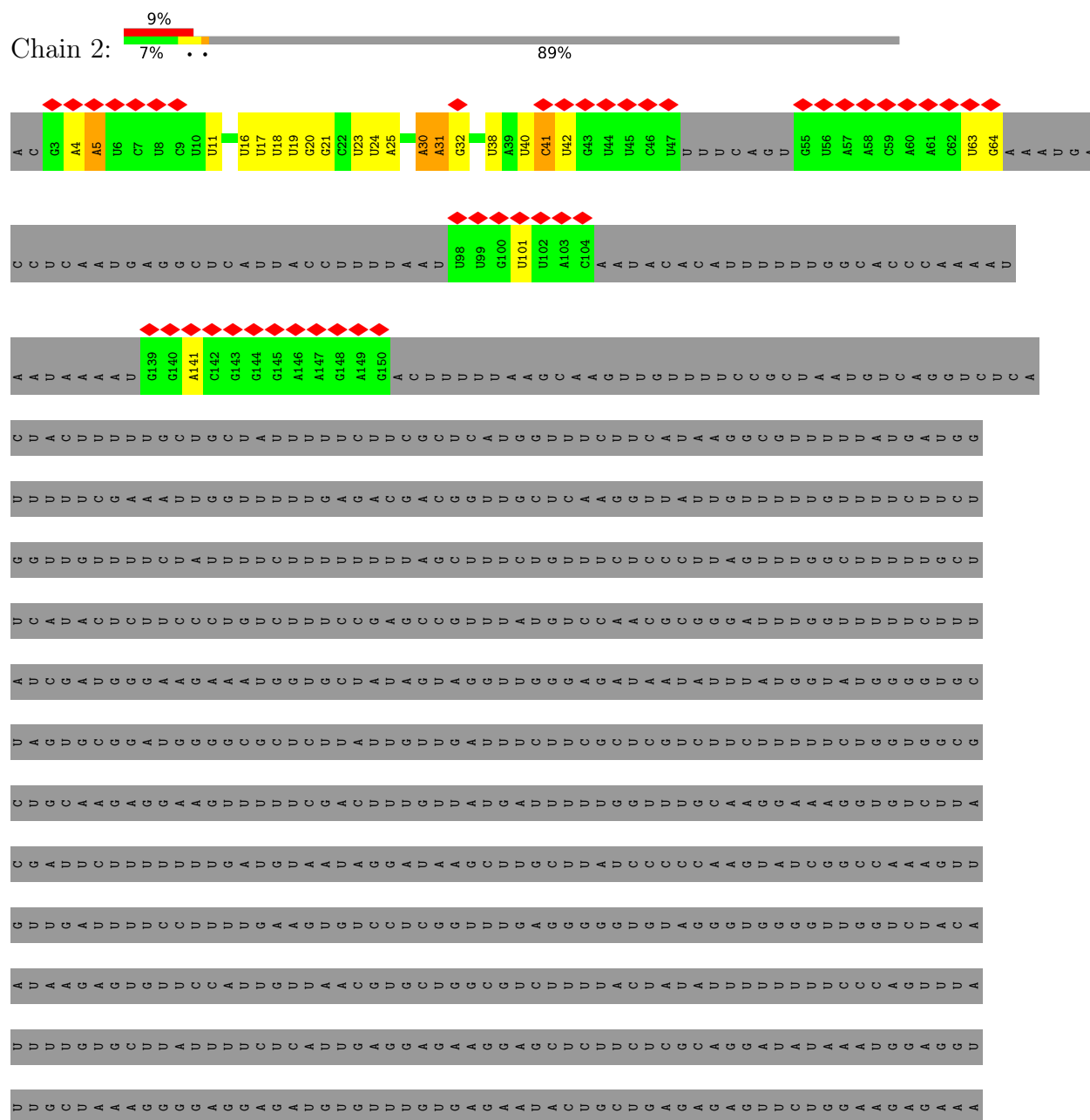
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

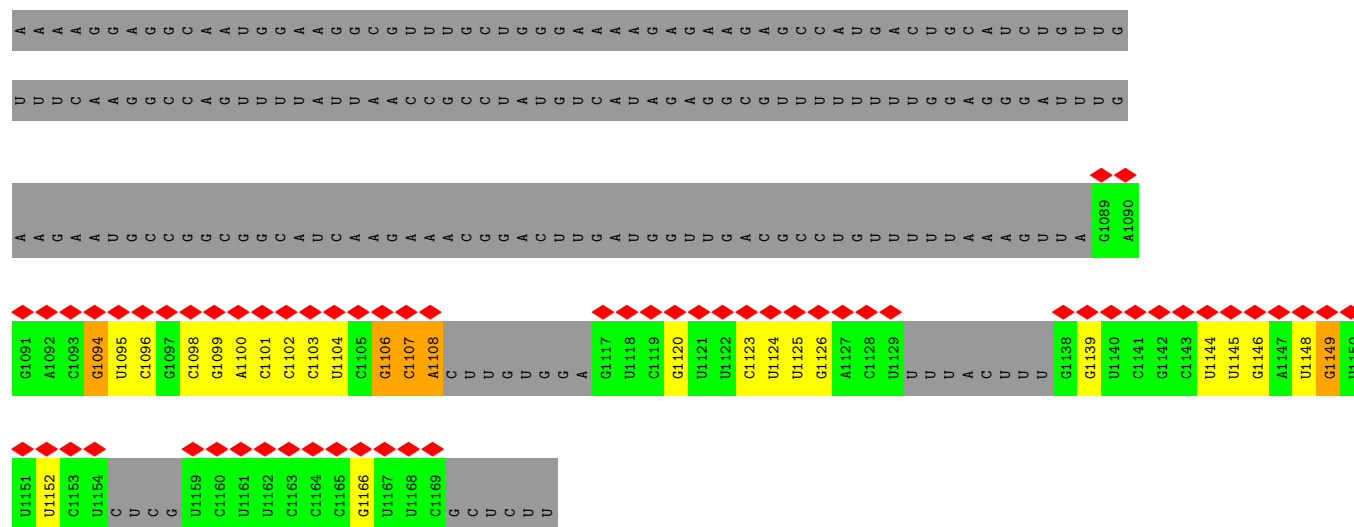
Mol	Chain	Residues	Atoms		AltConf
40	F	2	Total 2	Zn 2	0
40	G	1	Total 1	Zn 1	0
40	I	3	Total 3	Zn 3	0
40	O	1	Total 1	Zn 1	0

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.

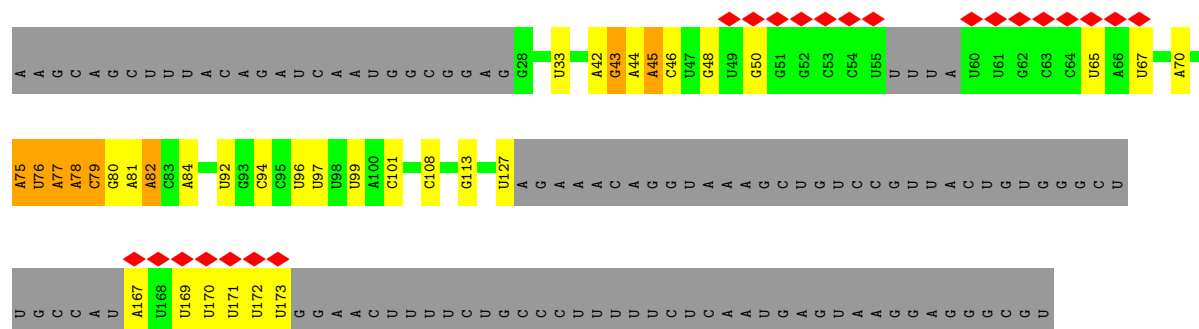
• Molecule 1: U2 snRNA





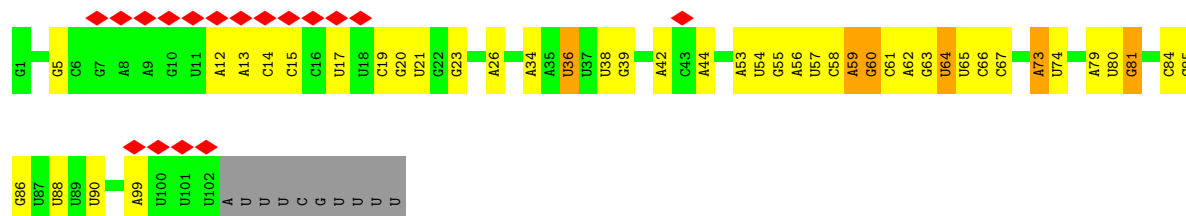
• Molecule 2: U5 snRNA

Chain 5: 10% 32% 13% 52%



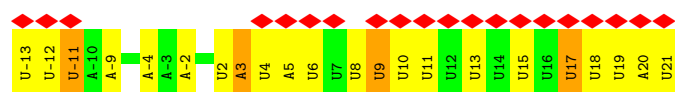
• Molecule 3: U6 snRNA

Chain 6: 15% 53% 33% 5% 9%



• Molecule 4: RNA (34-MER)

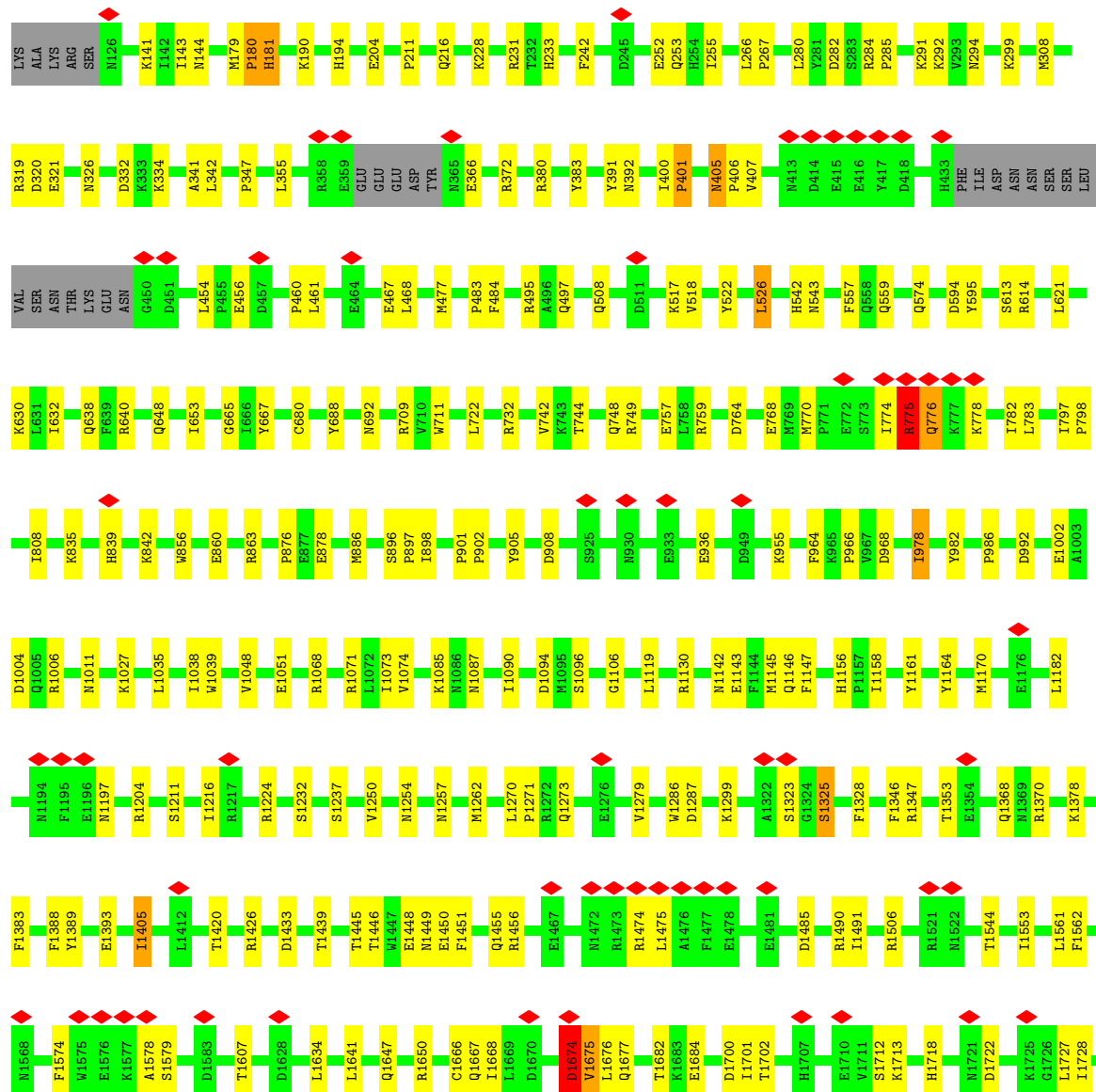
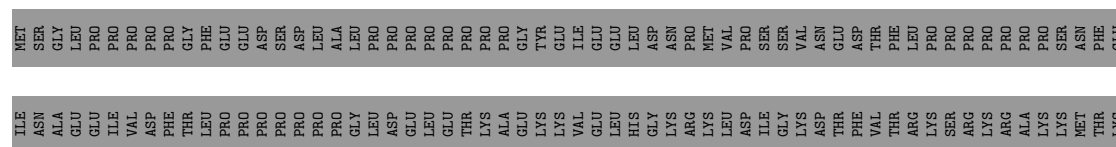
Chain e: 35% 59% 53% 12%

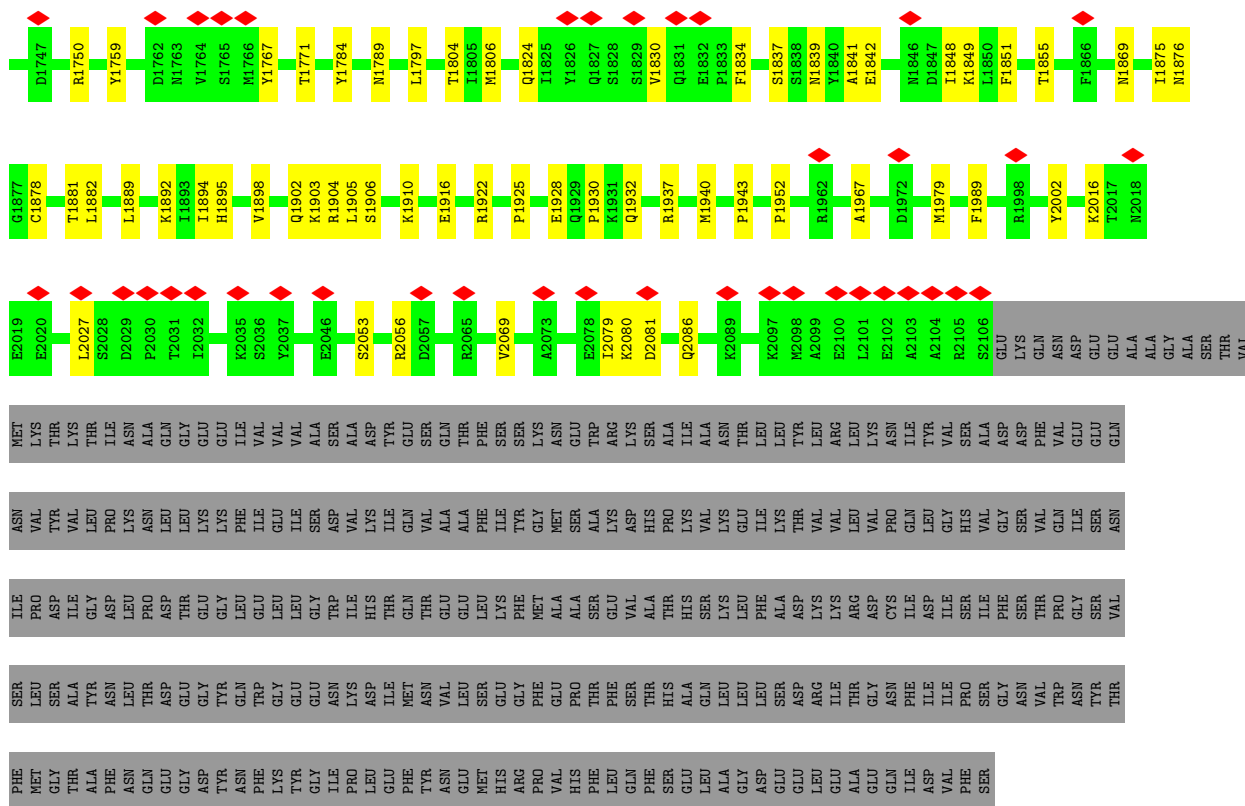


• Molecule 5: RNA (59-MER)

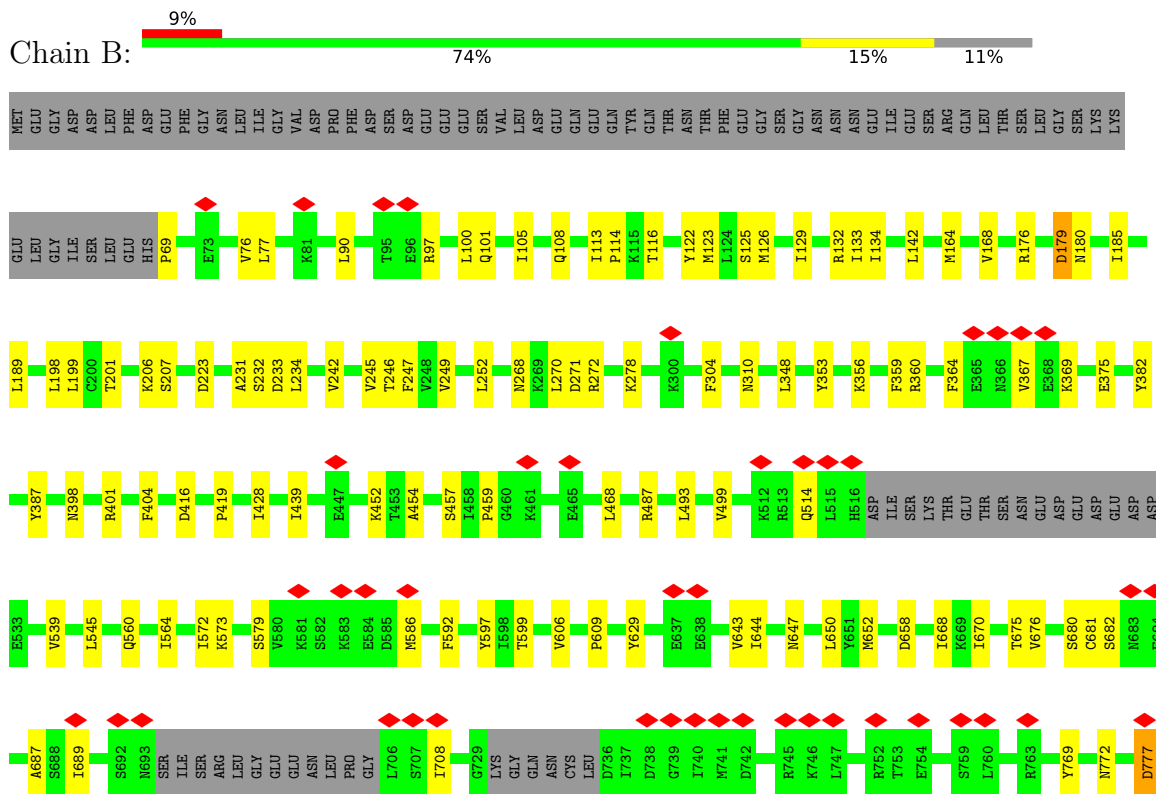


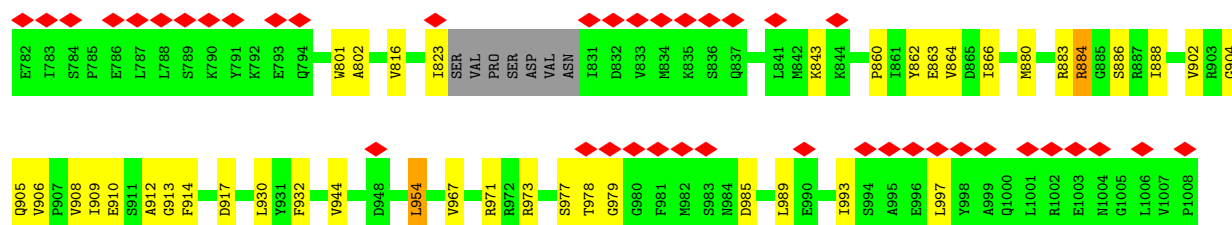
• Molecule 6: Pre-mRNA-splicing factor Prp8



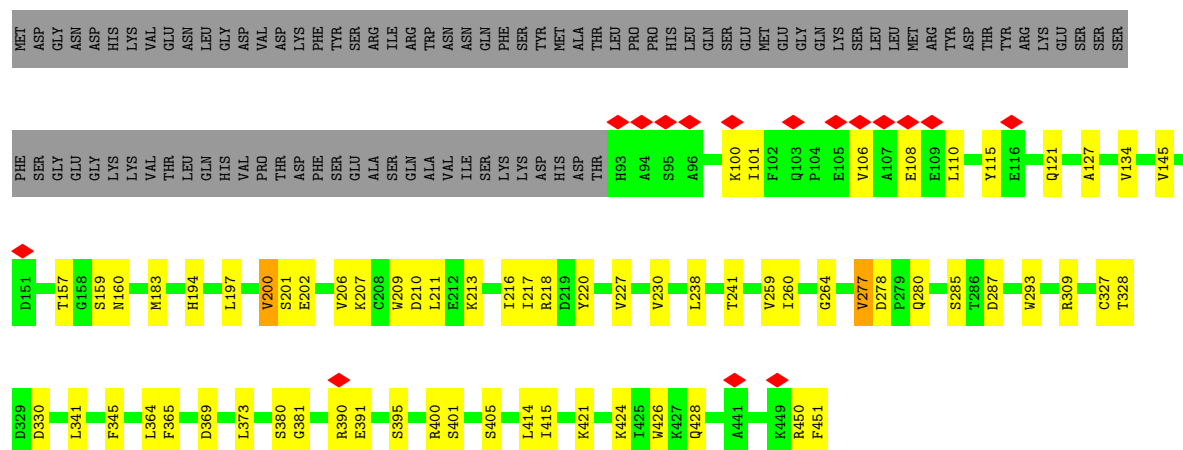


- Molecule 7: Pre-mRNA-splicing factor SNU114

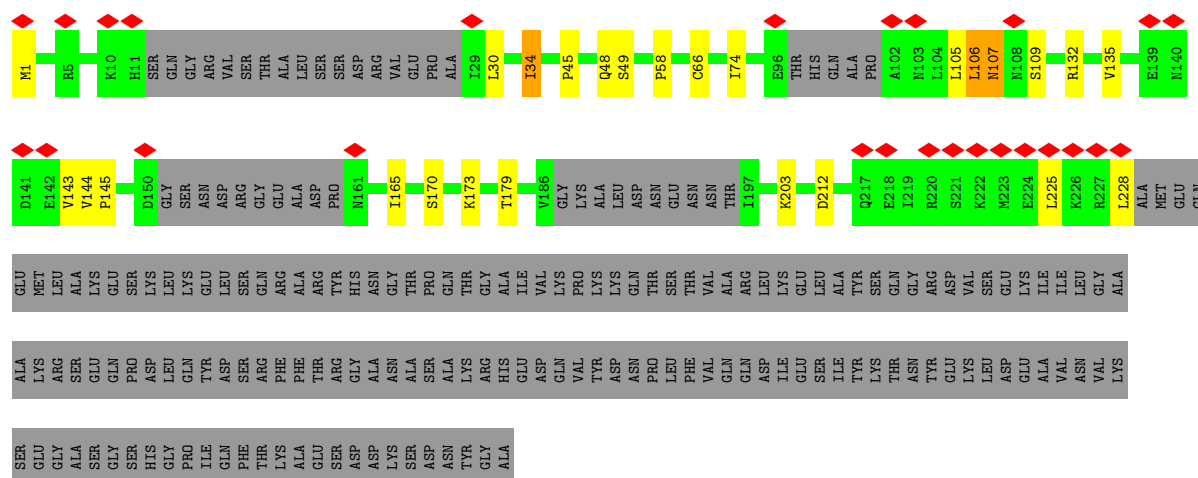
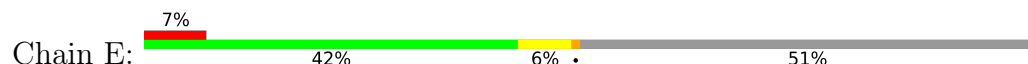




• Molecule 8: Pre-mRNA-splicing factor PRP46

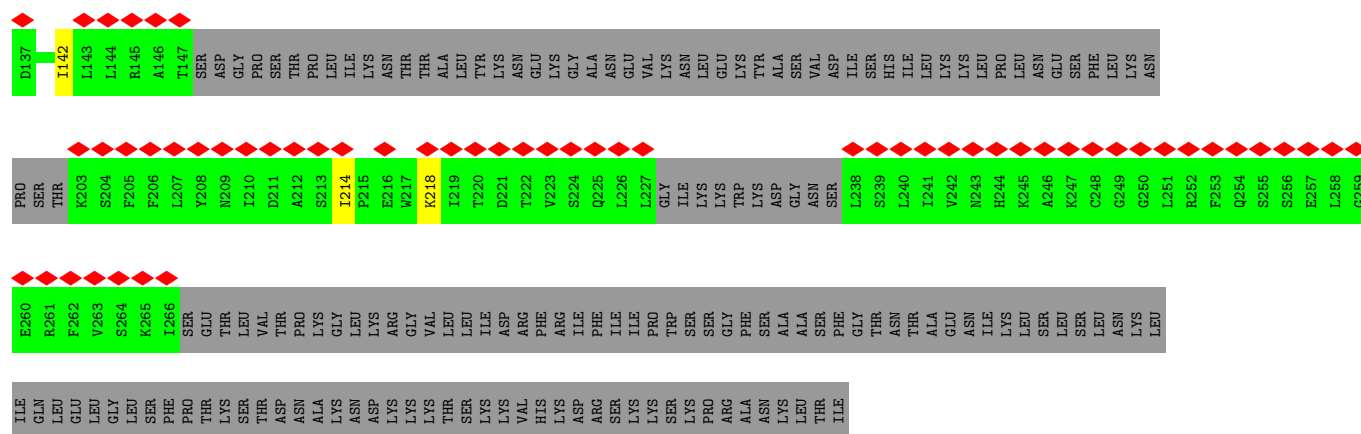


• Molecule 9: Pre-mRNA-processing protein 45

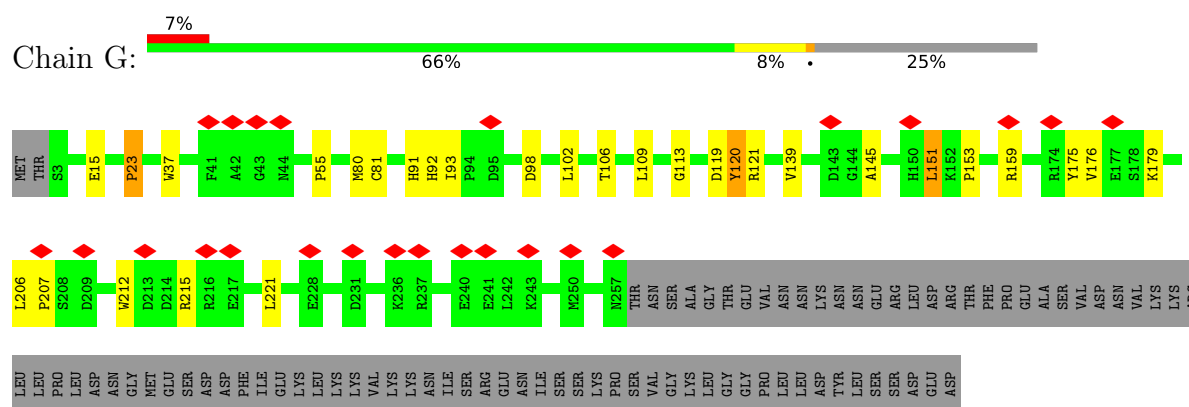


• Molecule 10: Pre-mRNA-splicing factor SLT11

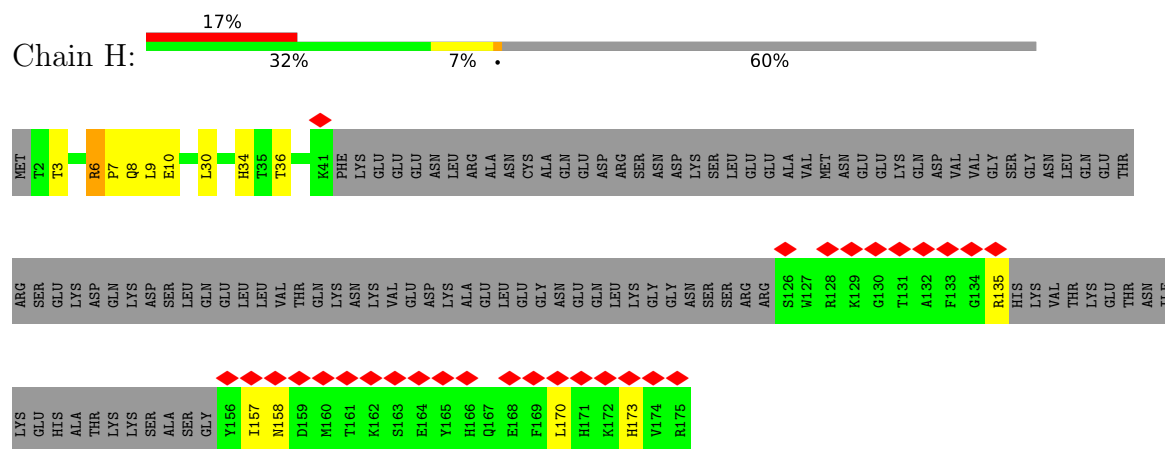




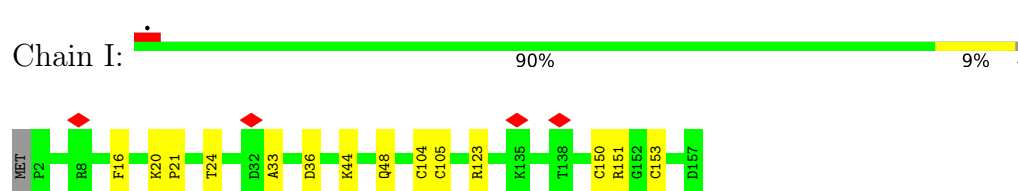
• Molecule 11: Pre-mRNA-splicing factor CWC2



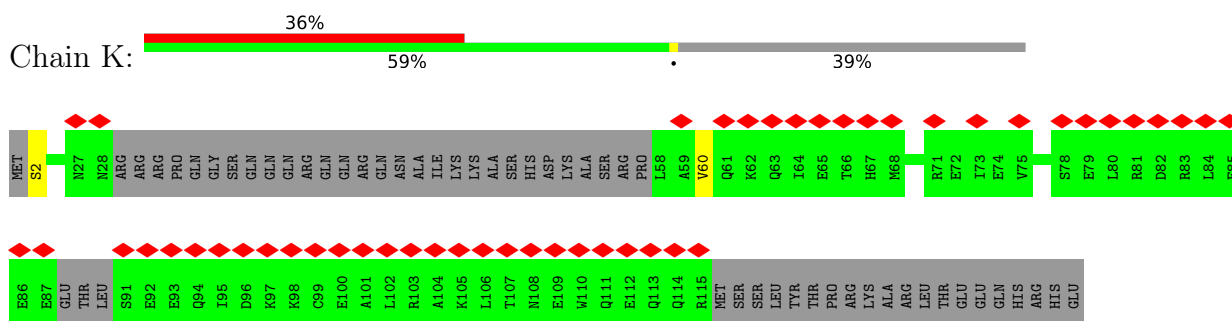
• Molecule 12: Pre-mRNA-splicing factor CWC15



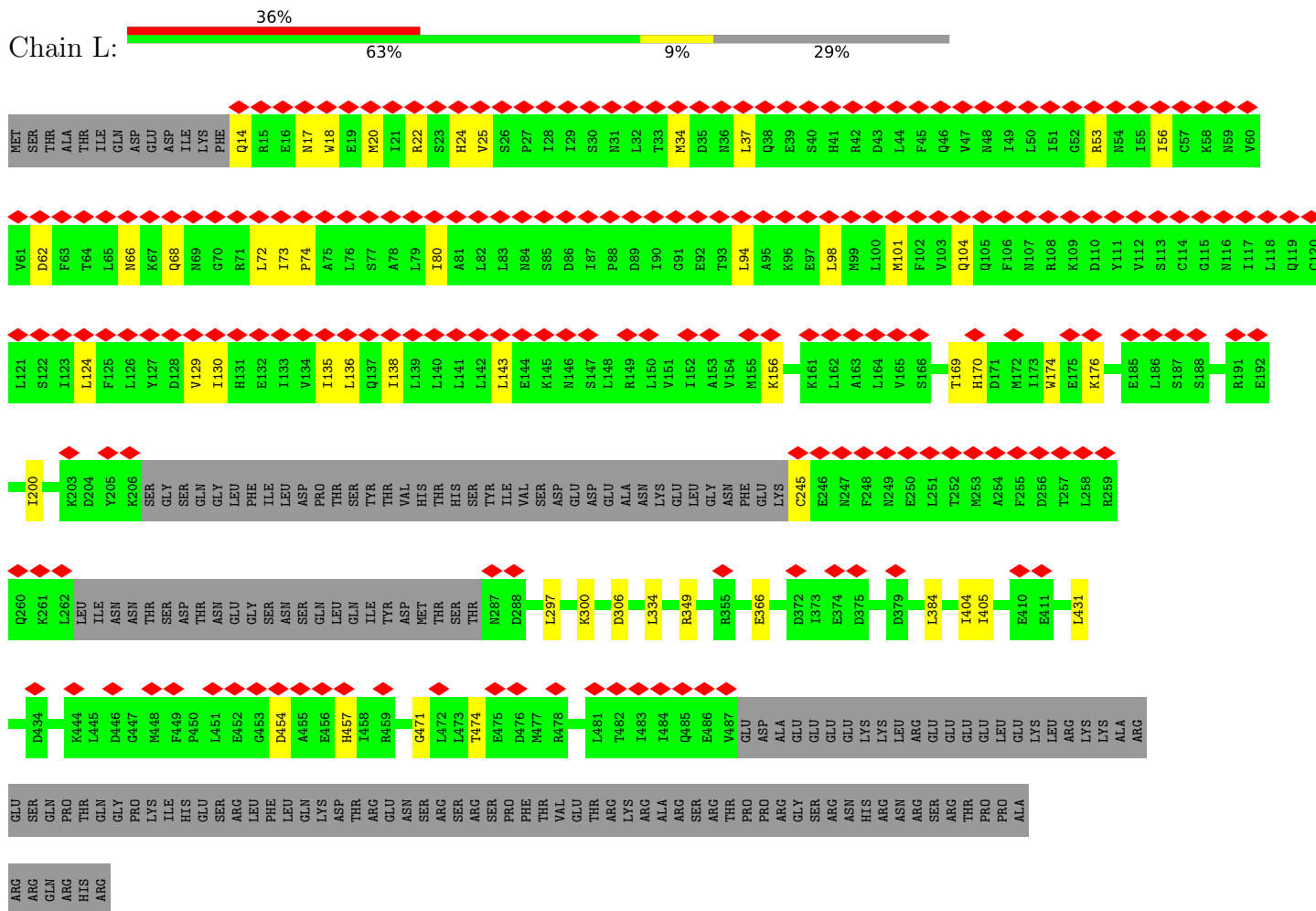
• Molecule 13: Pre-mRNA-splicing factor BUD31



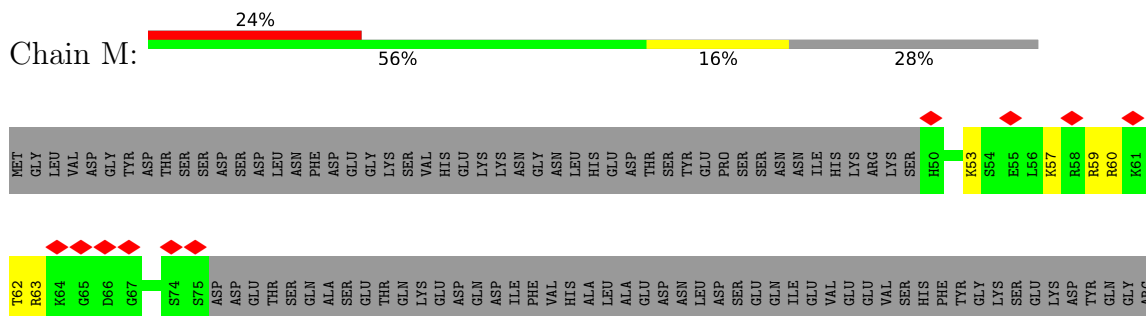
• Molecule 14: Pre-mRNA-splicing factor CWC21

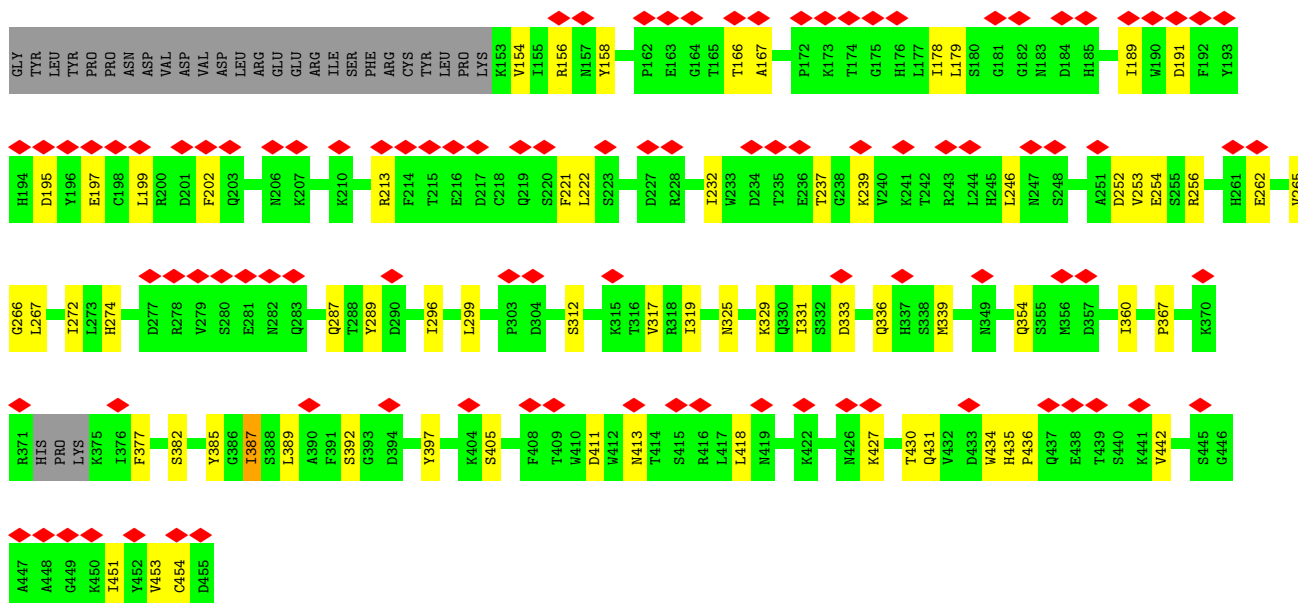


- Molecule 15: Pre-mRNA-splicing factor CWC22

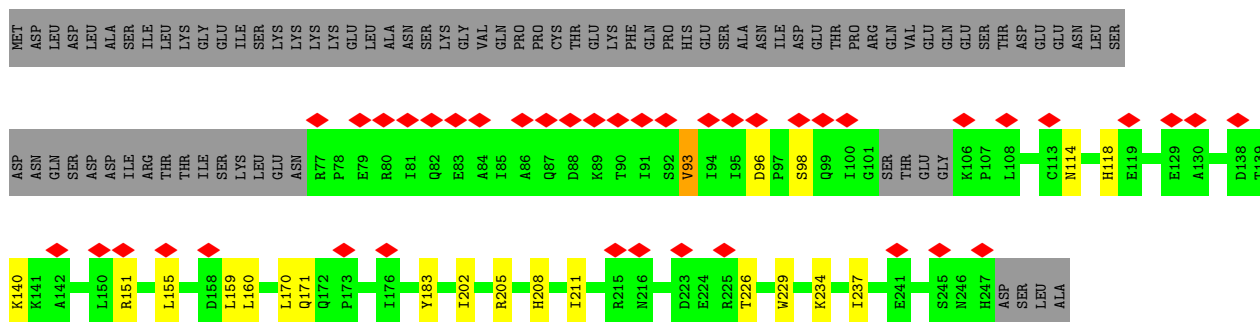


- Molecule 16: Pre-mRNA-processing factor Prp17

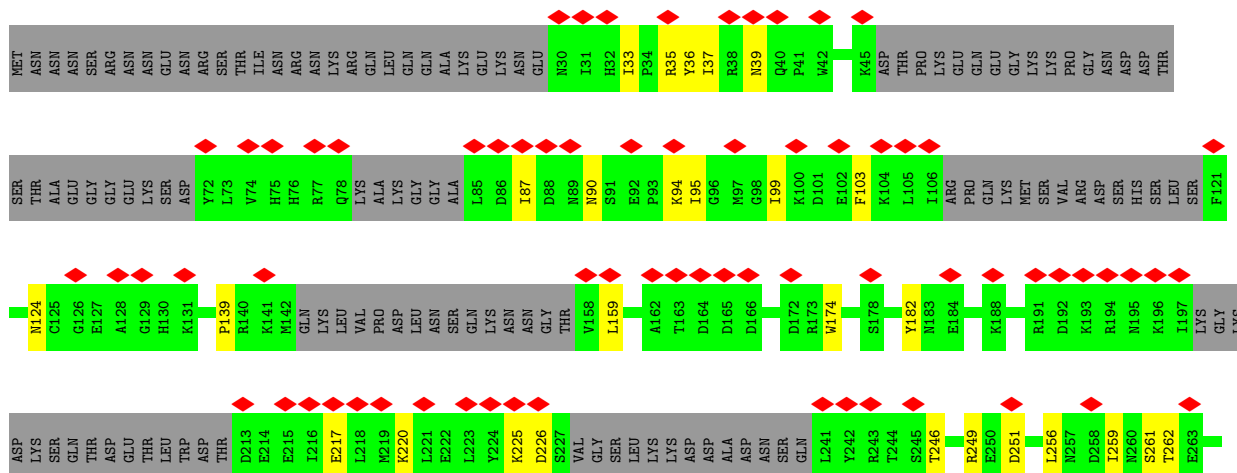




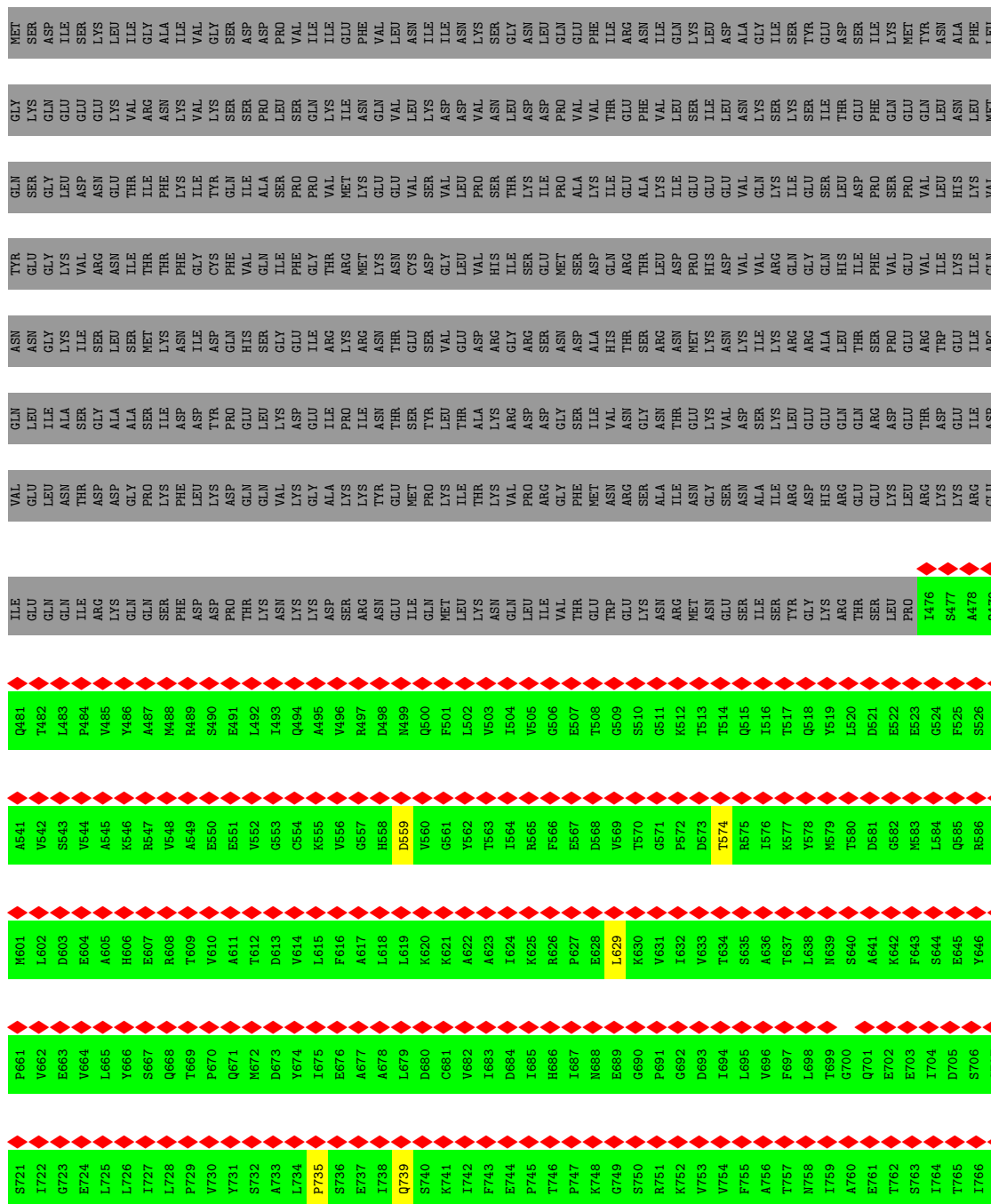
- Molecule 17: Pre-mRNA-splicing factor Prp18

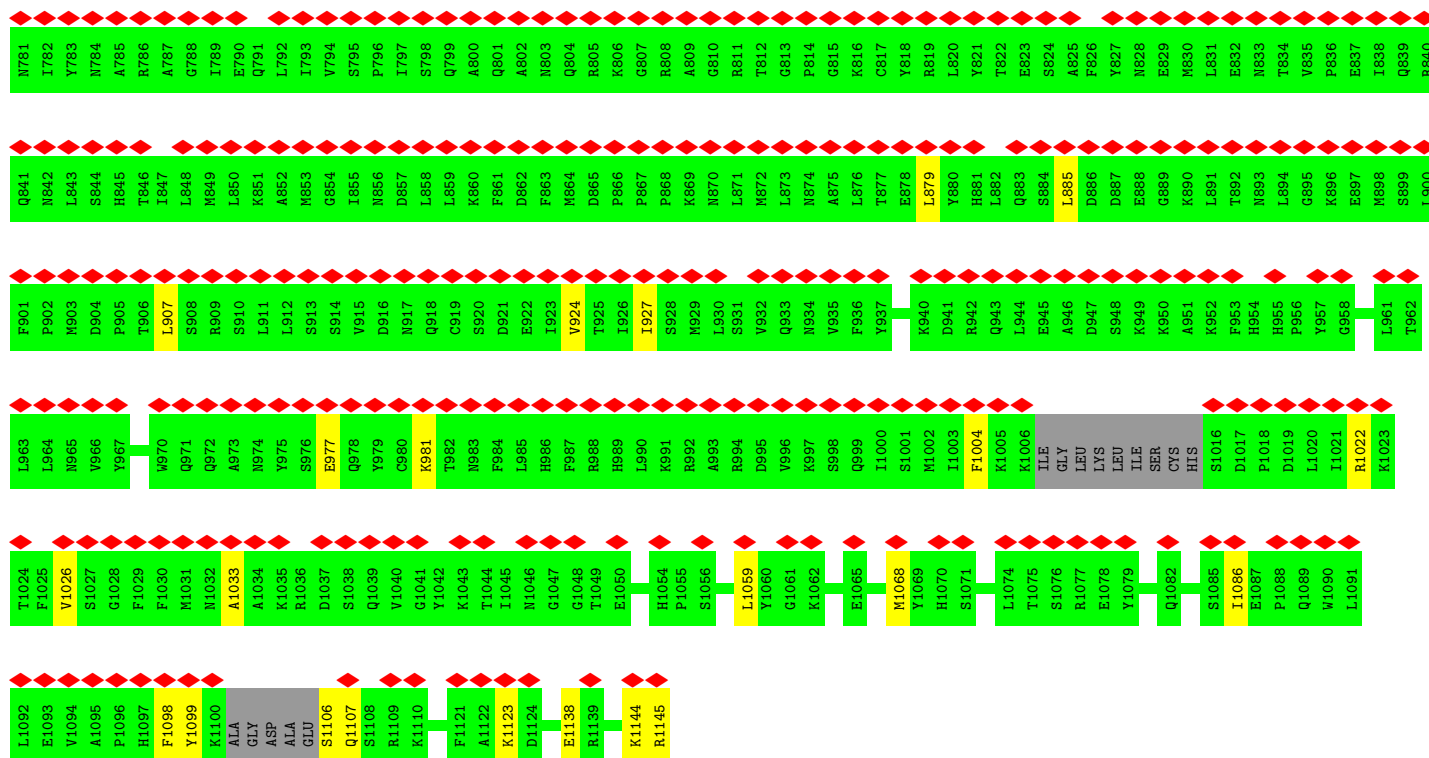


- Molecule 18: Pre-mRNA-splicing factor SLU7

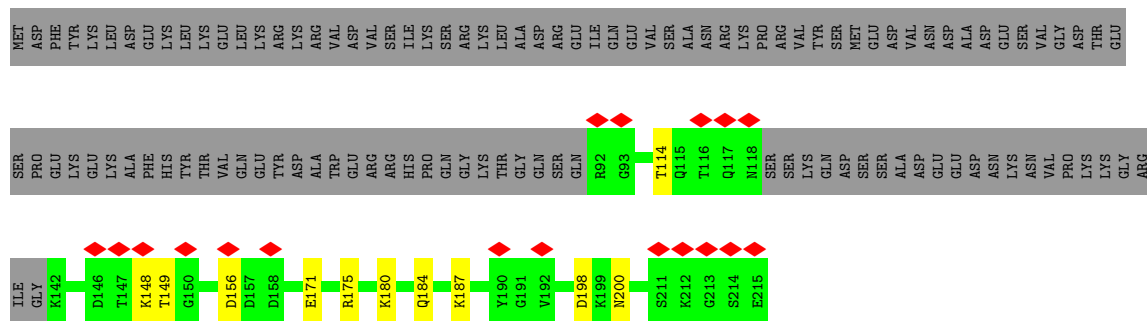
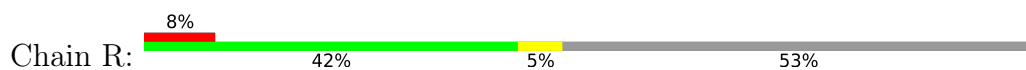


- Molecule 19: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22

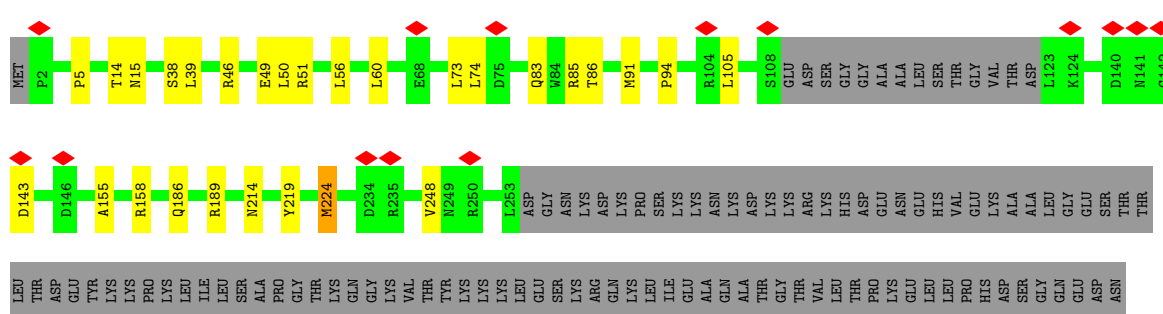
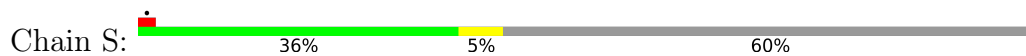




• Molecule 20: Pre-mRNA-splicing factor SYF2

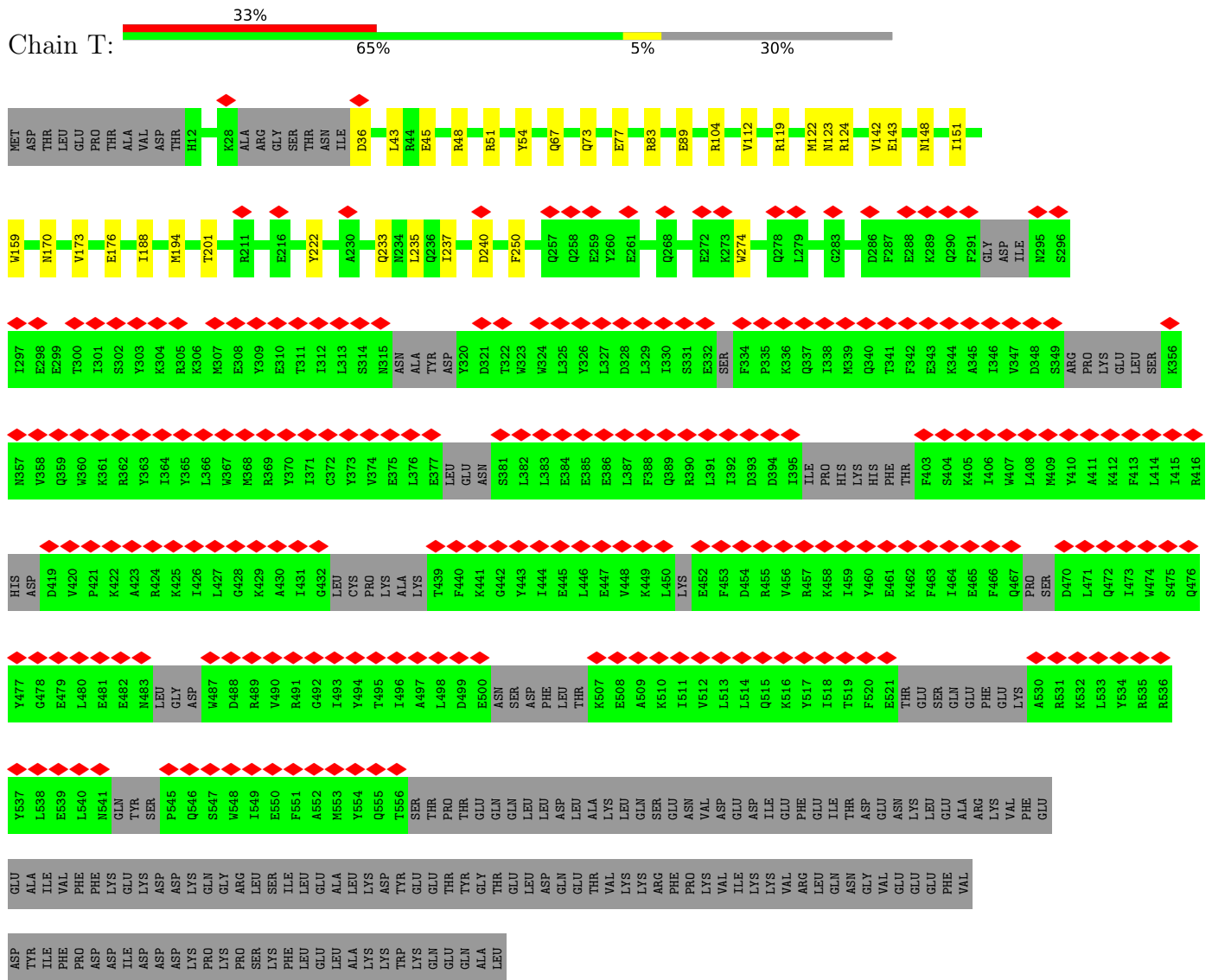


• Molecule 21: Pre-mRNA-splicing factor CEF1



[illegible]

- Molecule 22: Pre-mRNA-splicing factor CLF1



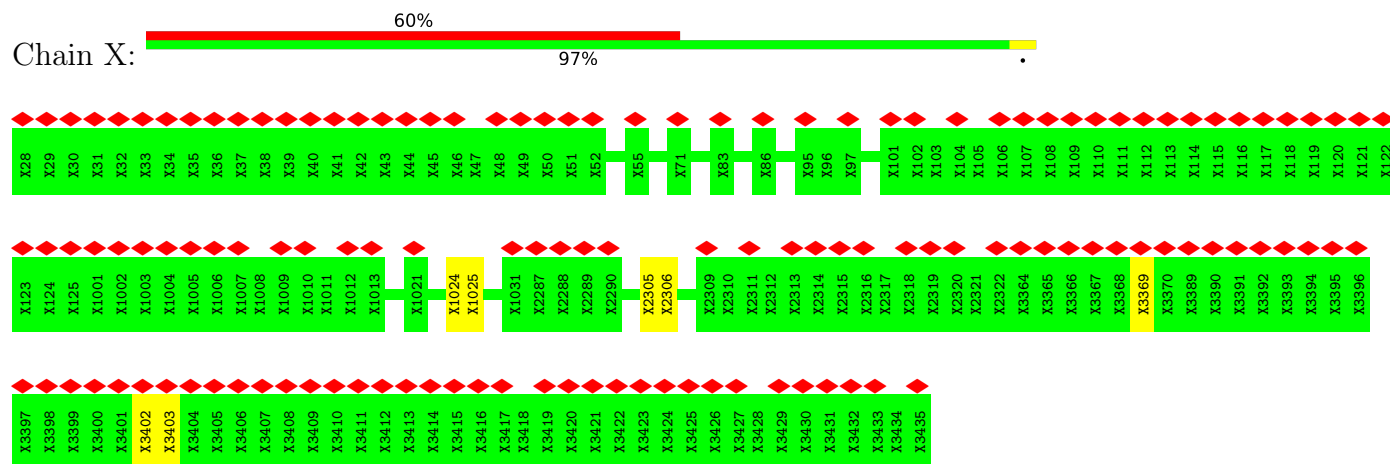
- Molecule 23: Pre-mRNA-splicing factor SYF1



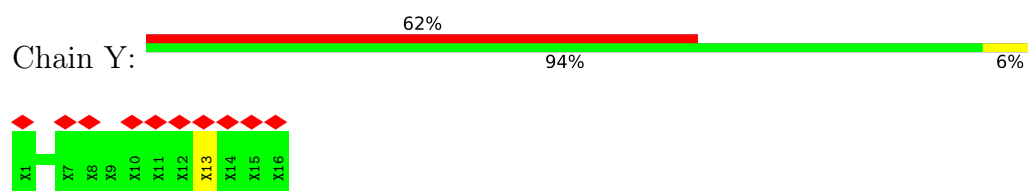


THR
GLN
SER
THR
SER
SER
TVR
SER
ILE
ASN
PRO
ASP
GLU
ILE
GLU
LEU
ASP
ILE

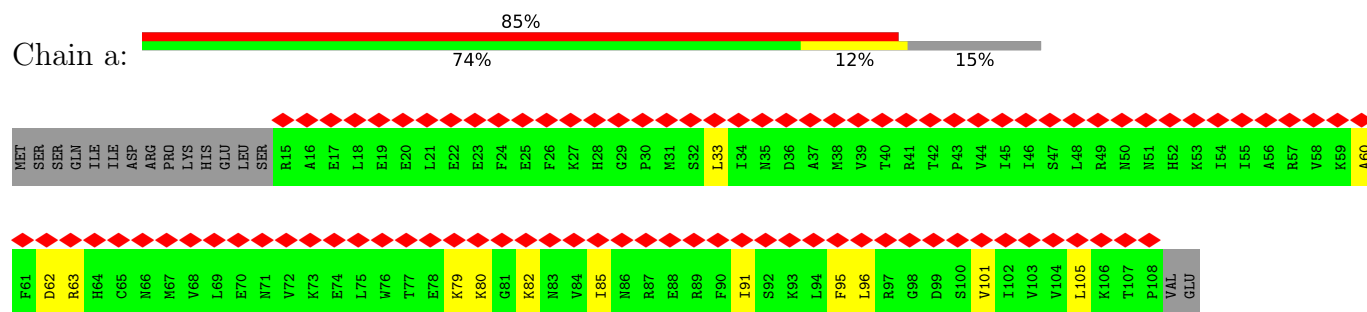
• Molecule 24: Unknown protein fragment



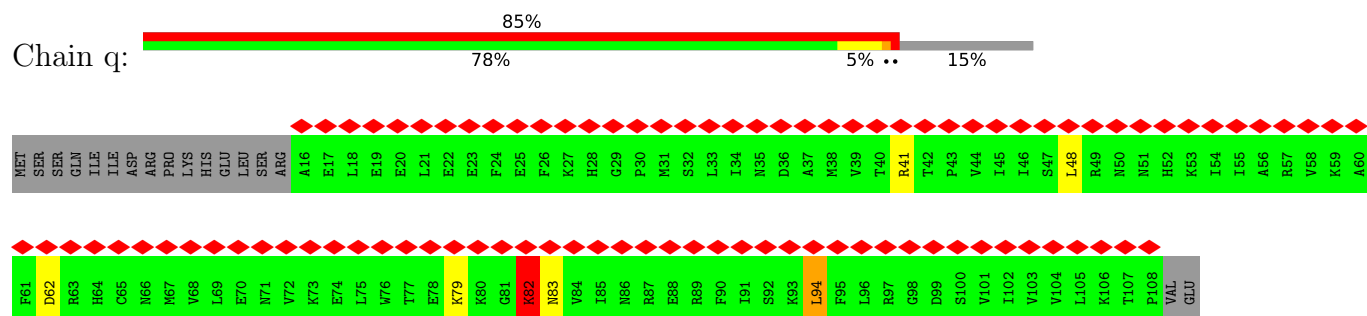
• Molecule 25: Unknown protein fragment



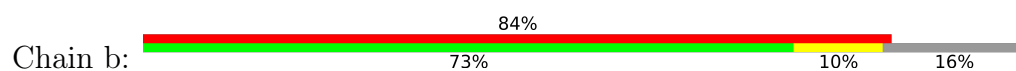
• Molecule 26: Small nuclear ribonucleoprotein Sm D2

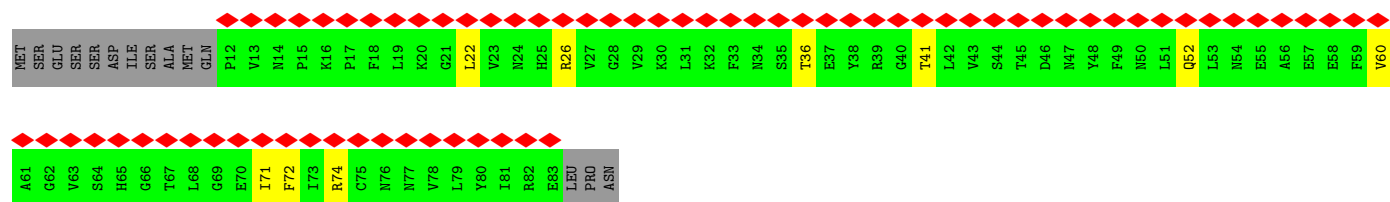


• Molecule 26: Small nuclear ribonucleoprotein Sm D2

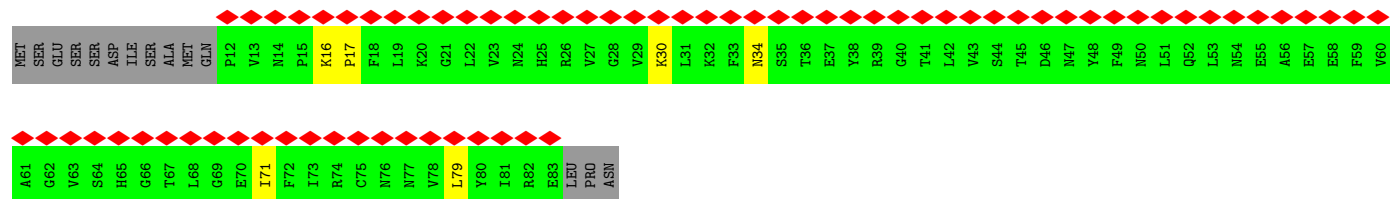
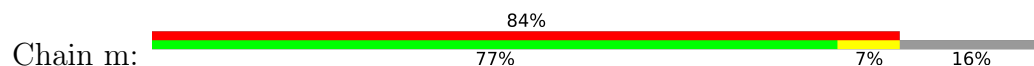


• Molecule 27: Small nuclear ribonucleoprotein F

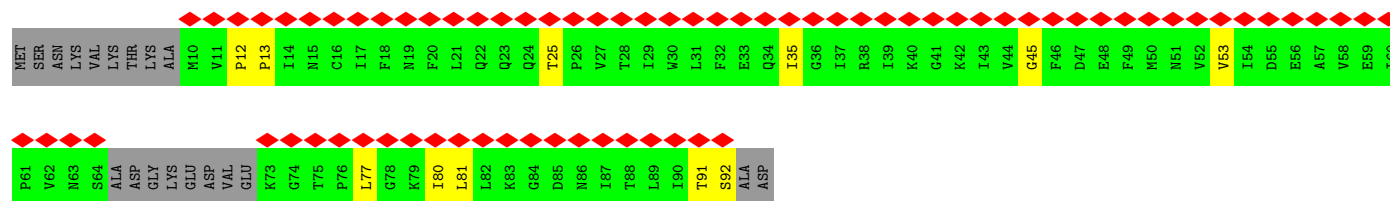
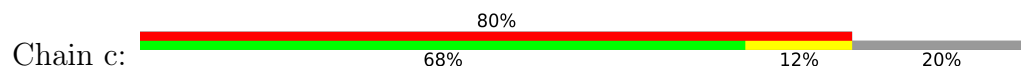




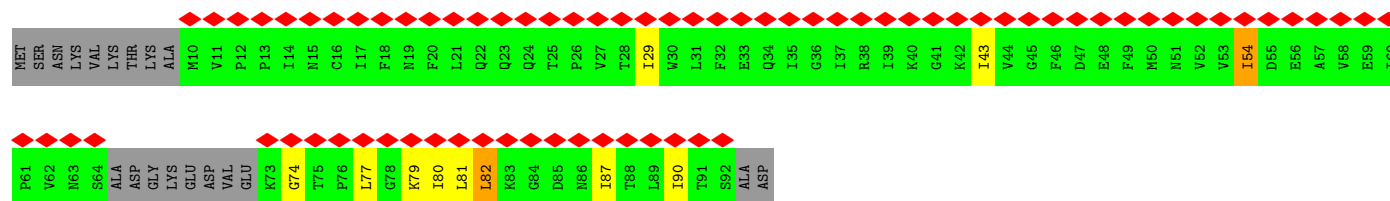
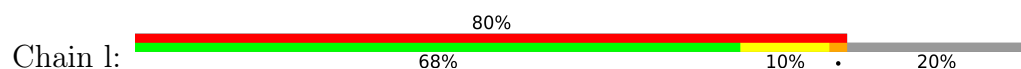
• Molecule 27: Small nuclear ribonucleoprotein F



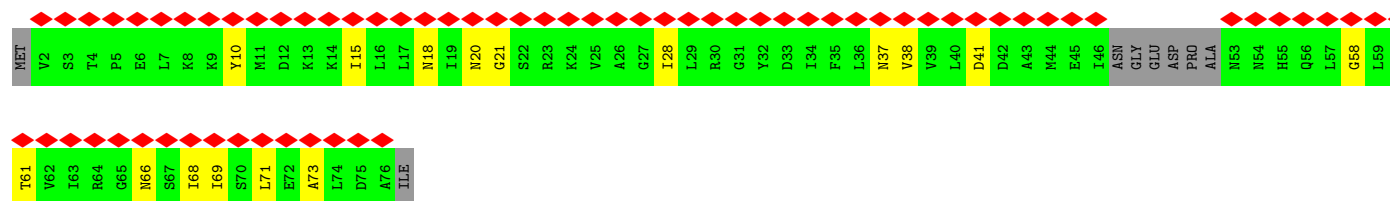
• Molecule 28: Small nuclear ribonucleoprotein E



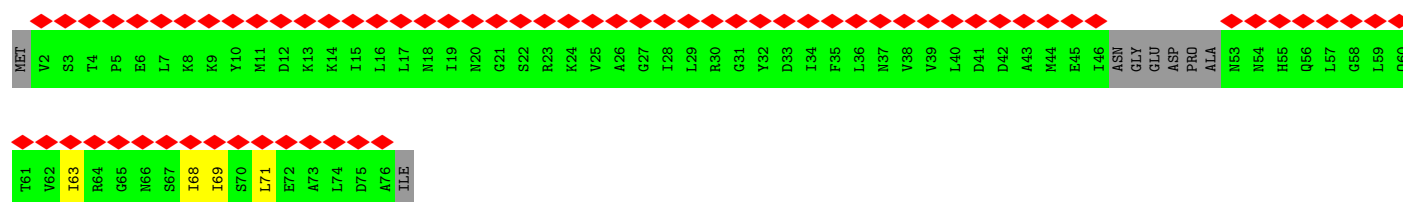
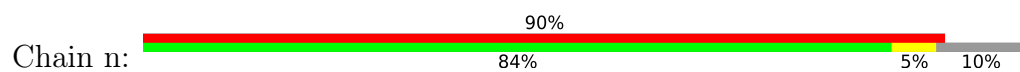
• Molecule 28: Small nuclear ribonucleoprotein E



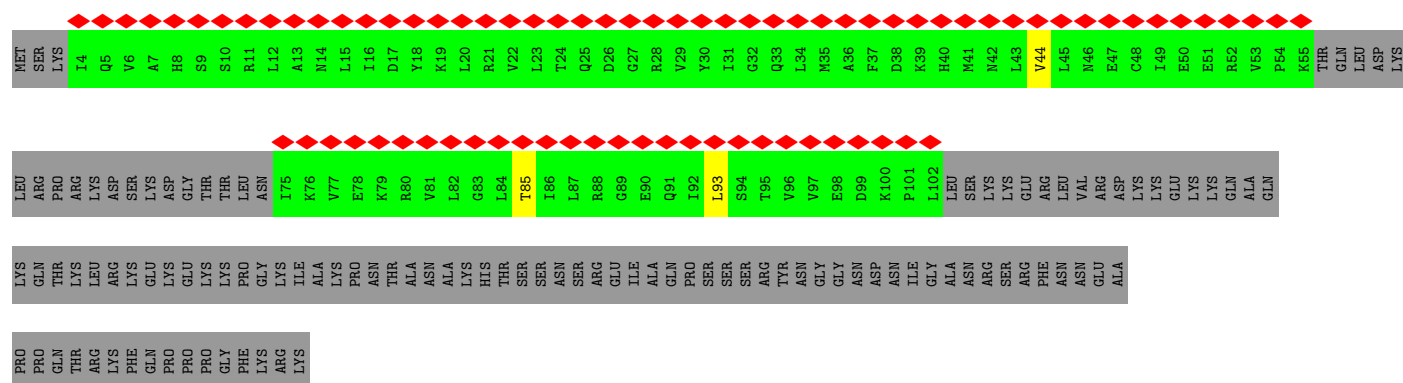
• Molecule 29: Small nuclear ribonucleoprotein G



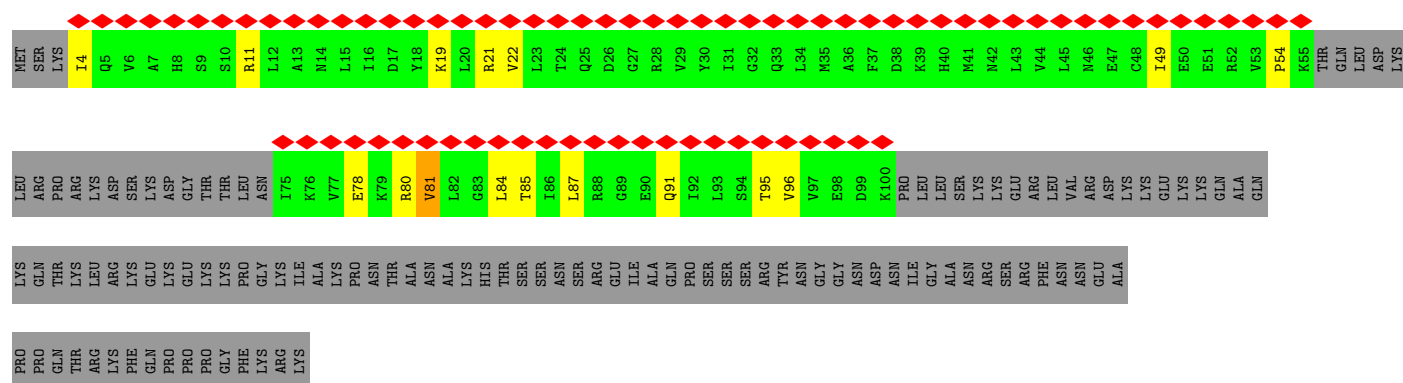
• Molecule 29: Small nuclear ribonucleoprotein G



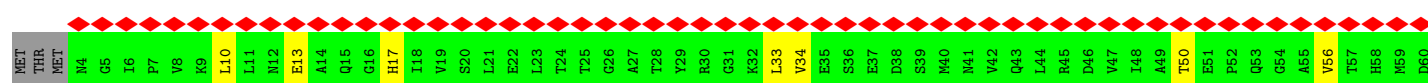
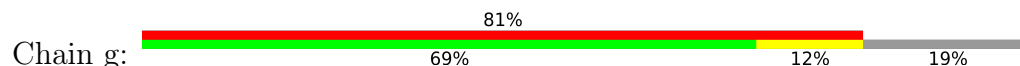
• Molecule 30: Small nuclear ribonucleoprotein-associated protein B

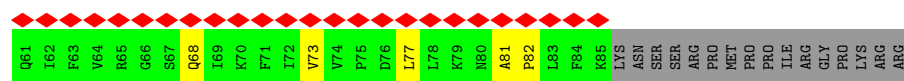


• Molecule 30: Small nuclear ribonucleoprotein-associated protein B

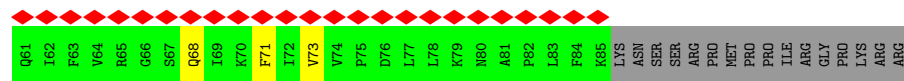
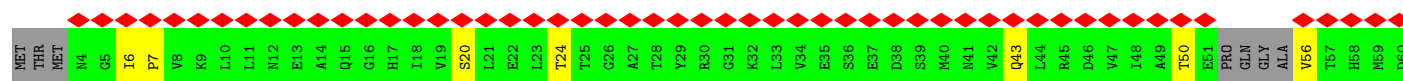
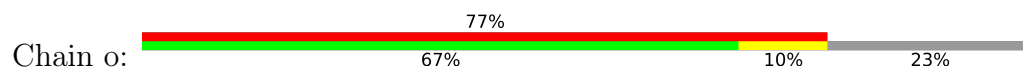


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

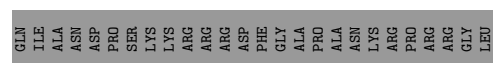
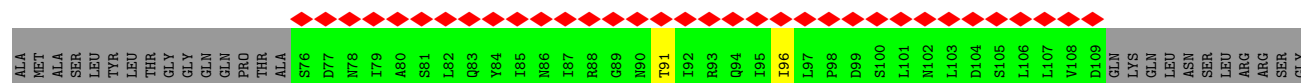




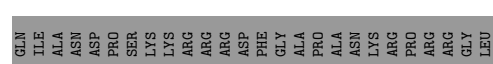
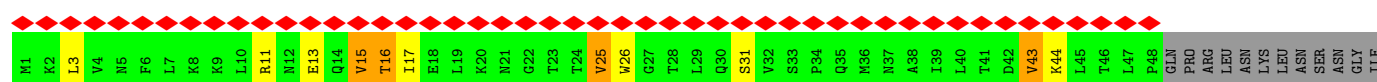
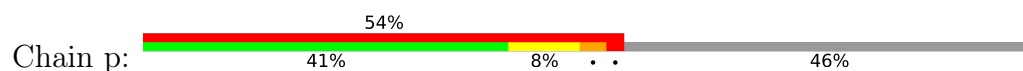
• Molecule 31: Small nuclear ribonucleoprotein Sm D3



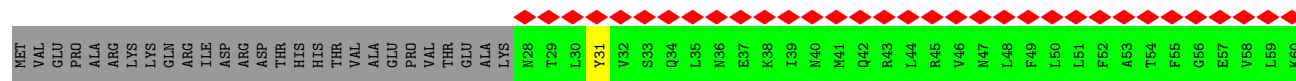
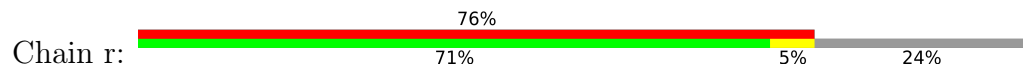
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

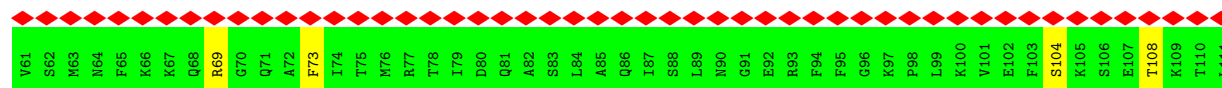


• Molecule 32: Small nuclear ribonucleoprotein Sm D1

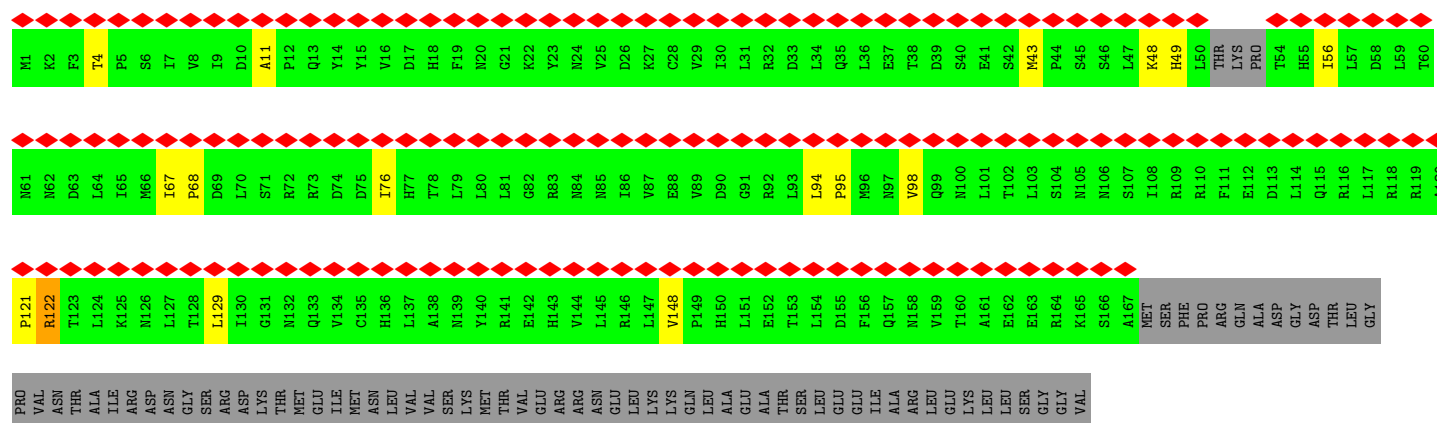


• Molecule 33: Lea1

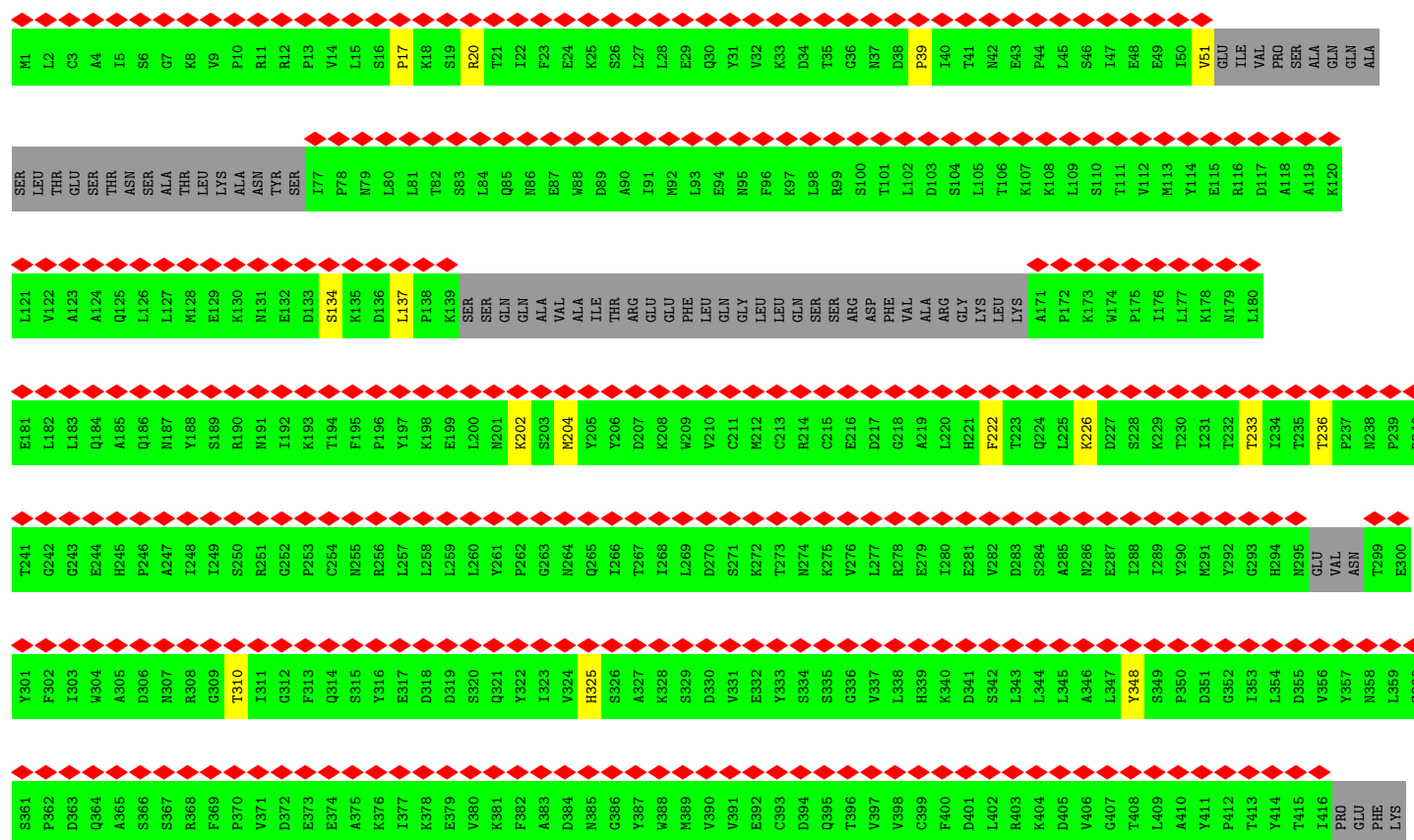
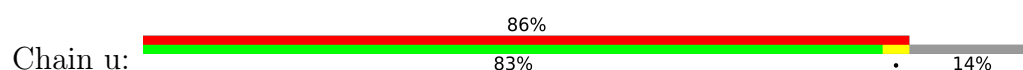




• Molecule 34: Msl1

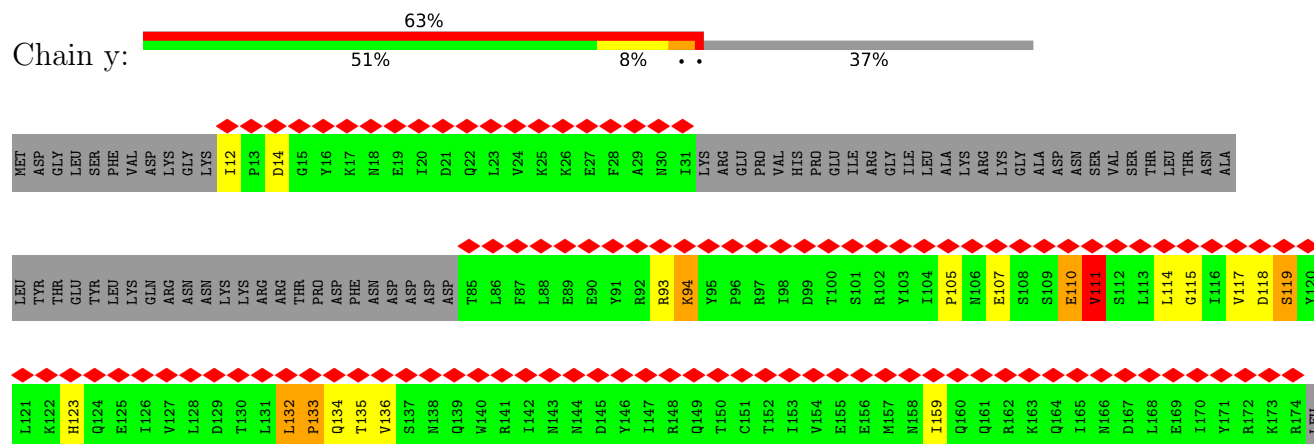


• Molecule 35: Pre-mRNA-processing factor Prp19





Chain y:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212219	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 ($e^-/\text{\AA}^2$)	2.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.197	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.40	0/3167	0.68	0/4911
2	5	0.45	0/2422	0.51	0/3762
3	6	0.45	0/2427	0.52	1/3778 (0.0%)
4	e	0.59	4/787 (0.5%)	0.67	1/1219 (0.1%)
5	i	0.30	0/1379	0.50	0/2131
6	A	0.48	0/16570	0.77	11/22456 (0.0%)
7	B	0.45	0/7331	0.76	4/9926 (0.0%)
8	D	0.52	0/2889	0.82	1/3924 (0.0%)
9	E	0.41	0/1517	0.73	0/2043
10	F	0.42	0/1598	0.78	4/2151 (0.2%)
11	G	0.42	0/2094	0.70	0/2815
12	H	0.43	0/584	0.89	1/781 (0.1%)
13	I	0.43	0/1307	0.71	0/1748
14	K	0.33	0/552	0.66	0/746
15	L	0.33	0/3406	0.67	0/4592
16	M	0.32	0/2678	0.70	1/3619 (0.0%)
17	N	0.34	0/1354	0.66	1/1838 (0.1%)
18	O	0.31	0/1967	0.71	0/2624
19	P	0.22	0/3918	0.56	0/5386
20	R	0.34	0/817	0.64	0/1083
21	S	0.41	0/1978	0.73	3/2655 (0.1%)
22	T	0.38	0/3411	0.61	2/4632 (0.0%)
23	U	0.21	0/3625	0.56	1/4963 (0.0%)
26	a	0.54	0/753	0.80	0/1013
26	q	0.57	0/738	0.87	1/995 (0.1%)
27	b	0.59	0/585	0.76	0/791
27	m	0.56	0/585	0.83	0/791
28	c	0.68	1/585 (0.2%)	0.84	0/795
28	l	0.62	0/585	0.79	0/795
29	d	0.70	2/532 (0.4%)	0.80	0/715
29	n	0.54	0/529	0.68	0/711
30	f	0.55	0/636	0.75	0/856

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	k	0.56	0/614	0.66	0/826
31	g	0.54	0/634	0.77	0/859
31	o	0.54	0/607	0.76	0/820
32	h	0.57	0/649	0.78	0/880
32	p	0.62	0/623	0.88	4/844 (0.5%)
33	r	0.50	0/415	1.08	0/577
34	s	0.50	0/814	1.19	10/1134 (0.9%)
35	u	0.76	0/2150	1.12	9/2989 (0.3%)
35	v	1.03	2/586 (0.3%)	1.56	7/816 (0.9%)
35	w	0.77	0/2165	1.20	12/3010 (0.4%)
35	x	0.96	1/576 (0.2%)	1.34	3/802 (0.4%)
36	y	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
All	All	0.48	11/83685 (0.0%)	0.77	88/115562 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	6
7	B	0	9
8	D	0	2
9	E	0	3
10	F	0	1
11	G	0	2
15	L	0	1
18	O	0	1
30	k	0	1
35	u	0	1
35	v	0	1
35	w	0	2
36	y	0	2
All	All	0	32

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	v	109	LEU	C-N	8.14	1.44	1.33
4	e	9	U	C1'-N1	7.24	1.59	1.48
4	e	-13	U	C1'-N1	7.01	1.58	1.48
4	e	-11	U	C1'-N1	6.25	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	v	134	SER	C-O	-5.79	1.17	1.24
36	y	133	PRO	CA-C	5.70	1.60	1.52
28	c	12	PRO	CA-C	5.60	1.54	1.51
4	e	17	U	C1'-N1	5.49	1.55	1.47
29	d	20	ASN	CG-OD1	5.21	1.33	1.23
29	d	18	ASN	CG-OD1	5.14	1.33	1.23
35	x	77	ILE	C-N	5.07	1.40	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	w	134	SER	CA-C-O	-16.70	103.49	120.70
35	v	134	SER	CA-C-O	-11.57	108.16	120.42
35	v	137	LEU	CA-C-N	10.19	130.36	119.05
35	v	137	LEU	C-N-CA	10.19	130.36	119.05
36	y	132	LEU	CA-C-N	10.15	132.53	119.84
36	y	132	LEU	C-N-CA	10.15	132.53	119.84
35	w	134	SER	O-C-N	9.46	132.30	122.09
35	x	137	LEU	CA-C-N	9.01	128.74	119.19
35	x	137	LEU	C-N-CA	9.01	128.74	119.19
34	s	43	MET	CA-C-N	8.58	128.72	119.28
34	s	43	MET	C-N-CA	8.58	128.72	119.28
35	v	110	SER	N-CA-C	8.56	120.61	111.28
35	w	137	LEU	CA-C-N	8.18	127.77	118.85
35	w	137	LEU	C-N-CA	8.18	127.77	118.85
34	s	4	THR	CA-C-N	7.86	127.42	118.85
34	s	4	THR	C-N-CA	7.86	127.42	118.85
35	v	134	SER	O-C-N	7.73	130.96	122.15
36	y	135	THR	CA-C-O	-7.70	112.31	120.55
35	x	134	SER	CA-C-O	-6.76	112.19	119.97
7	B	884	ARG	CA-CB-CG	6.72	127.55	114.10
22	T	112	VAL	N-CA-C	-6.67	106.02	112.29
34	s	11	ALA	CA-C-N	6.62	128.11	119.84
34	s	11	ALA	C-N-CA	6.62	128.11	119.84
6	A	1164	TYR	N-CA-C	-6.54	100.78	110.46
35	u	39	PRO	N-CA-CB	6.49	110.39	103.39
34	s	67	ILE	CA-C-N	6.23	127.62	119.84
34	s	67	ILE	C-N-CA	6.23	127.62	119.84
32	p	96	ILE	N-CA-C	6.16	117.99	108.44
21	S	143	ASP	CA-C-N	6.07	133.14	121.54
21	S	143	ASP	C-N-CA	6.07	133.14	121.54
34	s	148	VAL	CA-C-N	6.07	125.63	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	148	VAL	C-N-CA	6.07	125.63	119.19
35	u	137	LEU	CA-C-N	6.03	125.58	119.19
35	u	137	LEU	C-N-CA	6.03	125.58	119.19
6	A	1262	MET	CA-C-N	6.02	133.04	121.54
6	A	1262	MET	C-N-CA	6.02	133.04	121.54
35	w	226	LYS	N-CA-C	-5.96	106.62	114.31
35	u	226	LYS	N-CA-C	-5.90	106.70	114.31
36	y	132	LEU	N-CA-C	5.78	122.58	109.81
36	y	117	VAL	CA-C-O	5.77	124.14	119.29
7	B	954	LEU	CA-CB-CG	5.76	136.46	116.30
10	F	94	VAL	CA-C-N	5.73	135.85	126.86
10	F	94	VAL	C-N-CA	5.73	135.85	126.86
36	y	159	ILE	CA-C-O	5.70	127.37	121.05
22	T	159	TRP	CA-CB-CG	5.68	124.40	113.60
7	B	777	ASP	CA-C-N	5.66	132.35	121.54
7	B	777	ASP	C-N-CA	5.66	132.35	121.54
6	A	1903	LYS	CA-C-N	5.60	132.23	121.54
6	A	1903	LYS	C-N-CA	5.60	132.23	121.54
35	u	202	LYS	N-CA-C	-5.55	106.47	113.18
21	S	224	MET	CA-CB-CG	5.53	125.15	114.10
36	y	132	LEU	CA-C-O	5.49	127.68	120.16
36	y	135	THR	O-C-N	5.49	128.81	122.17
3	6	60	G	C4'-C3'-O3'	-5.47	104.79	113.00
35	w	202	LYS	N-CA-C	-5.47	106.56	113.18
17	N	93	VAL	N-CA-C	5.45	112.04	106.21
10	F	99	VAL	CA-C-N	5.38	129.33	121.31
10	F	99	VAL	C-N-CA	5.38	129.33	121.31
35	u	204	MET	N-CA-C	5.37	118.64	112.57
35	w	204	MET	N-CA-C	5.36	118.62	112.57
16	M	367	PRO	N-CA-CB	5.33	110.46	103.42
32	p	97	LEU	N-CA-C	5.29	121.51	109.81
36	y	134	GLN	N-CA-C	-5.28	104.77	111.11
32	p	98	PRO	CB-CA-C	5.27	120.26	111.56
6	A	1830	VAL	CA-C-N	5.27	128.72	120.82
6	A	1830	VAL	C-N-CA	5.27	128.72	120.82
35	w	348	TYR	N-CA-C	5.22	116.22	108.60
35	w	236	THR	CA-C-N	-5.20	114.88	120.03
35	w	236	THR	C-N-CA	-5.20	114.88	120.03
6	A	1674	ASP	CA-C-N	5.19	131.31	121.97
6	A	1674	ASP	C-N-CA	5.19	131.31	121.97
32	p	98	PRO	N-CA-C	-5.18	101.80	112.47
35	u	236	THR	CA-C-N	-5.18	114.90	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	u	236	THR	C-N-CA	-5.18	114.90	120.03
23	U	735	ILE	N-CA-C	5.16	114.22	106.42
26	q	82	LYS	N-CA-C	5.16	118.70	111.74
12	H	6	ARG	N-CA-C	5.14	117.38	110.29
35	u	348	TYR	N-CA-C	5.12	116.07	108.60
35	w	134	SER	CA-C-N	5.12	130.09	121.14
35	w	134	SER	C-N-CA	5.12	130.09	121.14
36	y	111	VAL	N-CA-C	5.10	119.94	109.34
6	A	1353	THR	CA-C-N	5.07	127.06	120.26
6	A	1353	THR	C-N-CA	5.07	127.06	120.26
4	e	17	U	P-O3'-C3'	5.06	127.80	120.20
8	D	421	LYS	CA-CB-CG	5.05	124.21	114.10
36	y	110	GLU	N-CA-C	5.05	117.75	110.28
35	v	109	LEU	CA-C-N	5.02	127.00	120.28
35	v	109	LEU	C-N-CA	5.02	127.00	120.28

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	1474	ARG	Peptide
6	A	405	ASN	Peptide
6	A	542	HIS	Peptide
6	A	774	ILE	Peptide
6	A	775	ARG	Peptide
7	B	114	PRO	Peptide
7	B	179	ASP	Peptide
7	B	572	ILE	Peptide
7	B	597	TYR	Peptide
7	B	682	SER	Peptide
7	B	769	TYR	Peptide
7	B	777	ASP	Peptide
7	B	977	SER	Peptide
7	B	978	THR	Peptide
8	D	277	VAL	Peptide
8	D	341	LEU	Peptide
9	E	106	LEU	Peptide
9	E	107	ASN	Peptide
9	E	143	VAL	Peptide
10	F	120	LEU	Peptide
11	G	206	LEU	Peptide

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Mol	Chain	Res	Type	Group
11	G	23	PRO	Peptide
15	L	300	LYS	Peptide
18	O	322	LYS	Peptide
30	k	84	LEU	Peptide
35	u	134	SER	Mainchain
35	v	109	LEU	Mainchain
35	w	134	SER	Mainchain
35	w	3	CYS	Mainchain
36	y	111	VAL	Peptide
36	y	132	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2848	0	1445	36	0
2	5	2173	0	1102	13	0
3	6	2170	0	1095	15	0
4	e	707	0	354	3	0
5	i	1239	0	624	6	0
6	A	16159	0	16162	193	0
7	B	7179	0	7361	87	0
8	D	2826	0	2816	48	0
9	E	1494	0	1540	22	0
10	F	1576	0	1607	15	0
11	G	2048	0	2011	18	0
12	H	570	0	556	11	0
13	I	1283	0	1301	11	0
14	K	550	0	454	2	0
15	L	3353	0	3421	28	0
16	M	2607	0	2512	43	0
17	N	1326	0	1367	15	0
18	O	1935	0	1894	34	0
19	P	3872	0	2618	17	0
20	R	813	0	837	7	0
21	S	1948	0	1979	22	0
22	T	3370	0	2727	24	0
23	U	3625	0	2248	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	1095	0	231	9	0
25	Y	80	0	18	1	0
26	a	741	0	778	16	0
26	q	726	0	754	5	0
27	b	573	0	572	7	0
27	m	573	0	572	2	0
28	c	575	0	597	9	0
28	l	575	0	597	4	0
29	d	529	0	557	9	0
29	n	526	0	555	2	0
30	f	631	0	670	3	0
30	k	610	0	638	23	0
31	g	625	0	647	14	0
31	o	600	0	623	9	0
32	h	644	0	686	10	0
32	p	618	0	660	43	0
33	r	416	0	182	14	0
34	s	816	0	341	5	0
35	u	2156	0	938	3	0
35	v	588	0	250	12	0
35	w	2171	0	945	4	0
35	x	578	0	246	3	0
36	y	548	0	219	17	0
37	6	4	0	0	0	0
37	B	1	0	0	0	0
38	A	36	0	6	3	0
39	B	32	0	12	0	0
40	F	2	0	0	0	0
40	G	1	0	0	0	0
40	I	3	0	0	0	0
40	O	1	0	0	0	0
All	All	82745	0	70325	715	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 5.

All (715) 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)
35:v:78:PRO:N	36:y:123:HIS:HA	1.46	1.26
32:p:16:THR:C	32:p:96:ILE:HD11	1.60	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:p:16:THR:CA	32:p:96:ILE:HD11	1.66	1.24
32:p:16:THR:HG22	32:p:96:ILE:CD1	1.67	1.24
9:E:212:ASP:OD2	24:X:1024:UNK:O	1.57	1.22
1:2:1107:C:C4	33:r:31:TYR:CB	2.23	1.21
1:2:1107:C:N3	33:r:31:TYR:CB	2.06	1.18
32:p:15:VAL:HG12	32:p:96:ILE:O	1.41	1.16
32:p:16:THR:HG22	32:p:96:ILE:CG1	1.78	1.14
32:p:16:THR:CG2	32:p:96:ILE:HD11	1.78	1.13
32:p:16:THR:N	32:p:96:ILE:CD1	2.13	1.11
32:p:16:THR:CA	32:p:96:ILE:CD1	2.29	1.10
32:p:16:THR:O	32:p:96:ILE:CD1	1.98	1.10
1:2:1148:U:H4'	30:k:78:GLU:HG3	1.35	1.07
30:k:4:ILE:HA	34:s:49:HIS:HA	1.38	1.05
32:p:16:THR:HG22	32:p:96:ILE:HG12	1.37	1.04
1:2:1106:G:C6	33:r:69:ARG:O	2.11	1.03
1:2:1149:G:OP1	30:k:54:PRO:HG3	1.61	1.01
32:p:16:THR:CG2	32:p:96:ILE:CD1	2.34	1.00
32:p:16:THR:CB	32:p:96:ILE:HD11	1.92	1.00
35:v:78:PRO:CA	36:y:123:HIS:HA	1.93	0.99
32:p:16:THR:C	32:p:96:ILE:CD1	2.36	0.97
7:B:122:TYR:CD2	31:g:81:ALA:HB3	1.99	0.97
35:v:78:PRO:N	36:y:123:HIS:CA	2.27	0.96
35:v:78:PRO:CB	36:y:123:HIS:HA	1.95	0.96
1:2:1106:G:O6	33:r:69:ARG:O	1.83	0.94
35:w:20:ARG:CB	35:x:52:GLU:O	2.16	0.94
32:p:16:THR:H	32:p:96:ILE:CD1	1.80	0.94
32:p:16:THR:H	32:p:96:ILE:HD13	1.33	0.91
32:p:13:GLU:HG2	32:p:98:PRO:O	1.70	0.90
36:y:114:LEU:O	36:y:118:ASP:N	2.04	0.90
13:I:150:CYS:SG	13:I:153:CYS:HB3	2.11	0.90
1:2:1148:U:H1'	30:k:78:GLU:OE2	1.71	0.89
32:p:15:VAL:CG1	32:p:96:ILE:O	2.20	0.89
1:2:1149:G:H5''	30:k:54:PRO:HB3	1.53	0.89
19:P:598:SER:O	19:P:629:LEU:HA	1.75	0.87
32:p:16:THR:O	32:p:96:ILE:HD11	1.63	0.87
1:2:1094:G:H4'	31:o:56:VAL:CG1	2.05	0.86
32:p:16:THR:O	32:p:96:ILE:HD12	1.76	0.85
30:k:4:ILE:CA	34:s:49:HIS:HA	2.07	0.85
26:q:82:LYS:O	26:q:82:LYS:NZ	2.08	0.84
1:2:1108:A:N6	33:r:108:THR:CB	2.39	0.84
11:G:81:CYS:SG	11:G:91:HIS:HE1	2.01	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:212:ASP:CG	24:X:1024:UNK:O	2.22	0.82
32:p:15:VAL:HA	32:p:96:ILE:O	1.80	0.81
32:p:16:THR:N	32:p:96:ILE:HD12	1.95	0.81
32:p:16:THR:CB	32:p:96:ILE:CD1	2.56	0.80
32:p:25:VAL:HG12	32:p:43:VAL:HG22	1.64	0.79
32:p:13:GLU:CG	32:p:98:PRO:O	2.33	0.76
1:2:1108:A:C2	33:r:73:PHE:CB	2.69	0.76
1:2:1094:G:H4'	31:o:56:VAL:HG11	1.67	0.76
1:2:1148:U:H4'	30:k:78:GLU:CG	2.13	0.76
32:p:15:VAL:HG12	32:p:96:ILE:C	2.11	0.75
1:2:1106:G:N1	33:r:69:ARG:O	2.19	0.75
6:A:517:LYS:NZ	38:A:3001:IHP:O45	2.20	0.74
35:v:78:PRO:CB	36:y:123:HIS:CA	2.65	0.74
9:E:212:ASP:OD2	24:X:1024:UNK:C	2.36	0.74
1:2:1148:U:C1'	30:k:78:GLU:OE2	2.36	0.73
2:5:48:G:H1	2:5:67:U:H3	1.37	0.72
8:D:217:ILE:HG22	8:D:218:ARG:HG3	1.70	0.72
1:2:1149:G:OP1	30:k:54:PRO:CG	2.38	0.72
35:u:51:VAL:CB	35:v:20:ARG:CB	2.68	0.71
23:U:729:TYR:CD2	23:U:748:PHE:HD1	2.09	0.71
7:B:207:SER:HB3	31:g:82:PRO:HG3	1.73	0.70
8:D:127:ALA:HB3	8:D:428:GLN:HE21	1.56	0.70
8:D:197:LEU:HB3	8:D:209:TRP:HB2	1.73	0.70
7:B:207:SER:CB	31:g:82:PRO:HG3	2.21	0.70
6:A:936:GLU:HG2	6:A:986:PRO:HB3	1.75	0.68
8:D:280:GLN:NE2	9:E:66:CYS:SG	2.67	0.67
1:2:1107:C:N4	33:r:31:TYR:CB	2.57	0.67
35:v:78:PRO:CA	36:y:123:HIS:CA	2.72	0.67
3:6:90:U:OP2	22:T:104:ARG:NH2	2.28	0.66
8:D:259:VAL:HG12	8:D:260:ILE:HG13	1.76	0.66
15:L:143:LEU:HD23	15:L:176:LYS:HD3	1.78	0.66
7:B:778:THR:HG23	7:B:780:PRO:HD3	1.77	0.66
31:g:50:THR:HG22	31:g:56:VAL:HG12	1.78	0.66
1:2:31:A:H4'	21:S:5:PRO:HB3	1.78	0.65
1:2:1095:U:OP1	31:o:50:THR:HG21	1.97	0.65
16:M:158:TYR:HB2	16:M:451:ILE:HB	1.80	0.64
36:y:107:GLU:CB	36:y:110:GLU:CB	2.76	0.64
6:A:1784:TYR:HB3	6:A:1806:MET:HE3	1.79	0.64
16:M:333:ASP:HB2	16:M:336:GLN:HB2	1.80	0.63
20:R:156:ASP:OD2	22:T:119:ARG:NH2	2.31	0.63
7:B:126:MET:HB3	7:B:132:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:105:ILE:O	7:B:180:ASN:ND2	2.30	0.63
7:B:971:ARG:NH1	7:B:985:ASP:O	2.31	0.63
6:A:1071:ARG:HB2	24:X:1025:UNK:CB	2.28	0.63
11:G:212:TRP:O	11:G:215:ARG:NH2	2.32	0.63
32:p:16:THR:CG2	32:p:96:ILE:HG12	2.23	0.63
8:D:159:SER:OG	8:D:160:ASN:N	2.31	0.62
24:X:2305:UNK:O	24:X:2306:UNK:CB	2.47	0.62
24:X:3402:UNK:O	24:X:3403:UNK:CB	2.45	0.62
1:2:1107:C:C2	33:r:31:TYR:CB	2.82	0.62
6:A:294:ASN:HD21	6:A:299:LYS:HB2	1.64	0.62
6:A:1851:PHE:O	6:A:1881:THR:HA	2.00	0.61
26:a:33:LEU:HD23	27:b:72:PHE:HB2	1.82	0.61
6:A:1011:ASN:ND2	6:A:1143:GLU:O	2.29	0.61
26:a:82:LYS:O	26:a:82:LYS:HG2	2.00	0.61
6:A:319:ARG:NH1	6:A:321:GLU:OE1	2.32	0.61
23:U:716:ALA:HB1	23:U:725:THR:HG22	1.82	0.61
6:A:1073:ILE:HG13	6:A:1074:VAL:HG13	1.82	0.61
9:E:34:ILE:O	22:T:123:ASN:ND2	2.33	0.61
17:N:151:ARG:HH11	18:O:220:LYS:HE3	1.66	0.61
13:I:151:ARG:O	16:M:63:ARG:NH1	2.34	0.61
20:R:187:LYS:NZ	20:R:198:ASP:OD1	2.34	0.61
6:A:1910:LYS:HB3	6:A:1943:PRO:HG2	1.84	0.60
6:A:141:LYS:HZ3	13:I:48:GLN:HB3	1.65	0.60
7:B:122:TYR:CE2	31:g:81:ALA:HB3	2.36	0.60
10:F:13:CYS:HB3	10:F:16:CYS:SG	2.40	0.60
5:i:502:G:H2'	5:i:503:A:H8	1.66	0.60
6:A:898:ILE:HA	6:A:1006:ARG:HH12	1.66	0.60
30:k:4:ILE:HG13	34:s:48:LYS:O	2.02	0.60
1:2:1108:A:H62	33:r:108:THR:CB	2.13	0.59
17:N:205:ARG:H	17:N:208:HIS:HD2	1.48	0.59
26:a:95:PHE:CZ	32:h:7:LEU:HD11	2.37	0.59
30:k:4:ILE:N	34:s:49:HIS:HA	2.17	0.59
15:L:366:GLU:HG2	15:L:404:ILE:HD13	1.82	0.59
7:B:468:LEU:HB3	7:B:579:SER:HB3	1.84	0.59
26:a:85:ILE:O	26:a:85:ILE:HG22	2.02	0.59
6:A:1090:ILE:O	6:A:1096:SER:HA	2.03	0.59
32:p:15:VAL:CA	32:p:96:ILE:O	2.48	0.59
6:A:1666:CYS:SG	18:O:249:ARG:NH1	2.75	0.59
20:R:171:GLU:OE2	20:R:175:ARG:NH2	2.35	0.59
6:A:1004:ASP:OD2	6:A:1506:ARG:NH1	2.36	0.59
6:A:1232:SER:OG	12:H:135:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:360:ILE:HB	16:M:377:PHE:HB2	1.84	0.59
2:5:75:A:H4'	2:5:76:U:H5'	1.85	0.59
8:D:121:GLN:NE2	9:E:49:SER:O	2.35	0.59
6:A:1051:GLU:OE2	6:A:1204:ARG:NH2	2.36	0.59
26:a:79:LYS:O	26:a:80:LYS:HG3	2.03	0.58
28:l:43:ILE:HD11	28:l:90:ILE:HD12	1.86	0.58
6:A:835:LYS:HD2	12:H:173:HIS:HE1	1.69	0.58
6:A:1405:ILE:HG23	6:A:1439:THR:HG21	1.85	0.58
7:B:234:LEU:HD21	7:B:439:ILE:HG23	1.86	0.58
13:I:104:CYS:SG	13:I:105:CYS:N	2.76	0.58
15:L:94:LEU:O	15:L:98:LEU:HB2	2.03	0.58
6:A:366:GLU:O	6:A:372:ARG:NH2	2.35	0.58
16:M:266:GLY:HA3	16:M:296:ILE:HD11	1.86	0.58
6:A:808:ILE:HD13	9:E:165:ILE:HD11	1.86	0.58
8:D:391:GLU:HB3	8:D:400:ARG:HB3	1.84	0.58
21:S:189:ARG:NH1	22:T:36:ASP:O	2.37	0.57
22:T:233:GLN:HG3	22:T:274:TRP:HE1	1.69	0.57
2:5:97:U:OP1	6:A:839:HIS:NE2	2.36	0.57
23:U:729:TYR:CD2	23:U:748:PHE:CD1	2.92	0.57
6:A:1211:SER:O	6:A:1257:ASN:ND2	2.36	0.57
6:A:228:LYS:NZ	6:A:692:ASN:OD1	2.33	0.57
6:A:1771:THR:HA	6:A:1789:ASN:HD22	1.70	0.57
6:A:2081:ASP:OD1	6:A:2086:GLN:NE2	2.36	0.57
7:B:514:GLN:NE2	7:B:586:MET:O	2.38	0.57
9:E:132:ARG:NH2	10:F:33:GLU:OE1	2.37	0.57
18:O:282:ASP:OD2	18:O:289:ARG:NH2	2.38	0.57
13:I:21:PRO:O	13:I:24:THR:HB	2.05	0.56
19:P:907:LEU:HD22	19:P:927:ILE:HG12	1.87	0.56
11:G:55:PRO:HB3	11:G:93:ILE:HD11	1.88	0.56
22:T:51:ARG:HH22	22:T:83:ARG:HD3	1.69	0.56
7:B:233:ASP:OD1	7:B:487:ARG:NH2	2.34	0.56
6:A:992:ASP:OD2	6:A:1085:LYS:NZ	2.39	0.56
7:B:90:LEU:HD12	8:D:211:LEU:HD22	1.88	0.56
8:D:414:LEU:HB3	8:D:426:TRP:HB2	1.88	0.56
7:B:242:VAL:HG21	7:B:272:ARG:HE	1.70	0.56
6:A:1789:ASN:ND2	18:O:182:TYR:OH	2.34	0.56
6:A:1842:GLU:O	6:A:1849:LYS:NZ	2.38	0.56
7:B:232:SER:O	7:B:452:LYS:NZ	2.38	0.56
16:M:262:GLU:OE1	16:M:274:HIS:NE2	2.39	0.56
10:F:25:MET:HB3	10:F:46:PHE:HB3	1.88	0.56
12:H:8:GLN:O	12:H:10:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:334:LEU:HD21	15:L:384:LEU:HG	1.88	0.56
1:2:1106:G:H1	33:r:69:ARG:CB	2.18	0.56
6:A:380:ARG:NH1	7:B:917:ASP:OD1	2.39	0.55
6:A:1889:LEU:HD12	6:A:1989:PHE:HB2	1.87	0.55
17:N:140:LYS:NZ	18:O:226:ASP:OD1	2.38	0.55
6:A:1848:ILE:HG23	6:A:1930:PRO:HA	1.88	0.55
6:A:1875:ILE:HD12	6:A:1979:MET:HE1	1.87	0.55
15:L:14:GLN:OE1	15:L:245:CYS:N	2.39	0.55
6:A:1393:GLU:OE1	18:O:36:TYR:OH	2.18	0.55
6:A:1578:ALA:O	6:A:1824:GLN:NE2	2.40	0.55
21:S:51:ARG:HG3	21:S:56:LEU:HD23	1.89	0.55
6:A:1682:THR:OG1	6:A:1702:THR:OG1	2.24	0.55
7:B:176:ARG:NH2	7:B:179:ASP:OD2	2.36	0.55
6:A:1323:SER:O	6:A:1370:ARG:NH1	2.39	0.55
1:2:101:U:OP1	30:k:11:ARG:NE	2.37	0.55
6:A:1876:ASN:HD21	6:A:1895:HIS:HD2	1.55	0.55
19:P:1138:GLU:OE1	19:P:1145:ARG:NH1	2.40	0.55
6:A:144:ASN:HB3	13:I:36:ASP:HB2	1.89	0.55
6:A:255:ILE:HG23	6:A:640:ARG:HG2	1.88	0.55
6:A:341:ALA:HA	6:A:355:LEU:HD21	1.88	0.55
8:D:395:SER:HB2	12:H:158:ASN:HD22	1.72	0.55
16:M:339:MET:SD	16:M:339:MET:N	2.80	0.55
22:T:89:GLU:OE2	22:T:124:ARG:NH2	2.39	0.55
29:d:15:ILE:HG21	29:d:71:LEU:HD13	1.88	0.55
8:D:345:PHE:O	8:D:450:ARG:NH1	2.33	0.54
35:v:78:PRO:CA	36:y:123:HIS:CB	2.84	0.54
36:y:114:LEU:O	36:y:118:ASP:CA	2.54	0.54
6:A:1142:ASN:HD21	6:A:1147:PHE:HA	1.72	0.54
15:L:18:TRP:HE1	15:L:22:ARG:HH21	1.55	0.54
6:A:216:GLN:NE2	6:A:280:LEU:O	2.35	0.54
8:D:309:ARG:HH11	8:D:328:THR:HG21	1.72	0.54
26:a:60:ALA:HB1	32:h:3:LEU:HD11	1.89	0.54
6:A:266:LEU:HD12	6:A:267:PRO:HD2	1.89	0.54
7:B:245:VAL:HG12	7:B:249:VAL:HG11	1.89	0.54
2:5:173:U:O2'	27:b:74:ARG:NH2	2.40	0.54
6:A:1841:ALA:HB2	18:O:299:LEU:HD22	1.89	0.54
13:I:150:CYS:SG	13:I:153:CYS:CB	2.85	0.54
34:s:121:PRO:O	34:s:122:ARG:CB	2.56	0.54
6:A:613:SER:O	6:A:613:SER:OG	2.24	0.54
6:A:1684:GLU:HB2	6:A:1700:ASP:HA	1.89	0.54
7:B:133:ILE:HD13	7:B:560:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:94:C:O2'	6:A:1378:LYS:NZ	2.40	0.54
15:L:25:VAL:HG21	15:L:56:ILE:HG22	1.89	0.54
20:R:180:LYS:O	20:R:184:GLN:NE2	2.40	0.54
7:B:499:VAL:HG12	7:B:579:SER:HB2	1.89	0.54
1:2:1107:C:N3	33:r:104:SER:HA	2.23	0.54
6:A:2002:TYR:HB2	18:O:299:LEU:HD12	1.90	0.54
7:B:129:ILE:HD11	31:g:17:HIS:CD2	2.43	0.54
16:M:253:VAL:HG23	16:M:265:VAL:HG22	1.89	0.54
23:U:436:ASP:O	23:U:441:GLY:N	2.39	0.53
2:5:43:G:C4	7:B:97:ARG:HD2	2.43	0.53
3:6:84:C:O2'	12:H:3:THR:O	2.21	0.53
7:B:76:VAL:HG12	8:D:134:VAL:HB	1.90	0.53
3:6:61:C:H5'	6:A:748:GLN:HE21	1.74	0.53
6:A:391:TYR:OH	7:B:912:ALA:O	2.26	0.53
6:A:460:PRO:HG2	7:B:375:GLU:HG2	1.89	0.53
6:A:835:LYS:HD2	12:H:173:HIS:CE1	2.43	0.53
6:A:1701:ILE:HB	6:A:1734:PHE:HB2	1.90	0.53
22:T:45:GLU:OE2	22:T:48:ARG:NH1	2.41	0.53
7:B:398:ASN:OD1	7:B:401:ARG:NH1	2.42	0.53
23:U:774:PRO:HG3	23:U:808:GLU:HA	1.90	0.53
6:A:204:GLU:OE2	6:A:284:ARG:NH1	2.42	0.53
6:A:1647:GLN:O	6:A:1650:ARG:NH1	2.40	0.53
6:A:1804:THR:HG21	18:O:259:ILE:HA	1.90	0.53
28:c:91:THR:HB	29:d:61:THR:HG22	1.89	0.53
6:A:1035:LEU:HD12	6:A:1038:ILE:HD12	1.91	0.53
7:B:866:ILE:HB	7:B:902:VAL:HB	1.91	0.53
8:D:285:SER:OG	8:D:287:ASP:OD1	2.24	0.53
16:M:392:SER:HB3	16:M:397:TYR:HB2	1.90	0.53
19:P:735:PRO:O	19:P:739:GLN:N	2.40	0.53
7:B:189:LEU:HD21	7:B:650:LEU:HD21	1.91	0.53
22:T:176:GLU:HG3	22:T:188:ILE:HD11	1.91	0.53
26:a:79:LYS:O	26:a:80:LYS:CG	2.57	0.53
32:p:16:THR:CG2	32:p:96:ILE:CG1	2.68	0.53
6:A:320:ASP:OD1	6:A:508:GLN:NE2	2.37	0.52
1:2:1094:G:H4'	31:o:56:VAL:HG13	1.88	0.52
6:A:856:TRP:HA	12:H:170:LEU:HD21	1.90	0.52
6:A:680:CYS:SG	6:A:711:TRP:NE1	2.83	0.52
6:A:1910:LYS:HA	6:A:1940:MET:HE1	1.91	0.52
6:A:1197:ASN:O	6:A:1224:ARG:NH2	2.42	0.52
8:D:183:MET:HE2	8:D:202:GLU:HG2	1.91	0.52
32:p:15:VAL:CB	32:p:96:ILE:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1108:A:N1	33:r:73:PHE:CB	2.71	0.52
6:A:190:LYS:HD3	6:A:559:GLN:HE21	1.74	0.52
6:A:1579:SER:HA	6:A:1824:GLN:HE22	1.73	0.52
6:A:757:GLU:HG2	8:D:202:GLU:CD	2.35	0.52
19:P:1106:SER:OG	19:P:1107:GLN:N	2.42	0.52
8:D:210:ASP:OD2	8:D:213:LYS:NZ	2.43	0.52
8:D:451:PHE:OXT	9:E:48:GLN:NE2	2.42	0.52
10:F:106:ASN:O	10:F:109:MET:N	2.35	0.52
6:A:1952:PRO:O	18:O:266:TYR:OH	2.21	0.52
28:l:54:ILE:HG23	28:l:80:ILE:HG23	1.92	0.51
2:5:43:G:H2'	2:5:45:A:H5''	1.91	0.51
16:M:166:THR:O	16:M:431:GLN:NE2	2.43	0.51
6:A:233:HIS:HE1	18:O:174:TRP:HA	1.75	0.51
7:B:493:LEU:HD21	7:B:539:VAL:HG21	1.92	0.51
23:U:780:LEU:O	23:U:784:PHE:HB2	2.11	0.51
6:A:2056:ARG:HD2	18:O:325:VAL:HG12	1.92	0.51
9:E:45:PRO:HG2	9:E:48:GLN:HB2	1.93	0.51
8:D:206:VAL:HB	8:D:220:TYR:HB2	1.92	0.51
16:M:256:ARG:HH11	16:M:262:GLU:HG3	1.75	0.51
36:y:93:ARG:O	36:y:94:LYS:CB	2.59	0.51
3:6:39:G:N1	11:G:120:TYR:O	2.43	0.51
18:O:35:ARG:O	18:O:39:ASN:ND2	2.43	0.51
8:D:145:VAL:HG23	8:D:157:THR:HB	1.93	0.51
21:S:248:VAL:HG11	22:T:43:LEU:HD22	1.93	0.51
35:v:78:PRO:HA	36:y:123:HIS:CB	2.41	0.51
6:A:595:TYR:O	6:A:630:LYS:NZ	2.44	0.50
6:A:1420:THR:HG22	7:B:954:LEU:HD21	1.93	0.50
11:G:151:LEU:HD11	11:G:159:ARG:HE	1.76	0.50
21:S:46:ARG:NH1	21:S:49:GLU:OE1	2.45	0.50
3:6:58:C:C2'	3:6:59:A:H5'	2.40	0.50
7:B:680:SER:OG	7:B:681:CYS:N	2.43	0.50
5:i:1115:A:H5'	17:N:202:ILE:HD12	1.93	0.50
6:A:744:THR:O	6:A:749:ARG:NH2	2.40	0.50
6:A:770:MET:O	8:D:309:ARG:NH2	2.44	0.50
7:B:454:ALA:HB1	7:B:459:PRO:HB3	1.93	0.50
23:U:742:VAL:HG21	23:U:772:LEU:HG	1.93	0.50
11:G:23:PRO:O	11:G:37:TRP:NE1	2.40	0.50
6:A:1712:SER:OG	6:A:1713:LYS:N	2.44	0.50
11:G:92:HIS:NE2	11:G:98:ASP:OD2	2.34	0.50
1:2:1108:A:H62	33:r:108:THR:CA	2.25	0.50
6:A:982:TYR:HB2	6:A:1106:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:202:PHE:HZ	16:M:221:PHE:HZ	1.59	0.50
2:5:50:G:H1	2:5:65:U:H3	1.58	0.50
6:A:456:GLU:HG3	7:B:356:LYS:HG2	1.93	0.50
6:A:1837:SER:O	6:A:2080:LYS:NZ	2.45	0.50
32:h:16:THR:HB	32:h:96:ILE:HB	1.93	0.50
6:A:1048:VAL:HG22	6:A:1250:VAL:HG22	1.93	0.50
7:B:883:ARG:HD2	7:B:914:PHE:HD1	1.77	0.50
26:a:96:LEU:HD21	26:a:101:VAL:CG2	2.42	0.50
5:i:507:A:H2'	5:i:508:G:C8	2.47	0.49
6:A:1347:ARG:NE	6:A:1445:THR:O	2.44	0.49
11:G:139:VAL:HG13	11:G:221:LEU:HD13	1.94	0.49
15:L:73:ILE:HG13	15:L:74:PRO:HD3	1.93	0.49
15:L:129:VAL:HG12	15:L:130:ILE:HG12	1.93	0.49
16:M:317:VAL:HB	16:M:331:ILE:HB	1.94	0.49
6:A:1878:CYS:HA	6:A:1892:LYS:O	2.12	0.49
8:D:309:ARG:HD2	8:D:328:THR:HG21	1.94	0.49
16:M:179:LEU:HB3	16:M:189:ILE:HD12	1.94	0.49
36:y:114:LEU:O	36:y:118:ASP:CB	2.60	0.49
7:B:708:ILE:HG23	7:B:823:ILE:HG22	1.94	0.49
7:B:944:VAL:HG13	7:B:967:VAL:HG21	1.94	0.49
9:E:170:SER:OG	9:E:173:LYS:O	2.30	0.49
15:L:62:ASP:O	15:L:66:ASN:ND2	2.45	0.49
15:L:156:LYS:HG2	15:L:200:ILE:HD11	1.95	0.49
6:A:905:TYR:OH	6:A:1002:GLU:OE2	2.30	0.49
7:B:862:TYR:HD2	7:B:930:LEU:HD23	1.77	0.49
9:E:225:LEU:HD13	9:E:228:LEU:HD12	1.94	0.49
21:S:73:LEU:HA	21:S:91:MET:HE1	1.93	0.49
35:v:108:LYS:C	35:v:110:SER:N	2.70	0.49
3:6:38:U:H5'	11:G:121:ARG:HH12	1.78	0.49
8:D:115:TYR:HD2	22:T:235:LEU:HD23	1.76	0.49
16:M:354:GLN:HB2	16:M:389:LEU:HD23	1.94	0.49
17:N:155:LEU:HB3	17:N:160:LEU:HD12	1.93	0.49
26:a:62:ASP:HB3	32:h:3:LEU:HD13	1.95	0.49
10:F:214:ILE:HG13	10:F:218:LYS:HD3	1.94	0.49
18:O:324:LYS:HA	18:O:327:HIS:HD2	1.78	0.49
7:B:100:LEU:HD22	7:B:108:GLN:HE21	1.77	0.49
19:P:559:ASP:HA	19:P:574:THR:HA	1.95	0.49
35:w:51:VAL:CB	35:x:20:ARG:CB	2.91	0.49
3:6:36:U:H5	11:G:80:MET:HE1	1.78	0.49
6:A:342:LEU:HD13	6:A:392:ASN:HD21	1.78	0.49
21:S:60:LEU:HD22	21:S:94:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:621:U:OP2	19:P:1144:LYS:NZ	2.38	0.48
6:A:461:LEU:HD13	7:B:404:PHE:HE1	1.78	0.48
6:A:1216:ILE:HD12	6:A:1254:ASN:HB3	1.94	0.48
15:L:143:LEU:O	15:L:176:LYS:NZ	2.41	0.48
5:i:502:G:O2'	16:M:413:ASN:O	2.31	0.48
6:A:211:PRO:HG3	6:A:308:MET:HE1	1.95	0.48
6:A:1574:PHE:HD2	18:O:33:ILE:HG22	1.77	0.48
6:A:1668:ILE:HD11	18:O:256:LEU:HD22	1.95	0.48
11:G:176:VAL:HG12	11:G:179:LYS:H	1.77	0.48
1:2:38:U:OP1	16:M:329:LYS:NZ	2.38	0.48
16:M:272:ILE:HB	16:M:289:TYR:HB2	1.94	0.48
15:L:454:ASP:HB3	15:L:457:HIS:HD2	1.78	0.48
23:U:36:ASN:O	23:U:38:LEU:N	2.47	0.48
23:U:686:ILE:HG13	23:U:689:ARG:HH21	1.78	0.48
6:A:1667:GLN:NE2	18:O:251:ASP:O	2.46	0.48
7:B:231:ALA:O	7:B:487:ARG:NH1	2.46	0.48
7:B:246:THR:OG1	7:B:247:PHE:N	2.46	0.48
18:O:293:THR:OG1	18:O:294:GLY:N	2.43	0.48
26:a:105:LEU:HB3	27:b:71:ILE:HG22	1.95	0.48
6:A:901:PRO:HB2	6:A:955:LYS:HE2	1.96	0.48
16:M:154:VAL:HA	16:M:454:CYS:HA	1.95	0.48
32:p:16:THR:N	32:p:96:ILE:HD13	1.98	0.48
6:A:1674:ASP:O	6:A:1677:GLN:N	2.44	0.48
6:A:1922:ARG:HD2	18:O:246:THR:HG23	1.96	0.48
8:D:327:CYS:HB3	8:D:330:ASP:HB3	1.96	0.48
16:M:213:ARG:HG3	16:M:254:GLU:HA	1.96	0.48
23:U:663:LYS:HB2	23:U:708:LEU:HD21	1.95	0.48
15:L:20:MET:O	15:L:24:HIS:HB2	2.13	0.47
3:6:23:G:O6	16:M:53:LYS:NZ	2.40	0.47
3:6:63:G:H2'	3:6:64:U:C6	2.49	0.47
7:B:207:SER:OG	31:g:82:PRO:HG3	2.14	0.47
18:O:124:ASN:HD22	18:O:139:PRO:HA	1.78	0.47
1:2:5:A:H5'	20:R:114:THR:HG21	1.95	0.47
6:A:978:ILE:N	12:H:173:HIS:O	2.43	0.47
16:M:385:TYR:O	21:S:186:GLN:NE2	2.48	0.47
32:p:25:VAL:HG12	32:p:43:VAL:CG2	2.40	0.47
2:5:99:U:O2'	3:6:73:A:N6	2.36	0.47
7:B:689:ILE:HD13	7:B:993:ILE:HD12	1.96	0.47
32:p:16:THR:CB	32:p:96:ILE:HD13	2.41	0.47
1:2:1149:G:OP1	30:k:54:PRO:HD3	2.15	0.47
6:A:1039:TRP:O	6:A:1273:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:67:GLN:NE2	10:F:116:LYS:O	2.48	0.47
15:L:101:MET:HA	15:L:104:GLN:HG2	1.96	0.47
16:M:405:SER:OG	16:M:427:LYS:O	2.32	0.47
26:a:33:LEU:HD22	27:b:52:GLN:HG3	1.96	0.47
1:2:1149:G:C5'	30:k:54:PRO:HB3	2.36	0.47
6:A:1722:ASP:N	6:A:1722:ASP:OD1	2.47	0.47
6:A:1967:ALA:HB2	6:A:2016:LYS:HB2	1.96	0.47
26:a:91:ILE:CG2	32:h:96:ILE:HG23	2.44	0.47
2:5:78:A:O2'	2:5:79:C:O5'	2.27	0.47
4:e:3:A:OP1	6:A:842:LYS:NZ	2.42	0.47
6:A:477:MET:HE2	7:B:278:LYS:HE3	1.96	0.47
6:A:517:LYS:HG3	6:A:518:VAL:HG23	1.97	0.47
6:A:1145:MET:HE3	6:A:1145:MET:HB2	1.73	0.47
11:G:109:LEU:HD13	11:G:113:GLY:HA2	1.96	0.47
32:p:17:ILE:HD13	32:p:92:ILE:CD1	2.44	0.47
19:P:879:LEU:HD23	19:P:885:LEU:HB2	1.97	0.47
21:S:39:LEU:HD11	21:S:155:ALA:HA	1.97	0.47
6:A:1925:PRO:HD2	6:A:1928:GLU:HB3	1.97	0.47
10:F:91:ILE:HB	10:F:99:VAL:HG11	1.97	0.47
21:S:38:SER:OG	21:S:158:ARG:NH1	2.48	0.47
6:A:467:GLU:O	7:B:387:TYR:OH	2.25	0.47
6:A:2053:SER:OG	6:A:2056:ARG:NH1	2.48	0.47
15:L:98:LEU:HA	15:L:101:MET:HG2	1.97	0.47
32:p:3:LEU:HD13	26:q:62:ASP:HB3	1.97	0.47
6:A:1676:LEU:HD11	6:A:1797:LEU:HD13	1.97	0.46
10:F:88:ASP:OD2	10:F:101:THR:OG1	2.29	0.46
9:E:135:VAL:HG21	21:S:219:TYR:CE1	2.51	0.46
9:E:135:VAL:HG21	21:S:219:TYR:HE1	1.80	0.46
6:A:1485:ASP:O	6:A:1490:ARG:NH2	2.47	0.46
28:l:29:ILE:HG21	28:l:82:LEU:HD13	1.98	0.46
6:A:143:ILE:HD11	6:A:574:GLN:HE21	1.80	0.46
6:A:905:TYR:HB3	6:A:908:ASP:HB2	1.97	0.46
36:y:115:GLY:O	36:y:119:SER:CB	2.63	0.46
7:B:675:THR:HG22	7:B:909:ILE:HD12	1.97	0.46
23:U:713:ILE:HD12	23:U:729:TYR:CE1	2.51	0.46
6:A:1759:TYR:HB3	6:A:1767:TYR:HE2	1.81	0.46
23:U:709:TRP:NE1	23:U:732:CYS:SG	2.89	0.46
30:k:85:THR:HG22	31:o:73:VAL:HG22	1.98	0.46
32:p:16:THR:HG22	32:p:96:ILE:HD13	1.80	0.46
35:w:222:PHE:O	35:w:233:THR:HA	2.16	0.46
30:f:93:LEU:HA	32:h:91:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1142:ASN:ND2	6:A:1146:GLN:O	2.49	0.46
6:A:1451:PHE:O	6:A:1455:GLN:NE2	2.49	0.46
7:B:223:ASP:N	7:B:223:ASP:OD1	2.47	0.46
22:T:122:MET:HE1	22:T:142:VAL:HG11	1.97	0.46
35:u:222:PHE:O	35:u:233:THR:HA	2.16	0.46
6:A:1347:ARG:NH1	6:A:1450:GLU:OE1	2.49	0.46
6:A:1446:THR:OG1	6:A:1449:ASN:ND2	2.49	0.46
6:A:1869:ASN:N	6:A:1869:ASN:OD1	2.45	0.46
7:B:599:THR:OG1	7:B:647:ASN:ND2	2.49	0.46
8:D:238:LEU:HD21	9:E:74:ILE:HD13	1.98	0.46
22:T:119:ARG:NH1	22:T:143:GLU:OE2	2.49	0.46
26:a:95:PHE:CE1	32:h:7:LEU:HD11	2.51	0.46
31:o:6:ILE:N	31:o:7:PRO:CD	2.78	0.46
32:p:96:ILE:HD12	32:p:96:ILE:H	1.80	0.46
6:A:252:GLU:HG3	6:A:253:GLN:HG3	1.97	0.46
7:B:69:PRO:O	8:D:390:ARG:NH1	2.48	0.46
10:F:13:CYS:HB2	10:F:71:CYS:SG	2.56	0.46
10:F:42:THR:O	10:F:42:THR:OG1	2.34	0.46
27:b:36:THR:HG23	27:b:60:VAL:HA	1.98	0.46
7:B:539:VAL:HG13	7:B:564:ILE:HG23	1.98	0.45
15:L:34:MET:HA	15:L:37:LEU:HD12	1.97	0.45
15:L:68:GLN:HA	15:L:72:LEU:HD23	1.98	0.45
6:A:759:ARG:HH12	12:H:7:PRO:HB3	1.82	0.45
7:B:122:TYR:CG	31:g:81:ALA:HB3	2.50	0.45
7:B:125:SER:HB2	31:g:77:LEU:HD22	1.98	0.45
8:D:218:ARG:NH2	12:H:34:HIS:O	2.49	0.45
15:L:170:HIS:CE1	15:L:174:TRP:HE1	2.34	0.45
16:M:167:ALA:HA	16:M:431:GLN:HG2	1.98	0.45
16:M:191:ASP:HB3	16:M:199:LEU:HD11	1.97	0.45
18:O:217:GLU:HA	18:O:220:LYS:HE2	1.98	0.45
19:P:1086:ILE:HD12	19:P:1086:ILE:HA	1.82	0.45
30:k:21:ARG:N	30:k:96:VAL:O	2.49	0.45
26:q:79:LYS:CB	26:q:83:ASN:O	2.65	0.45
2:5:77:A:H61	7:B:101:GLN:NE2	2.14	0.45
6:A:179:MET:HE2	6:A:632:ILE:HG21	1.98	0.45
8:D:201:SER:OG	8:D:202:GLU:N	2.49	0.45
16:M:213:ARG:HB2	16:M:222:LEU:HD12	1.99	0.45
6:A:454:LEU:HD13	7:B:359:PHE:HE2	1.81	0.45
7:B:886:SER:HB3	7:B:906:VAL:HG23	1.98	0.45
8:D:330:ASP:OD1	8:D:450:ARG:NH2	2.37	0.45
16:M:319:ILE:HB	16:M:329:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:v:78:PRO:CB	36:y:123:HIS:O	2.64	0.45
36:y:12:ILE:C	36:y:14:ASP:H	2.24	0.45
4:e:2:U:C6	6:A:1325:SER:HB3	2.52	0.45
7:B:457:SER:HB3	7:B:592:PHE:HA	1.98	0.45
26:a:91:ILE:HG23	32:h:96:ILE:HG23	1.98	0.45
6:A:775:ARG:HE	6:A:776:GLN:H	1.65	0.45
30:f:85:THR:HG22	31:g:73:VAL:HA	1.97	0.45
1:2:1149:G:OP1	30:k:54:PRO:CD	2.64	0.45
6:A:968:ASP:OD1	21:S:46:ARG:NH2	2.49	0.45
8:D:207:LYS:HD3	8:D:216:ILE:HD13	1.98	0.45
11:G:119:ASP:OD1	11:G:119:ASP:N	2.49	0.45
17:N:93:VAL:O	17:N:171:GLN:NE2	2.49	0.45
6:A:332:ASP:OD1	6:A:332:ASP:N	2.49	0.45
30:k:91:GLN:NE2	31:o:24:THR:HG22	2.32	0.45
6:A:1383:PHE:HB3	6:A:1388:PHE:HE2	1.81	0.45
15:L:53:ARG:HA	15:L:56:ILE:HG12	1.99	0.45
16:M:411:ASP:HB2	16:M:418:LEU:HD11	1.99	0.45
7:B:164:MET:HG3	7:B:168:VAL:HG23	1.98	0.45
8:D:380:SER:OG	8:D:381:GLY:N	2.50	0.45
11:G:207:PRO:HA	11:G:212:TRP:CG	2.52	0.45
15:L:404:ILE:HG13	15:L:405:ILE:HG23	1.99	0.45
17:N:118:HIS:HD2	18:O:225:LYS:HE3	1.82	0.45
22:T:235:LEU:HD22	22:T:237:ILE:HD11	1.99	0.45
8:D:200:VAL:HG23	8:D:206:VAL:HG22	2.00	0.44
16:M:287:GLN:HE21	16:M:325:ASN:HB2	1.81	0.44
32:p:26:TRP:HH2	32:p:97:LEU:HG	1.81	0.44
35:w:310:THR:HA	35:w:325:HIS:O	2.17	0.44
6:A:400:ILE:HA	6:A:401:PRO:HD3	1.86	0.44
6:A:1904:ARG:O	6:A:1906:SER:N	2.41	0.44
20:R:148:LYS:HD2	20:R:149:THR:HG23	1.99	0.44
35:u:310:THR:HA	35:u:325:HIS:O	2.17	0.44
3:6:5:G:O6	3:6:21:U:O2	2.34	0.44
28:c:35:ILE:HD11	29:d:21:GLY:HA3	1.98	0.44
3:6:79:A:OP1	3:6:81:G:O2'	2.33	0.44
6:A:886:MET:HE1	6:A:1119:LEU:HD22	1.98	0.44
6:A:1068:ARG:HA	24:X:1025:UNK:CB	2.47	0.44
6:A:1087:ASN:HD21	21:S:86:THR:H	1.65	0.44
19:P:924:VAL:HG21	19:P:1004:PHE:HE2	1.83	0.44
22:T:148:ASN:HB3	22:T:151:ILE:HD13	2.00	0.44
26:q:82:LYS:HB3	26:q:82:LYS:HE3	1.62	0.44
6:A:764:ASP:O	6:A:768:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:802:ALA:HB2	7:B:843:LYS:HA	2.00	0.44
11:G:15:GLU:OE1	13:I:44:LYS:NZ	2.39	0.44
5:i:501:A:H2'	5:i:502:G:C8	2.52	0.44
26:a:79:LYS:C	26:a:80:LYS:HG3	2.42	0.44
17:N:159:LEU:HD21	17:N:229:TRP:HH2	1.82	0.44
29:n:69:ILE:HD12	31:o:68:GLN:HG3	1.98	0.44
6:A:347:PRO:HG3	14:K:2:SER:HB3	2.00	0.44
6:A:1892:LYS:HG2	6:A:1916:GLU:HG2	1.98	0.44
6:A:1932:GLN:OE1	18:O:290:ARG:NH2	2.49	0.44
7:B:675:THR:OG1	7:B:676:VAL:N	2.51	0.44
12:H:6:ARG:HA	12:H:7:PRO:HD3	1.75	0.44
19:P:1099:TYR:HB3	24:X:3369:UNK:HA	2.00	0.44
29:d:28:ILE:HG22	29:d:41:ASP:HB3	1.99	0.44
6:A:1287:ASP:OD1	6:A:1287:ASP:N	2.36	0.44
15:L:306:ASP:OD1	15:L:349:ARG:NE	2.51	0.44
16:M:195:ASP:HB3	16:M:197:GLU:HG3	1.98	0.44
30:k:22:VAL:HG22	30:k:95:THR:HG22	2.00	0.44
30:k:22:VAL:HG11	30:k:87:LEU:HD21	2.00	0.44
9:E:144:VAL:HA	9:E:145:PRO:HD3	1.92	0.43
32:h:16:THR:HB	32:h:96:ILE:HD12	2.00	0.43
1:2:30:A:H62	21:S:38:SER:HB3	1.81	0.43
6:A:1279:VAL:O	6:A:1299:LYS:NZ	2.51	0.43
7:B:993:ILE:HD11	7:B:997:LEU:HD22	2.00	0.43
10:F:104:ALA:HB1	10:F:109:MET:HG3	1.99	0.43
11:G:102:LEU:HB3	11:G:106:THR:HG23	2.00	0.43
11:G:153:PRO:HB3	11:G:175:TYR:HE2	1.83	0.43
19:P:1098:PHE:HD2	19:P:1099:TYR:HD1	1.66	0.43
35:v:78:PRO:N	36:y:123:HIS:N	2.65	0.43
6:A:621:LEU:HD23	6:A:722:LEU:HD21	2.00	0.43
8:D:327:CYS:SG	8:D:328:THR:N	2.88	0.43
30:f:44:VAL:HG11	31:g:10:LEU:HD13	2.01	0.43
32:p:17:ILE:O	32:p:17:ILE:HD12	2.19	0.43
16:M:339:MET:HE3	16:M:339:MET:HB3	1.94	0.43
29:d:38:VAL:HG23	29:d:68:ILE:HD11	2.00	0.43
29:n:63:ILE:HB	29:n:68:ILE:HD11	2.00	0.43
7:B:367:VAL:HG11	7:B:369:LYS:HE2	2.00	0.43
9:E:105:LEU:HD21	9:E:109:SER:HA	2.01	0.43
16:M:382:SER:HB3	16:M:387:ILE:HD13	2.00	0.43
30:k:85:THR:HG21	31:o:71:PHE:CD1	2.53	0.43
8:D:390:ARG:O	8:D:424:LYS:NZ	2.52	0.43
9:E:179:THR:H	20:R:200:ASN:HD21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:69:ILE:HA	31:g:68:GLN:HG3	2.01	0.43
32:p:26:TRP:CZ3	32:p:97:LEU:HB2	2.54	0.43
6:A:1882:LEU:HB3	6:A:1889:LEU:HD23	2.00	0.43
17:N:226:THR:HA	17:N:229:TRP:CD1	2.53	0.43
18:O:36:TYR:CD1	18:O:37:ILE:HG13	2.54	0.43
32:p:94:GLN:CD	26:q:94:LEU:HD12	2.44	0.43
6:A:1094:ASP:OD1	6:A:1094:ASP:N	2.42	0.43
6:A:1750:ARG:HD2	18:O:99:ILE:HG12	2.01	0.43
8:D:277:VAL:HG12	8:D:278:ASP:H	1.84	0.43
27:b:26:ARG:HA	27:b:41:THR:HA	2.01	0.43
35:x:107:LYS:C	35:x:109:LEU:H	2.25	0.43
3:6:19:C:H2'	3:6:20:G:C8	2.54	0.43
6:A:495:ARG:NH2	6:A:497:GLN:HE21	2.17	0.43
6:A:1270:LEU:HD22	6:A:1271:PRO:HD2	1.99	0.43
7:B:863:GLU:HG2	7:B:905:GLN:HG2	2.01	0.43
15:L:135:ILE:HA	15:L:138:ILE:HG12	2.01	0.43
16:M:222:LEU:HD23	16:M:232:ILE:HG12	2.01	0.43
16:M:296:ILE:HA	16:M:312:SER:HA	2.01	0.43
17:N:114:ASN:O	17:N:118:HIS:ND1	2.52	0.43
22:T:222:TYR:HB3	22:T:250:PHE:CD2	2.54	0.43
23:U:437:PRO:HA	23:U:441:GLY:HA3	1.99	0.43
32:p:98:PRO:HG2	32:p:99:ASP:H	1.84	0.43
6:A:383:TYR:CZ	7:B:913:GLY:HA3	2.53	0.43
7:B:801:TRP:CD1	7:B:843:LYS:HD3	2.53	0.43
8:D:264:GLY:HA3	8:D:293:TRP:HH2	1.84	0.43
17:N:183:TYR:CZ	17:N:234:LYS:HB2	2.54	0.43
21:S:74:LEU:HG	21:S:105:LEU:HD13	2.01	0.43
23:U:751:PHE:O	23:U:754:SER:OG	2.29	0.43
6:A:665:GLY:HA2	6:A:667:TYR:CE2	2.54	0.42
16:M:246:LEU:HD13	16:M:267:LEU:HD11	2.01	0.42
28:l:82:LEU:HD22	28:l:87:ILE:HG13	2.02	0.42
6:A:468:LEU:HD11	7:B:382:TYR:HB3	2.02	0.42
8:D:197:LEU:HD23	8:D:209:TRP:CD1	2.53	0.42
13:I:16:PHE:O	13:I:20:LYS:N	2.52	0.42
16:M:59:ARG:O	16:M:62:THR:OG1	2.31	0.42
16:M:252:ASP:HB3	16:M:299:LEU:HD23	2.02	0.42
3:6:26:A:O2'	13:I:123:ARG:NH2	2.50	0.42
6:A:1161:TYR:CD1	6:A:1170:MET:HG2	2.55	0.42
6:A:1286:TRP:CD1	6:A:1448:GLU:HB2	2.54	0.42
6:A:1902:GLN:HG2	17:N:211:ILE:HD11	2.02	0.42
11:G:145:ALA:HB2	11:G:221:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:96:ASP:OD2	17:N:98:SER:OG	2.35	0.42
8:D:106:VAL:HG12	8:D:108:GLU:H	1.84	0.42
19:P:907:LEU:HD13	19:P:927:ILE:HG23	2.02	0.42
28:c:45:GLY:HA3	28:c:53:VAL:HG12	2.01	0.42
6:A:194:HIS:HD2	6:A:557:PHE:HE1	1.66	0.42
6:A:231:ARG:HH22	6:A:648:GLN:HE21	1.66	0.42
6:A:326:ASN:ND2	6:A:405:ASN:O	2.41	0.42
6:A:1068:ARG:NE	24:X:1024:UNK:CB	2.83	0.42
6:A:2079:ILE:HB	18:O:328:VAL:HG21	2.01	0.42
7:B:860:PRO:HG2	7:B:908:VAL:HG11	2.00	0.42
6:A:688:TYR:HE2	38:A:3001:IHP:O32	2.02	0.42
7:B:360:ARG:HD2	7:B:364:PHE:HD1	1.83	0.42
7:B:862:TYR:CD1	7:B:932:PHE:HB2	2.55	0.42
10:F:107:ASP:HA	10:F:110:LYS:HG2	2.02	0.42
32:h:17:ILE:O	32:h:24:THR:HA	2.20	0.42
6:A:1027:LYS:O	6:A:1145:MET:HE1	2.19	0.42
6:A:1894:ILE:HG23	6:A:1898:VAL:HG21	2.02	0.42
8:D:100:LYS:HG3	8:D:101:ILE:HG13	2.01	0.42
19:P:977:GLU:O	19:P:981:LYS:CB	2.68	0.42
21:S:14:THR:OG1	21:S:15:ASN:N	2.53	0.42
6:A:778:LYS:O	6:A:782:ILE:HG12	2.20	0.42
6:A:876:PRO:HG2	9:E:203:LYS:HG3	2.02	0.42
6:A:1727:LEU:HD22	6:A:1728:ILE:H	1.84	0.42
17:N:170:LEU:HD13	17:N:237:ILE:HG12	2.01	0.42
27:m:16:LYS:N	27:m:17:PRO:CD	2.83	0.42
6:A:143:ILE:HD13	6:A:143:ILE:HA	1.87	0.42
6:A:1433:ASP:OD1	6:A:1433:ASP:N	2.52	0.42
23:U:780:LEU:O	23:U:784:PHE:CB	2.68	0.42
28:c:77:LEU:HD21	28:c:80:ILE:CD1	2.50	0.42
6:A:282:ASP:HB2	6:A:285:PRO:HA	2.01	0.42
6:A:1161:TYR:HD1	6:A:1170:MET:HG2	1.85	0.42
6:A:1855:THR:HG22	6:A:1937:ARG:HD2	2.02	0.42
7:B:416:ASP:HB2	7:B:419:PRO:HD2	2.01	0.42
7:B:864:VAL:HB	7:B:904:GLY:O	2.20	0.42
23:U:729:TYR:O	23:U:732:CYS:HB3	2.20	0.42
7:B:772:ASN:HB3	7:B:816:VAL:H	1.85	0.41
7:B:973:ARG:HA	7:B:973:ARG:HD2	1.85	0.41
16:M:435:HIS:HD2	16:M:436:PRO:HD2	1.85	0.41
28:c:91:THR:O	28:c:91:THR:HG23	2.20	0.41
3:6:73:A:OP1	6:A:732:ARG:NE	2.41	0.41
6:A:896:SER:HA	6:A:897:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1674:ASP:O	6:A:1676:LEU:N	2.53	0.41
7:B:201:THR:HG22	7:B:207:SER:HB3	2.01	0.41
16:M:387:ILE:HG13	16:M:430:THR:HG22	2.02	0.41
31:g:33:LEU:HD23	31:g:34:VAL:N	2.35	0.41
30:k:49:ILE:HG23	30:k:80:ARG:O	2.20	0.41
4:e:-2:A:OP1	6:A:614:ARG:NH1	2.53	0.41
6:A:1368:GLN:NE2	6:A:1389:TYR:OH	2.54	0.41
6:A:1562:PHE:HE2	18:O:87:ILE:HG22	1.85	0.41
8:D:365:PHE:HE1	8:D:373:LEU:HB2	1.85	0.41
16:M:392:SER:HA	16:M:434:TRP:CE2	2.55	0.41
18:O:261:SER:HG	18:O:262:THR:H	1.68	0.41
6:A:141:LYS:NZ	13:I:33:ALA:O	2.50	0.41
6:A:594:ASP:OD1	6:A:594:ASP:N	2.53	0.41
6:A:878:GLU:OE1	6:A:1237:SER:OG	2.36	0.41
6:A:1834:PHE:O	6:A:1839:ASN:ND2	2.50	0.41
7:B:134:ILE:HD11	7:B:234:LEU:HD23	2.01	0.41
8:D:277:VAL:HG21	9:E:58:PRO:HB2	2.02	0.41
8:D:345:PHE:HE2	8:D:364:LEU:HD13	1.85	0.41
10:F:11:ASN:OD1	10:F:11:ASN:N	2.53	0.41
10:F:51:ARG:HA	10:F:51:ARG:HD3	1.76	0.41
15:L:80:ILE:HB	15:L:124:LEU:HD21	2.01	0.41
15:L:297:LEU:HD13	15:L:297:LEU:HA	1.89	0.41
18:O:103:PHE:HB3	18:O:159:LEU:HB3	2.02	0.41
2:5:82:A:O3'	6:A:709:ARG:NH2	2.54	0.41
7:B:606:VAL:HG22	7:B:643:VAL:HG12	2.02	0.41
6:A:966:PRO:HD2	21:S:50:LEU:HD21	2.02	0.41
32:p:16:THR:O	32:p:96:ILE:CG1	2.65	0.41
32:p:96:ILE:HD12	32:p:96:ILE:N	2.34	0.41
1:2:4:A:H2'	1:2:5:A:C8	2.55	0.41
7:B:123:MET:HB2	7:B:199:LEU:HD23	2.03	0.41
7:B:883:ARG:NH1	7:B:910:GLU:O	2.52	0.41
10:F:77:ASP:OD1	10:F:87:ARG:NH1	2.49	0.41
19:P:1022:ARG:O	19:P:1026:VAL:HG23	2.21	0.41
22:T:240:ASP:OD1	22:T:240:ASP:N	2.51	0.41
27:b:22:LEU:HD22	28:c:81:LEU:HD21	2.03	0.41
6:A:1675:VAL:H	6:A:1675:VAL:HG23	1.59	0.41
7:B:271:ASP:OD1	7:B:271:ASP:N	2.50	0.41
7:B:687:ALA:HB1	14:K:60:VAL:HB	2.02	0.41
8:D:405:SER:HA	8:D:415:ILE:O	2.21	0.41
15:L:471:GLY:O	15:L:474:THR:OG1	2.34	0.41
16:M:156:ARG:HE	16:M:453:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:332:ASN:OD1	18:O:332:ASN:N	2.54	0.41
6:A:180:PRO:O	6:A:181:HIS:ND1	2.44	0.41
6:A:688:TYR:CE2	38:A:3001:IHP:O32	2.74	0.41
6:A:1087:ASN:HD22	21:S:83:GLN:HB3	1.85	0.41
6:A:1130:ARG:HD2	6:A:1130:ARG:HA	1.87	0.41
6:A:1567:PHE:O	18:O:90:ASN:HB3	2.21	0.41
7:B:176:ARG:HH12	7:B:185:ILE:HA	1.86	0.41
9:E:30:LEU:HD21	22:T:151:ILE:HG13	2.02	0.41
19:P:530:MET:H	19:P:597:TYR:HA	1.86	0.41
21:S:224:MET:HE2	22:T:124:ARG:HH11	1.85	0.41
22:T:54:TYR:HD1	22:T:67:GLN:HE21	1.69	0.41
28:c:91:THR:HG21	29:d:58:GLY:HA3	2.02	0.41
27:m:71:ILE:C	27:m:71:ILE:HD12	2.45	0.41
1:2:41:C:H6	1:2:41:C:H2'	1.72	0.41
6:A:835:LYS:HE2	6:A:835:LYS:HB3	1.91	0.41
6:A:902:PRO:HD2	6:A:905:TYR:HD1	1.85	0.41
6:A:1607:THR:HG22	6:A:1641:LEU:HD13	2.03	0.41
7:B:304:PHE:HD2	7:B:310:ASN:HB3	1.85	0.41
7:B:644:ILE:HG13	7:B:652:MET:HE1	2.02	0.41
22:T:73:GLN:O	22:T:77:GLU:HG2	2.21	0.41
28:c:13:PRO:HG2	29:d:37:ASN:HB2	2.02	0.41
28:c:77:LEU:HD21	28:c:80:ILE:HD12	2.02	0.41
6:A:1156:HIS:CD2	6:A:1158:ILE:H	2.39	0.40
16:M:57:LYS:HG2	16:M:60:ARG:NH1	2.35	0.40
18:O:94:LYS:HD3	18:O:94:LYS:HA	1.84	0.40
6:A:242:PHE:HE1	6:A:638:GLN:HE21	1.68	0.40
6:A:319:ARG:HH11	6:A:319:ARG:HD2	1.76	0.40
6:A:1370:ARG:HD2	6:A:1370:ARG:HA	1.82	0.40
6:A:1718:HIS:NE2	18:O:95:ILE:HD11	2.36	0.40
7:B:252:LEU:HD23	7:B:252:LEU:HA	1.94	0.40
7:B:609:PRO:HA	7:B:668:ILE:HG22	2.04	0.40
8:D:110:LEU:HD11	22:T:194:MET:HB3	2.04	0.40
8:D:365:PHE:CE1	8:D:373:LEU:HB2	2.56	0.40
9:E:1:MET:HG3	25:Y:13:UNK:CB	2.52	0.40
15:L:17:ASN:HA	15:L:20:MET:HG2	2.03	0.40
17:N:159:LEU:HD21	17:N:229:TRP:CH2	2.55	0.40
21:S:214:ASN:ND2	22:T:48:ARG:HB2	2.37	0.40
22:T:170:ASN:HA	22:T:173:VAL:HG22	2.02	0.40
30:k:81:VAL:O	30:k:81:VAL:HG13	2.21	0.40
1:2:4:A:H2'	1:2:5:A:H8	1.86	0.40
2:5:167:A:N6	26:a:63:ARG:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:291:LYS:HE2	6:A:292:LYS:HE3	2.04	0.40
7:B:206:LYS:HG3	31:g:13:GLU:HA	2.03	0.40
15:L:136:LEU:HD22	15:L:169:THR:HG21	2.03	0.40
6:A:860:GLU:OE2	6:A:863:ARG:NH2	2.51	0.40
7:B:629:TYR:OH	7:B:658:ASP:OD2	2.29	0.40
7:B:880:MET:HG3	7:B:888:ILE:HD11	2.04	0.40
16:M:237:THR:HG21	16:M:239:LYS:HE2	2.03	0.40
19:P:1033:ALA:HA	19:P:1068:MET:HA	2.03	0.40
29:d:10:TYR:HE1	29:d:73:ALA:HB2	1.86	0.40
6:A:522:TYR:O	6:A:526:LEU:HB2	2.22	0.40
6:A:797:ILE:HA	6:A:798:PRO:HD3	1.89	0.40
6:A:902:PRO:HD2	6:A:905:TYR:CD1	2.57	0.40
6:A:964:PHE:O	21:S:85:ARG:NH2	2.44	0.40
6:A:1544:THR:HG22	18:O:36:TYR:O	2.22	0.40
8:D:230:VAL:HG22	8:D:241:THR:HG22	2.02	0.40
8:D:369:ASP:HA	8:D:401:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
6	A	1954/2413 (81%)	1813 (93%)	126 (6%)	15 (1%)	16	45
7	B	889/1008 (88%)	830 (93%)	55 (6%)	4 (0%)	30	60
8	D	357/451 (79%)	329 (92%)	28 (8%)	0	100	100
9	E	176/379 (46%)	164 (93%)	11 (6%)	1 (1%)	21	52
10	F	193/364 (53%)	173 (90%)	19 (10%)	1 (0%)	24	55
11	G	253/339 (75%)	229 (90%)	23 (9%)	1 (0%)	30	60
12	H	64/175 (37%)	55 (86%)	8 (12%)	1 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	154/157 (98%)	140 (91%)	14 (9%)	0	100	100
14	K	76/135 (56%)	72 (95%)	4 (5%)	0	100	100
15	L	406/577 (70%)	380 (94%)	26 (6%)	0	100	100
16	M	320/455 (70%)	302 (94%)	18 (6%)	0	100	100
17	N	163/251 (65%)	157 (96%)	6 (4%)	0	100	100
18	O	215/382 (56%)	196 (91%)	19 (9%)	0	100	100
19	P	645/1145 (56%)	610 (95%)	35 (5%)	0	100	100
20	R	97/215 (45%)	94 (97%)	3 (3%)	0	100	100
21	S	234/590 (40%)	223 (95%)	11 (5%)	0	100	100
22	T	451/687 (66%)	442 (98%)	9 (2%)	0	100	100
23	U	587/859 (68%)	555 (94%)	30 (5%)	2 (0%)	36	65
26	a	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
26	q	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
27	b	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	m	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	c	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
28	l	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	9	33
29	d	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	n	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
30	f	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
30	k	74/196 (38%)	66 (89%)	7 (10%)	1 (1%)	9	33
31	g	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
31	o	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
32	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
32	p	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	4	22
33	r	82/111 (74%)	76 (93%)	6 (7%)	0	100	100
34	s	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	11
35	u	423/503 (84%)	413 (98%)	8 (2%)	2 (0%)	24	55
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	4	23
35	w	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
35	x	112/503 (22%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	y	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	9
All	All	9709/14738 (66%)	9051 (93%)	610 (6%)	48 (0%)	26	55

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	1905	LEU
12	H	9	LEU
23	U	37	ILE
34	s	76	ILE
36	y	94	LYS
36	y	111	VAL
36	y	133	PRO
6	A	483	PRO
6	A	775	ARG
6	A	1675	VAL
7	B	778	THR
9	E	107	ASN
34	s	122	ARG
35	v	109	LEU
36	y	105	PRO
36	y	136	VAL
6	A	180	PRO
6	A	401	PRO
6	A	1475	LEU
6	A	1674	ASP
7	B	573	LYS
30	k	81	VAL
34	s	95	PRO
35	v	20	ARG
6	A	543	ASN
6	A	776	GLN
7	B	116	THR
10	F	120	LEU
11	G	120	TYR
23	U	300	ASP
32	p	31	SER
34	s	68	PRO
34	s	94	LEU
34	s	129	LEU
35	u	20	ARG
36	y	119	SER

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Mol	Chain	Res	Type
6	A	406	PRO
6	A	1328	PHE
6	A	1491	ILE
7	B	979	GLY
32	p	98	PRO
35	u	17	PRO
6	A	181	HIS
6	A	484	PHE
28	l	74	GLY
34	s	56	ILE
34	s	98	VAL
35	v	36	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	
6	A	1778/2182 (82%)	1761 (99%)	17 (1%)	68	76
7	B	809/910 (89%)	796 (98%)	13 (2%)	55	72
8	D	313/397 (79%)	310 (99%)	3 (1%)	68	76
9	E	168/328 (51%)	166 (99%)	2 (1%)	63	75
10	F	183/332 (55%)	182 (100%)	1 (0%)	81	83
11	G	219/296 (74%)	218 (100%)	1 (0%)	81	83
12	H	58/151 (38%)	55 (95%)	3 (5%)	21	49
13	I	140/141 (99%)	140 (100%)	0	100	100
14	K	44/121 (36%)	44 (100%)	0	100	100
15	L	379/538 (70%)	378 (100%)	1 (0%)	86	86
16	M	288/413 (70%)	285 (99%)	3 (1%)	68	76
17	N	144/225 (64%)	144 (100%)	0	100	100
18	O	210/346 (61%)	208 (99%)	2 (1%)	68	76
19	P	178/1029 (17%)	176 (99%)	2 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	90/193 (47%)	90 (100%)	0	100	100
21	S	208/525 (40%)	208 (100%)	0	100	100
22	T	248/633 (39%)	247 (100%)	1 (0%)	84	84
23	U	131/786 (17%)	127 (97%)	4 (3%)	35	60
26	a	79/103 (77%)	79 (100%)	0	100	100
26	q	77/103 (75%)	73 (95%)	4 (5%)	21	49
27	b	63/77 (82%)	63 (100%)	0	100	100
27	m	63/77 (82%)	60 (95%)	3 (5%)	23	52
28	c	65/83 (78%)	63 (97%)	2 (3%)	35	60
28	l	65/83 (78%)	60 (92%)	5 (8%)	12	37
29	d	58/66 (88%)	57 (98%)	1 (2%)	53	71
29	n	57/66 (86%)	56 (98%)	1 (2%)	51	70
30	f	70/176 (40%)	70 (100%)	0	100	100
30	k	67/176 (38%)	66 (98%)	1 (2%)	57	72
31	g	69/89 (78%)	69 (100%)	0	100	100
31	o	67/89 (75%)	65 (97%)	2 (3%)	36	61
32	h	77/129 (60%)	76 (99%)	1 (1%)	61	74
32	p	73/129 (57%)	63 (86%)	10 (14%)	3	16
All	All	6538/10992 (60%)	6455 (99%)	83 (1%)	59	74

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	334	LYS
6	A	407	VAL
6	A	526	LEU
6	A	653	ILE
6	A	742	VAL
6	A	783	LEU
6	A	978	ILE
6	A	1182	LEU
6	A	1346	PHE
6	A	1405	ILE
6	A	1426	ARG
6	A	1456	ARG
6	A	1553	ILE

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Mol	Chain	Res	Type
6	A	1561	LEU
6	A	1634	LEU
6	A	2027	LEU
6	A	2069	VAL
7	B	77	LEU
7	B	113	ILE
7	B	142	LEU
7	B	198	LEU
7	B	268	ASN
7	B	270	LEU
7	B	348	LEU
7	B	353	TYR
7	B	428	ILE
7	B	545	LEU
7	B	670	ILE
7	B	884	ARG
7	B	989	LEU
8	D	194	HIS
8	D	200	VAL
8	D	227	VAL
9	E	34	ILE
9	E	106	LEU
10	F	142	ILE
11	G	151	LEU
12	H	30	LEU
12	H	36	THR
12	H	157	ILE
15	L	431	LEU
16	M	178	ILE
16	M	387	ILE
16	M	442	VAL
18	O	278	LEU
18	O	311	LYS
19	P	1059	LEU
19	P	1123	LYS
22	T	201	THR
23	U	686	ILE
23	U	777	ASN
23	U	801	LEU
23	U	807	LEU
28	c	25	THR
28	c	92	SER

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Mol	Chain	Res	Type
29	d	66	ASN
32	h	16	THR
30	k	19	LYS
28	l	54	ILE
28	l	77	LEU
28	l	79	LYS
28	l	81	LEU
28	l	82	LEU
27	m	30	LYS
27	m	34	ASN
27	m	79	LEU
29	n	71	LEU
31	o	20	SER
31	o	43	GLN
32	p	11	ARG
32	p	15	VAL
32	p	16	THR
32	p	25	VAL
32	p	43	VAL
32	p	44	LYS
32	p	95	ILE
32	p	96	ILE
32	p	97	LEU
32	p	101	LEU
26	q	41	ARG
26	q	48	LEU
26	q	82	LYS
26	q	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	170	HIS
6	A	265	ASN
6	A	310	ASN
6	A	343	ASN
6	A	429	ASN
6	A	481	HIS
6	A	497	GLN
6	A	535	HIS
6	A	543	ASN
6	A	553	ASN

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Mol	Chain	Res	Type
6	A	559	GLN
6	A	574	GLN
6	A	648	GLN
6	A	733	GLN
6	A	739	ASN
6	A	748	GLN
6	A	785	HIS
6	A	830	ASN
6	A	848	ASN
6	A	859	ASN
6	A	907	ASN
6	A	1086	ASN
6	A	1087	ASN
6	A	1142	ASN
6	A	1156	HIS
6	A	1368	GLN
6	A	1376	ASN
6	A	1449	ASN
6	A	1466	GLN
6	A	1529	ASN
6	A	1532	HIS
6	A	1568	ASN
6	A	1635	HIS
6	A	1667	GLN
6	A	1687	HIS
6	A	1695	ASN
6	A	1707	HIS
6	A	1782	ASN
6	A	1789	ASN
6	A	1800	ASN
6	A	1809	ASN
6	A	1824	GLN
6	A	1876	ASN
6	A	1895	HIS
6	A	2047	GLN
7	B	101	GLN
7	B	103	HIS
7	B	112	ASN
7	B	180	ASN
7	B	183	GLN
7	B	220	ASN
7	B	255	GLN

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Mol	Chain	Res	Type
7	B	268	ASN
7	B	289	ASN
7	B	294	ASN
7	B	358	ASN
7	B	471	HIS
7	B	511	GLN
7	B	514	GLN
7	B	647	ASN
7	B	693	ASN
7	B	764	ASN
7	B	869	HIS
7	B	960	ASN
8	D	126	HIS
8	D	382	HIS
8	D	428	GLN
9	E	87	ASN
9	E	107	ASN
9	E	171	ASN
10	F	85	GLN
10	F	89	HIS
10	F	134	ASN
11	G	39	GLN
11	G	44	ASN
11	G	252	HIS
11	G	256	ASN
12	H	173	HIS
13	I	46	ASN
13	I	56	HIS
13	I	58	GLN
13	I	112	ASN
13	I	143	HIS
14	K	67	HIS
15	L	14	GLN
15	L	66	ASN
15	L	202	GLN
15	L	354	HIS
15	L	390	HIS
15	L	441	ASN
15	L	457	HIS
16	M	219	GLN
16	M	261	HIS
16	M	325	ASN

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Mol	Chain	Res	Type
16	M	380	HIS
16	M	437	GLN
17	N	172	GLN
17	N	203	HIS
17	N	208	HIS
17	N	247	HIS
18	O	32	HIS
18	O	327	HIS
19	P	960	HIS
19	P	986	HIS
19	P	989	HIS
19	P	1082	GLN
20	R	184	GLN
21	S	186	GLN
22	T	17	GLN
22	T	79	HIS
22	T	183	ASN
22	T	210	ASN
22	T	212	HIS
22	T	277	ASN
23	U	730	GLN
23	U	777	ASN
27	b	54	ASN
27	b	65	HIS
28	c	34	GLN
28	c	86	ASN
29	d	66	ASN
31	g	17	HIS
32	h	86	ASN
30	k	25	GLN
27	m	34	ASN
29	n	55	HIS
32	p	14	GLN
32	p	21	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	127/1175 (10%)	44 (34%)	4 (3%)
2	5	100/214 (46%)	25 (25%)	2 (2%)
3	6	101/112 (90%)	28 (27%)	3 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	e	33/34 (97%)	19 (57%)	0
5	i	54/59 (91%)	18 (33%)	0
All	All	415/1594 (26%)	134 (32%)	9 (2%)

All (134) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	11	U
1	2	16	U
1	2	17	U
1	2	18	U
1	2	19	U
1	2	20	G
1	2	21	G
1	2	23	U
1	2	24	U
1	2	25	A
1	2	30	A
1	2	31	A
1	2	32	G
1	2	40	U
1	2	41	C
1	2	42	U
1	2	63	U
1	2	64	G
1	2	141	A
1	2	1094	G
1	2	1096	C
1	2	1098	C
1	2	1099	G
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1106	G
1	2	1107	C
1	2	1108	A
1	2	1120	G
1	2	1123	C
1	2	1124	U

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Mol	Chain	Res	Type
1	2	1125	U
1	2	1126	G
1	2	1139	G
1	2	1144	U
1	2	1145	U
1	2	1146	G
1	2	1149	G
1	2	1152	U
1	2	1166	G
2	5	33	U
2	5	42	A
2	5	43	G
2	5	44	A
2	5	45	A
2	5	46	C
2	5	70	A
2	5	75	A
2	5	76	U
2	5	77	A
2	5	79	C
2	5	80	G
2	5	81	A
2	5	82	A
2	5	84	A
2	5	92	U
2	5	96	U
2	5	101	C
2	5	108	C
2	5	113	G
2	5	127	U
2	5	169	U
2	5	170	U
2	5	171	U
2	5	172	U
3	6	12	A
3	6	13	A
3	6	14	C
3	6	15	C
3	6	17	U
3	6	34	A
3	6	36	U
3	6	42	A

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Mol	Chain	Res	Type
3	6	44	A
3	6	53	A
3	6	54	U
3	6	55	G
3	6	57	U
3	6	59	A
3	6	60	G
3	6	62	A
3	6	64	U
3	6	65	U
3	6	66	C
3	6	67	C
3	6	73	A
3	6	74	U
3	6	80	U
3	6	81	G
3	6	85	C
3	6	86	G
3	6	88	U
3	6	99	A
4	e	-12	U
4	e	-11	U
4	e	-9	A
4	e	-4	A
4	e	3	A
4	e	4	U
4	e	5	A
4	e	6	U
4	e	8	U
4	e	9	U
4	e	10	U
4	e	11	U
4	e	13	U
4	e	15	U
4	e	17	U
4	e	18	U
4	e	19	U
4	e	20	A
4	e	21	U
5	i	2	U
5	i	9	U
5	i	505	C

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Mol	Chain	Res	Type
5	i	508	G
5	i	509	U
5	i	511	A
5	i	514	A
5	i	515	A
5	i	516	C
5	i	518	U
5	i	1008	A
5	i	1111	U
5	i	1112	U
5	i	1113	A
5	i	1114	U
5	i	1115	A
5	i	1117	A
5	i	1118	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	41	C
1	2	1123	C
1	2	1124	U
1	2	1145	U
2	5	78	A
2	5	81	A
3	6	14	C
3	6	56	A
3	6	64	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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
38	IHP	A	3001	-	36,36,36	0.88	0	60,60,60	1.67	12 (20%)
39	GTP	B	2001	37	33,34,34	0.97	1 (3%)	50,54,54	1.60	10 (20%)

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	3001	-	-	7/30/54/54	0/1/1/1
39	GTP	B	2001	37	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	2001	GTP	O4'-C4'	-2.14	1.40	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	2001	GTP	C2-N3-C4	4.62	120.25	112.30
39	B	2001	GTP	C5-C4-N3	-4.21	121.69	128.39
38	A	3001	IHP	C4-C3-C2	3.66	118.45	110.43
38	A	3001	IHP	C5-C6-C1	3.62	118.38	110.43
38	A	3001	IHP	O15-C5-C6	3.61	116.44	108.76
38	A	3001	IHP	P6-O16-C6	-3.47	114.17	123.43
38	A	3001	IHP	C5-C4-C3	3.46	118.02	110.43
38	A	3001	IHP	C3-C2-C1	3.21	117.47	110.43
39	B	2001	GTP	N9-C8-N7	-3.11	107.64	113.40
39	B	2001	GTP	C2-N1-C6	-2.96	119.75	125.11
39	B	2001	GTP	C5-C6-N1	2.94	120.73	113.25
38	A	3001	IHP	O11-C1-C2	2.64	114.38	108.76
39	B	2001	GTP	C8-N7-C5	2.56	108.82	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	3001	IHP	O11-C1-C6	2.53	114.15	108.76
38	A	3001	IHP	O15-C5-C4	2.51	114.11	108.76
38	A	3001	IHP	P3-O13-C3	-2.42	116.98	123.43
39	B	2001	GTP	O6-C6-C5	-2.36	120.30	126.53
39	B	2001	GTP	N9-C4-N3	2.25	130.45	125.95
39	B	2001	GTP	C6-C5-N7	2.21	134.30	130.29
38	A	3001	IHP	O12-C2-C3	2.13	113.29	108.76
39	B	2001	GTP	N1-C2-N3	-2.08	119.52	123.32
38	A	3001	IHP	P2-O12-C2	-2.05	117.97	123.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	B	2001	GTP	PB-O3B-PG-O2G
38	A	3001	IHP	C1-O11-P1-O21
39	B	2001	GTP	C5'-O5'-PA-O3A
39	B	2001	GTP	C5'-O5'-PA-O1A
39	B	2001	GTP	C5'-O5'-PA-O2A
38	A	3001	IHP	C4-O14-P4-O34
38	A	3001	IHP	C6-O16-P6-O36
38	A	3001	IHP	C2-O12-P2-O22
38	A	3001	IHP	C3-O13-P3-O23
39	B	2001	GTP	PB-O3B-PG-O3G
38	A	3001	IHP	C1-O11-P1-O41
38	A	3001	IHP	C3-O13-P3-O33

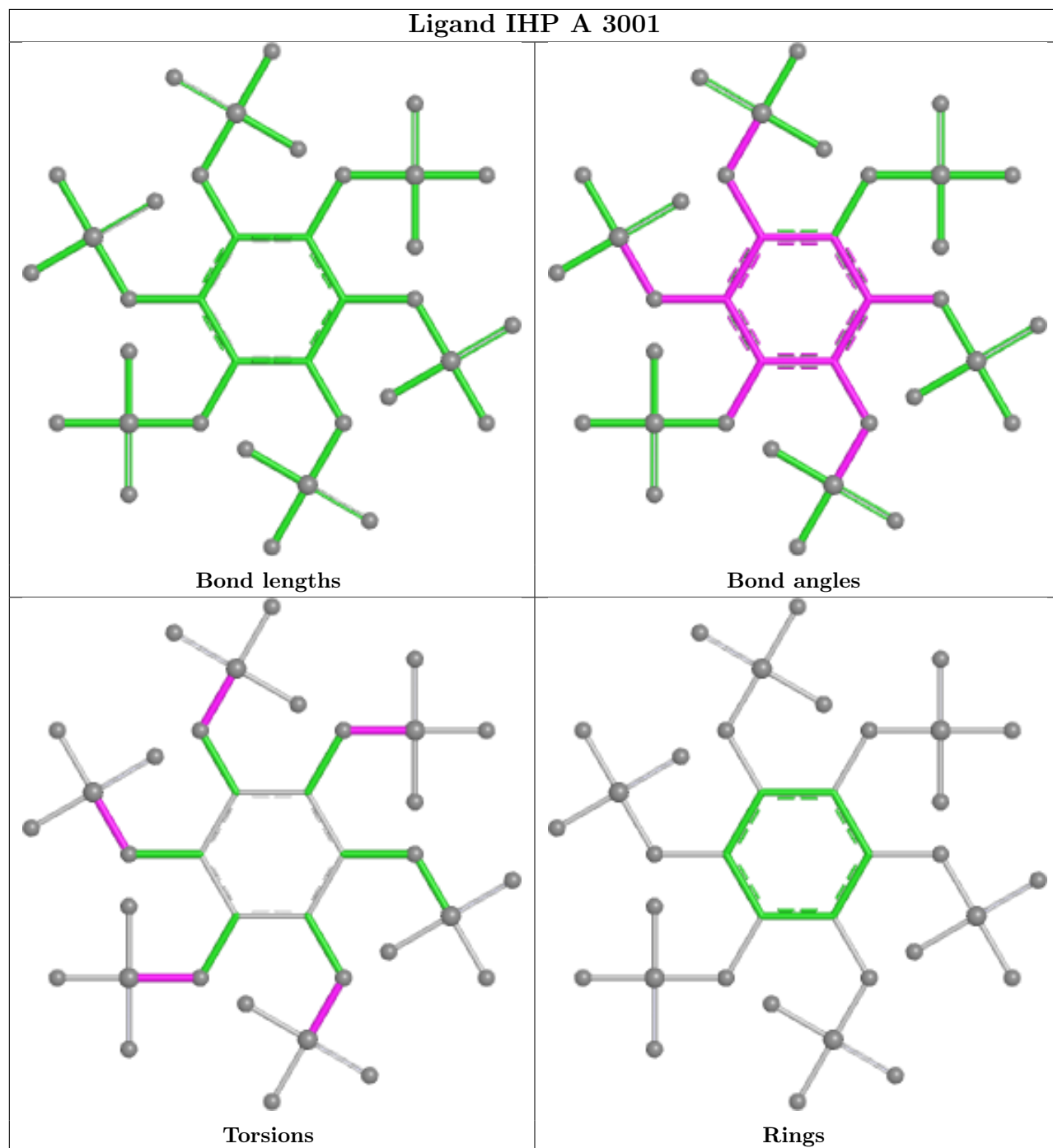
There are no ring outliers.

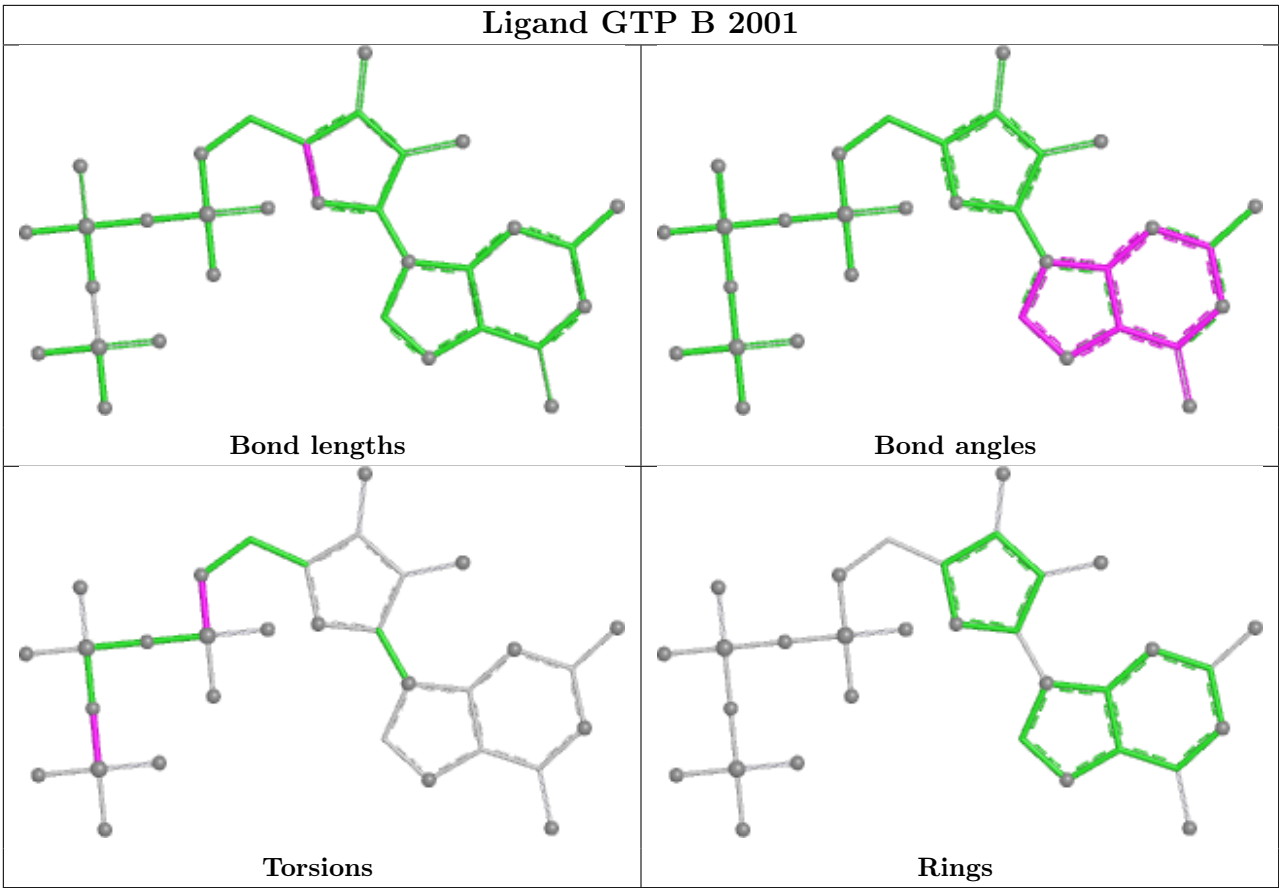
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A	3001	IHP	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	i	4
24	X	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	15:U	O3'	501:A	P	58.05
1	X	3370:UNK	C	3389:UNK	N	35.33
1	X	1031:UNK	C	2287:UNK	N	34.77
1	X	125:UNK	C	1001:UNK	N	25.13
1	X	2322:UNK	C	3364:UNK	N	19.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	628:U	O3'	1001:A	P	15.34
1	i	518:U	O3'	620:U	P	7.99
1	i	1008:A	O3'	1110:A	P	5.10

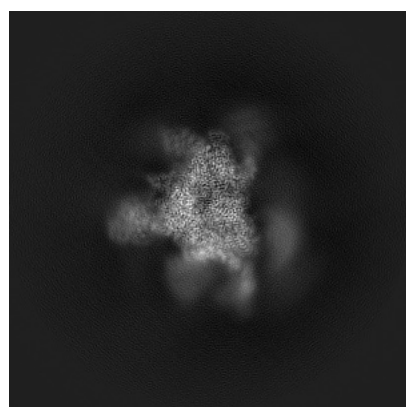
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7109. These allow visual inspection of the internal detail of the map and identification of artifacts.

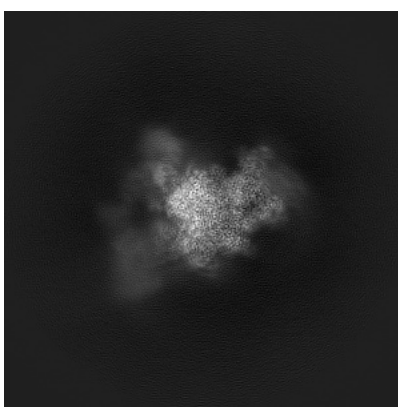
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

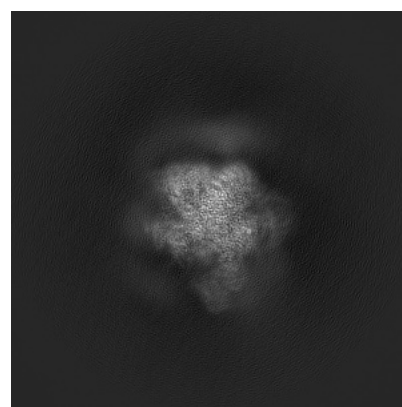
6.1.1 Primary map



X



Y

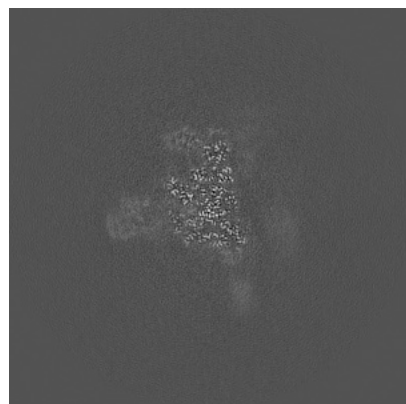


Z

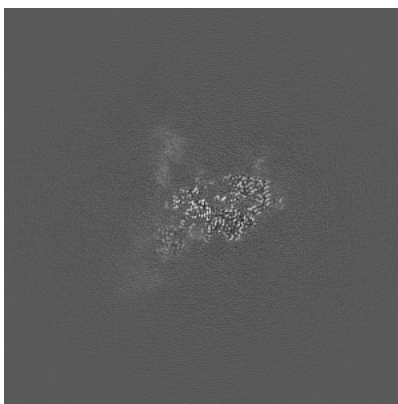
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

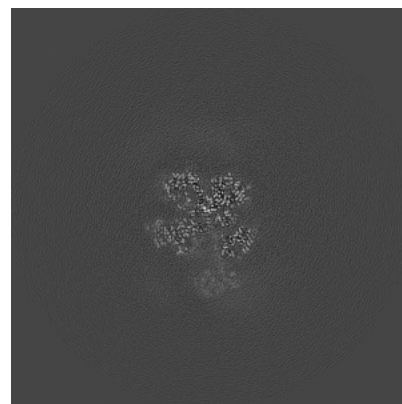
6.2.1 Primary map



X Index: 200



Y Index: 200

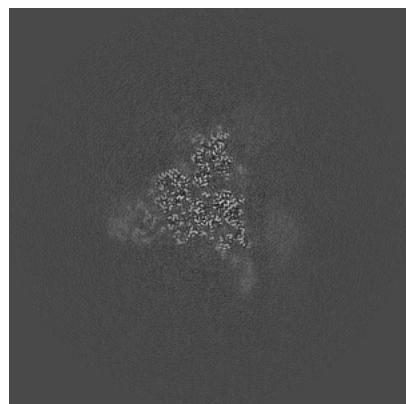


Z Index: 200

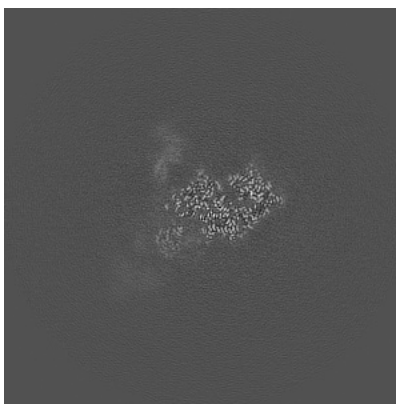
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

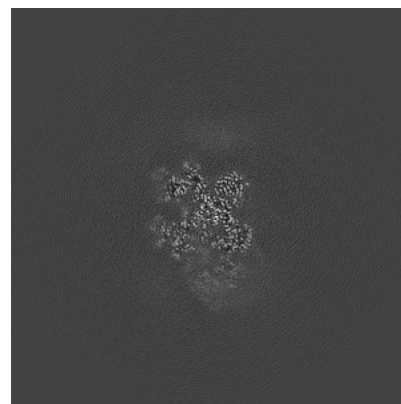
6.3.1 Primary map



X Index: 212



Y Index: 204

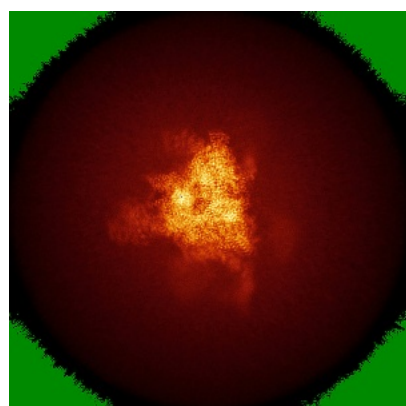


Z Index: 191

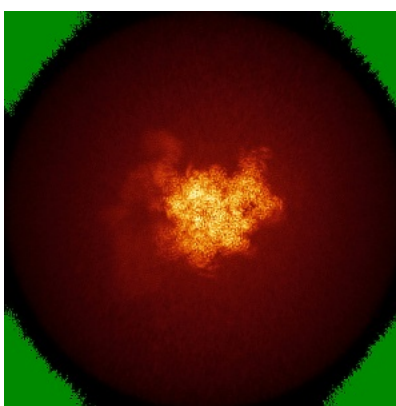
The images above show the largest variance slices of the map in three orthogonal directions.

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

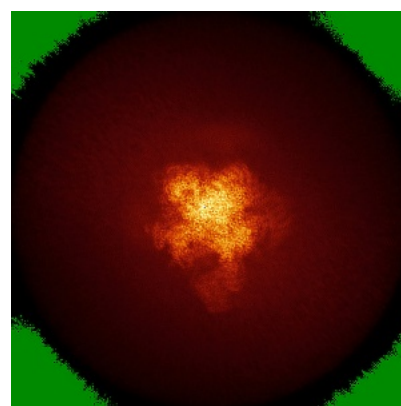
6.4.1 Primary map



X



Y

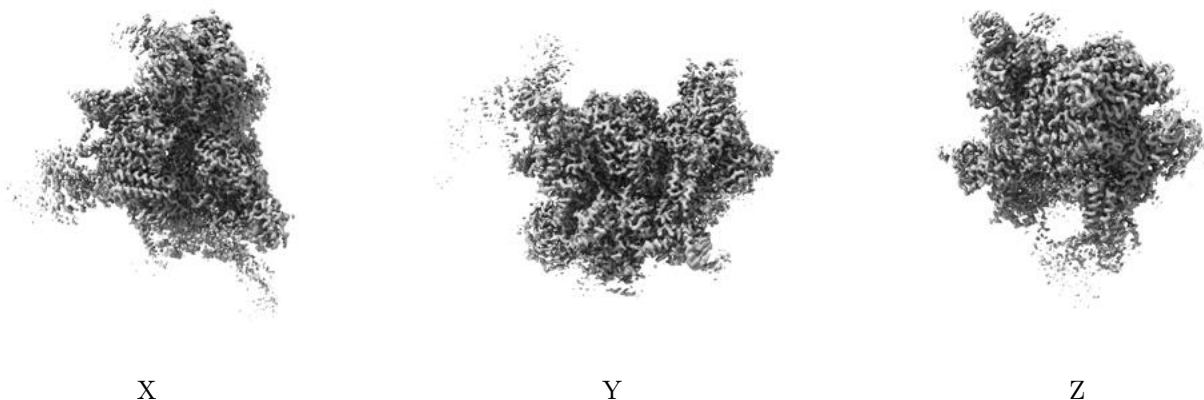


Z

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

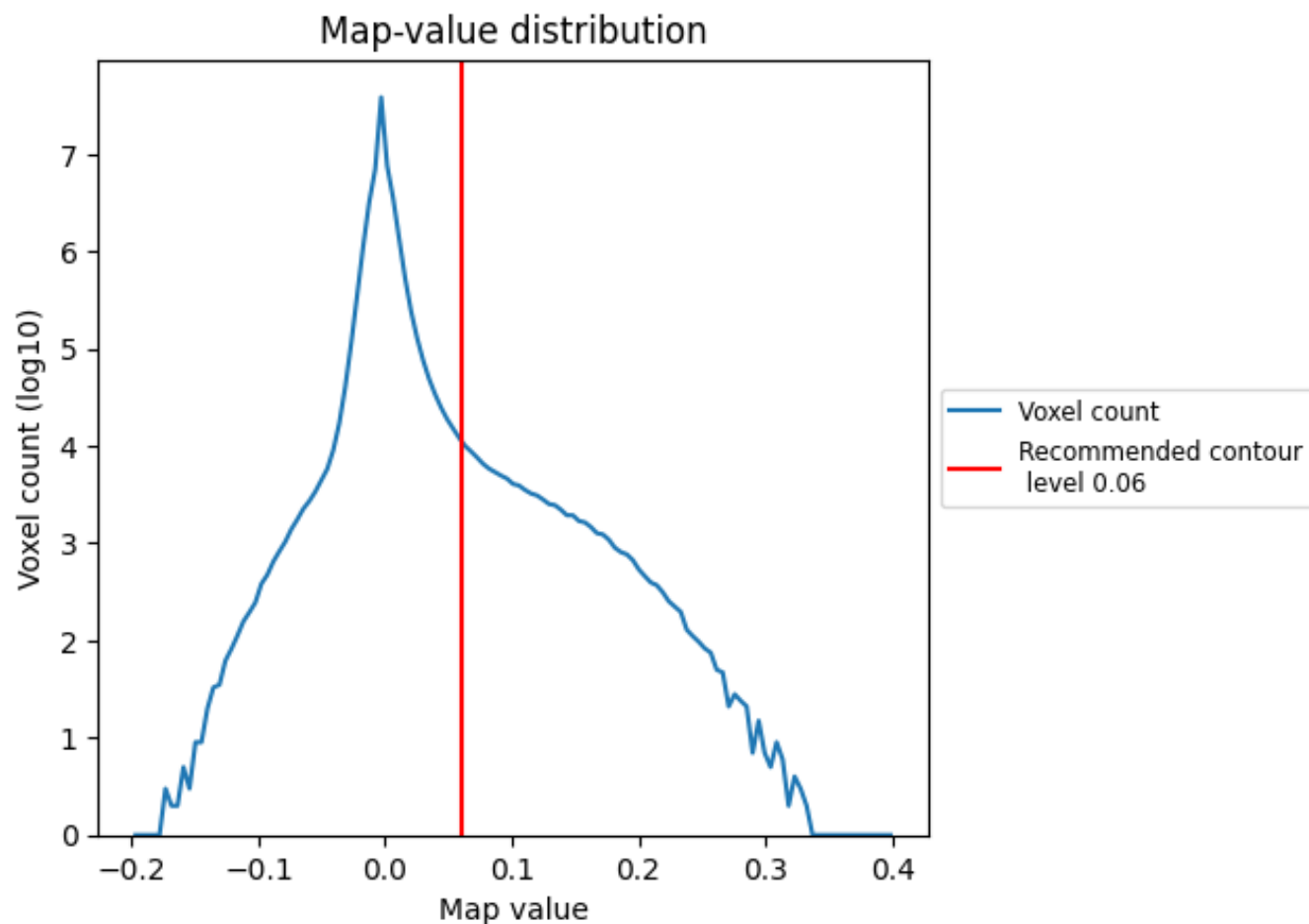
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

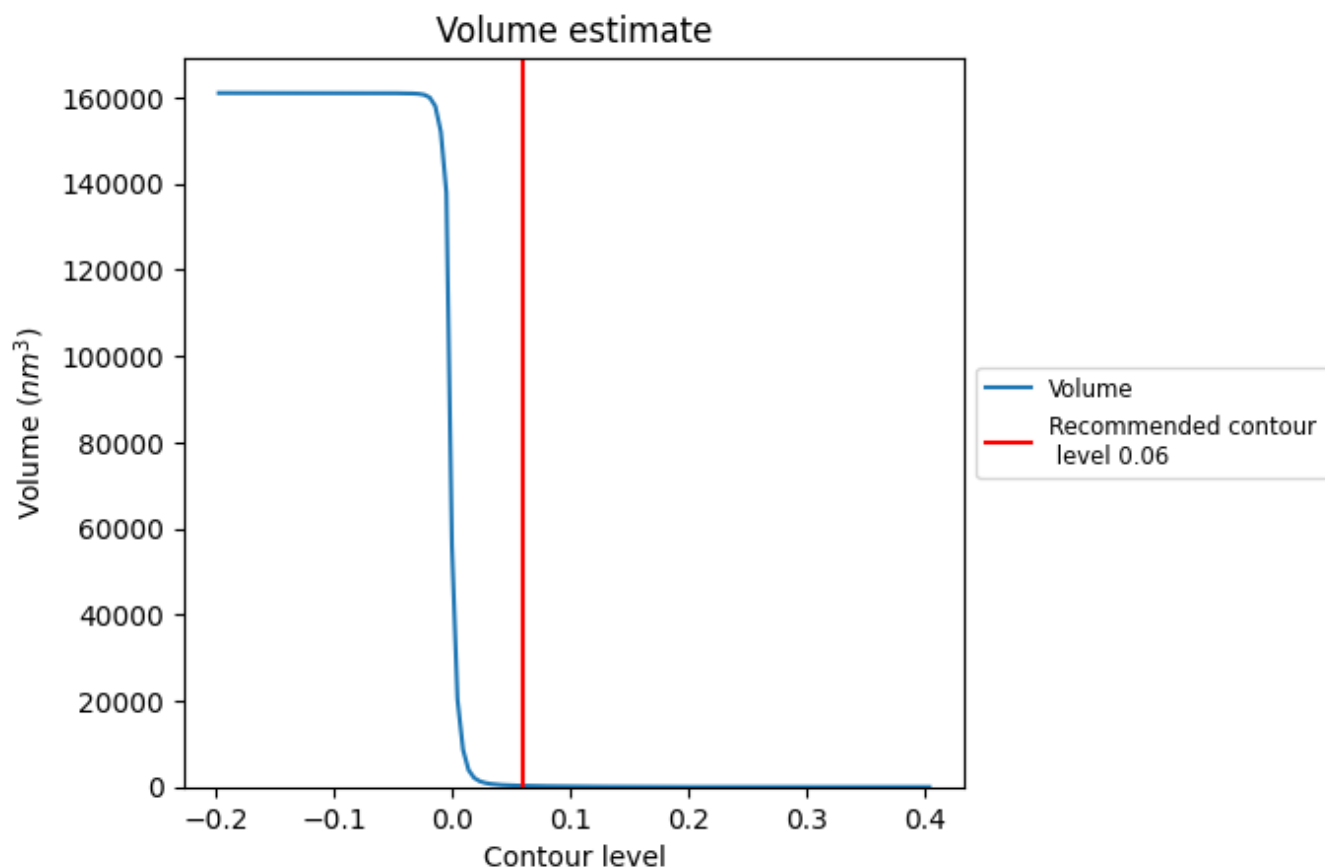
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

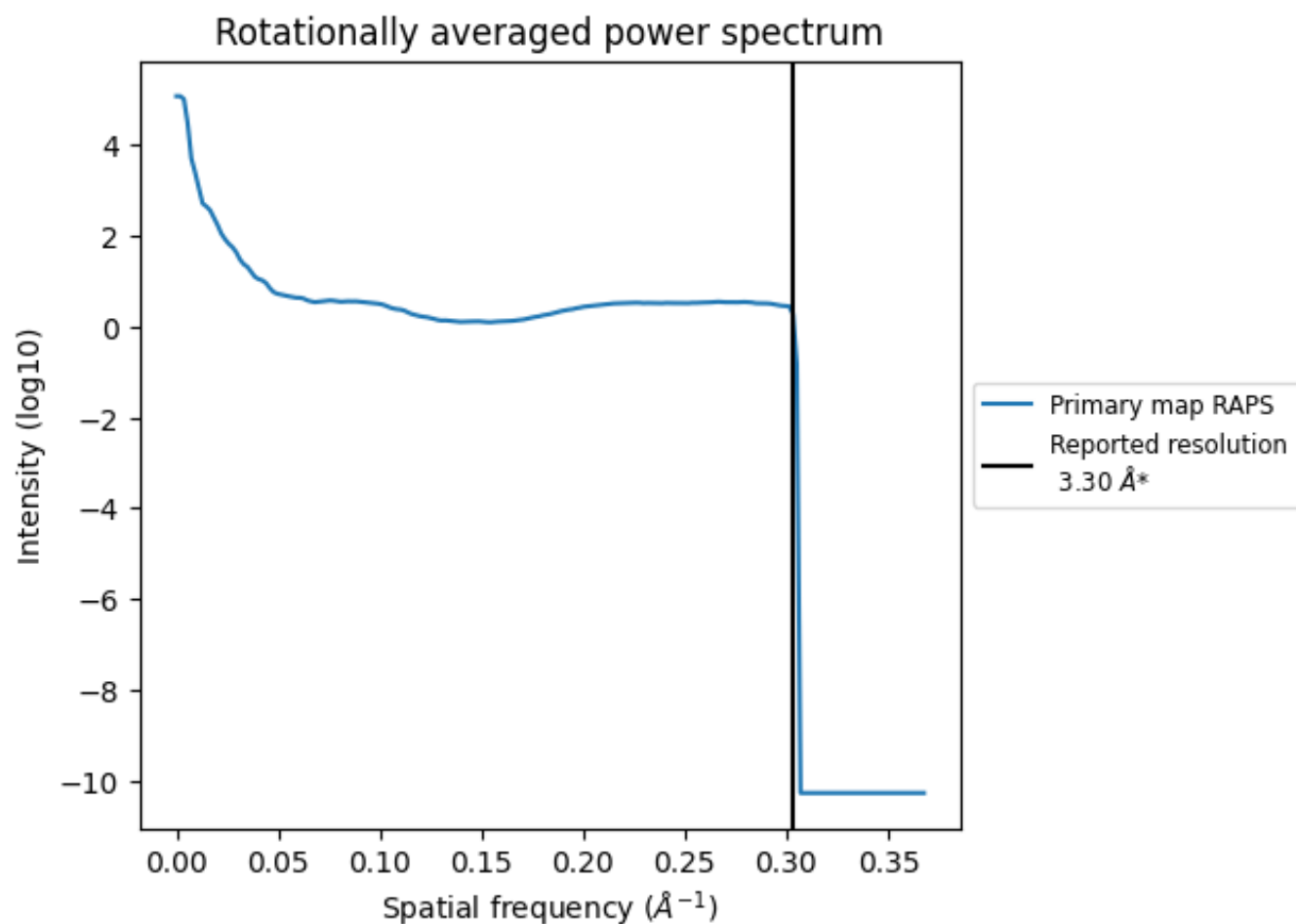
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm^3 ; this corresponds to an approximate mass of 246 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 0.303 Å⁻¹

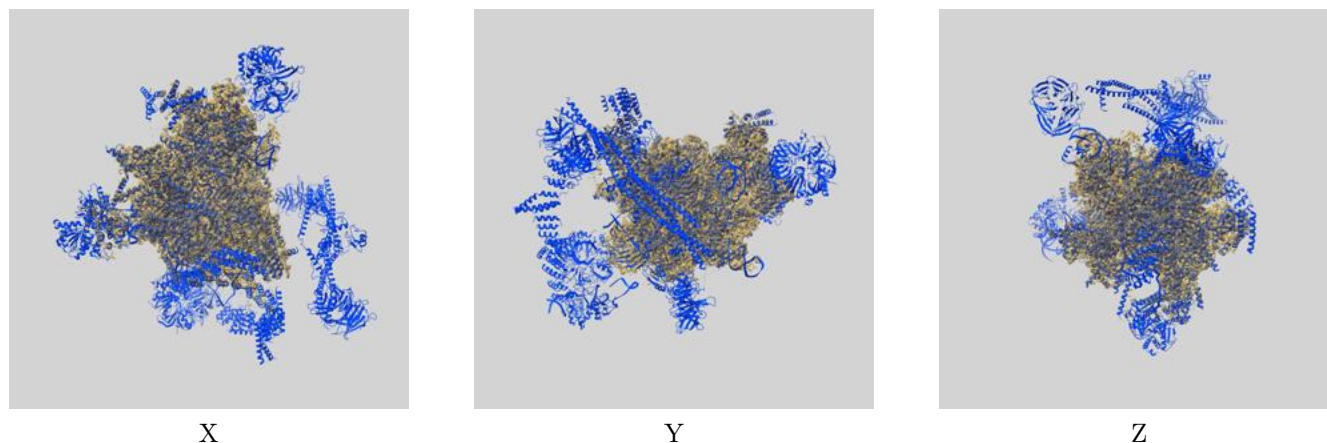
8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

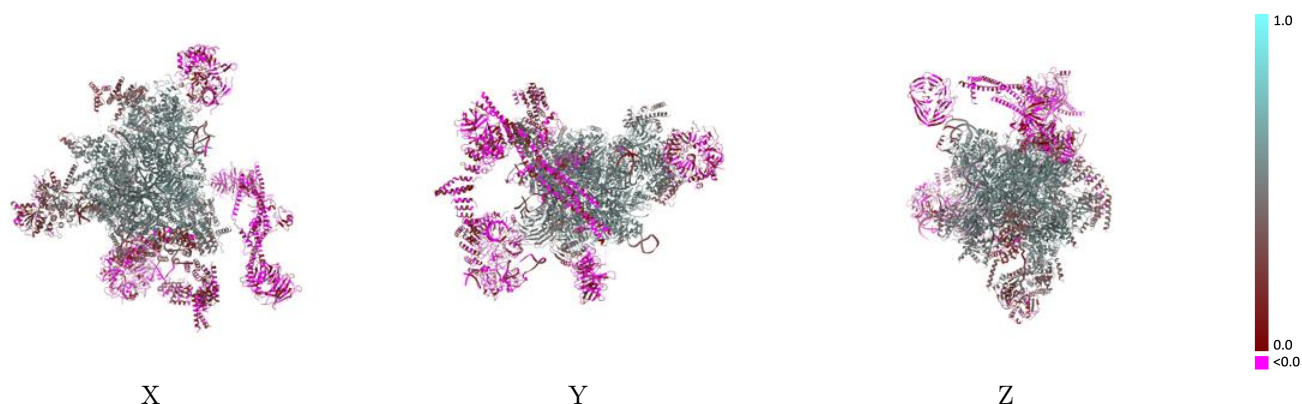
This section contains information regarding the fit between EMDB map EMD-7109 and PDB model 6BK8. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay ⓘ



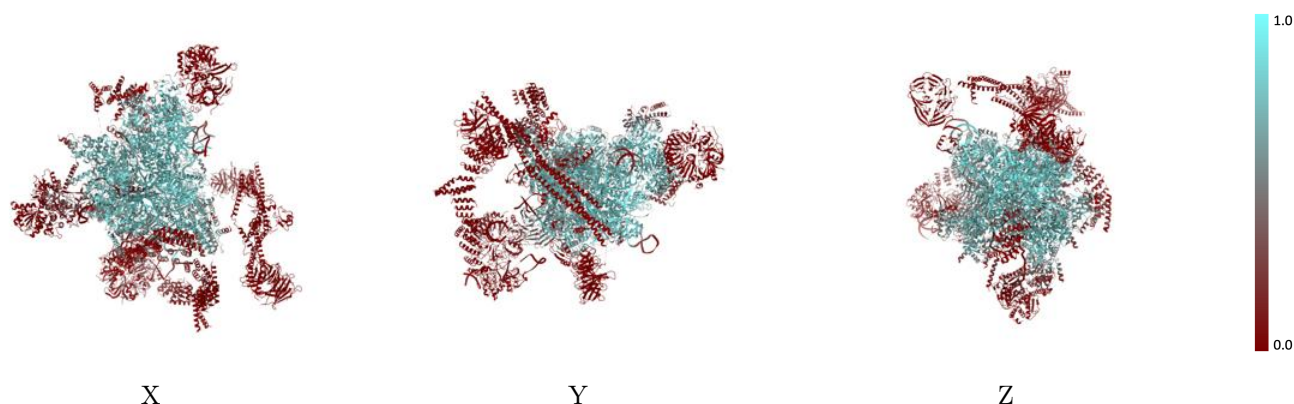
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



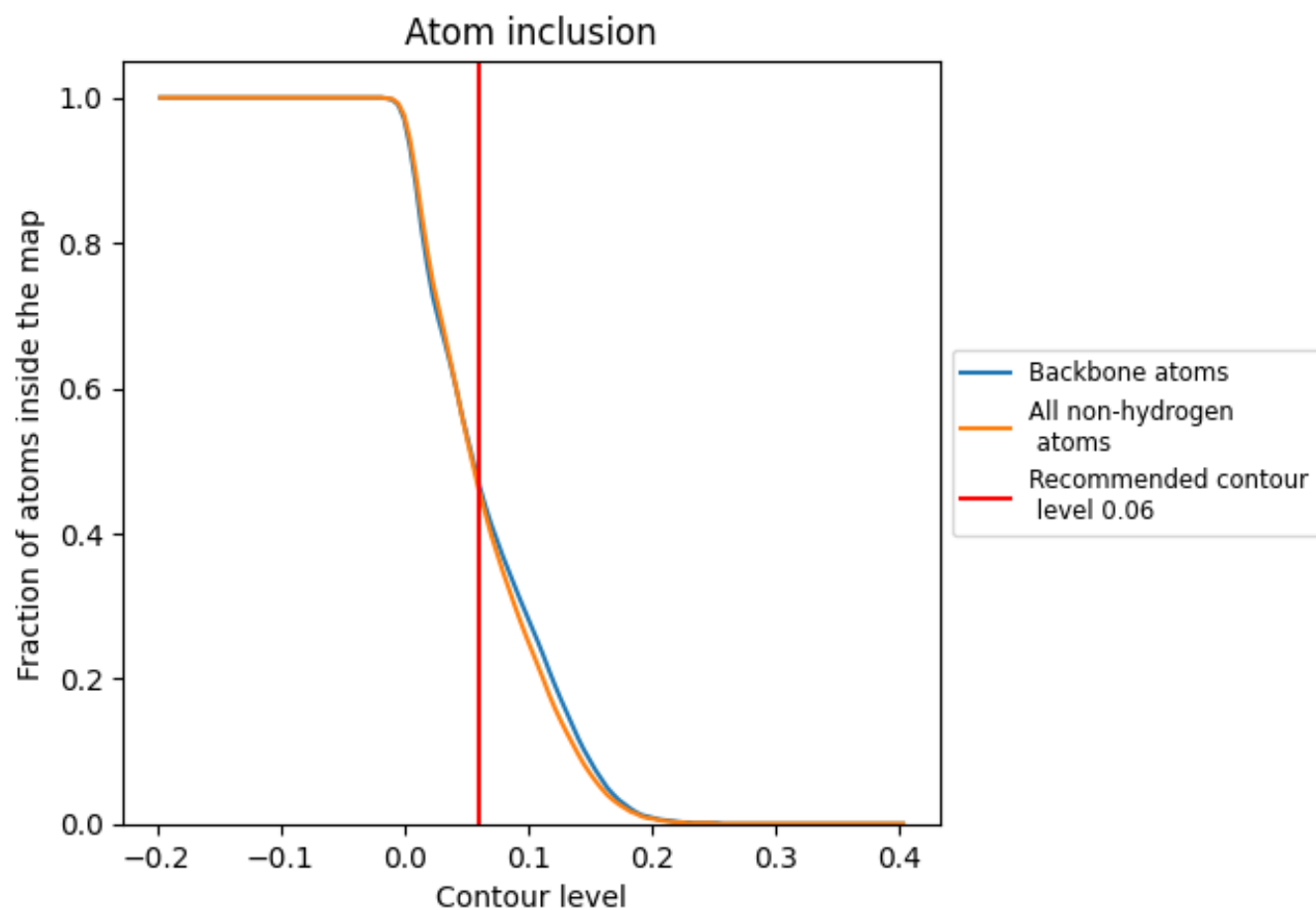
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 46% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4630	 0.3790
2	 0.2020	 0.1350
5	 0.7190	 0.4800
6	 0.7540	 0.5110
A	 0.7660	 0.5480
B	 0.7220	 0.5340
D	 0.7990	 0.5590
E	 0.6660	 0.5200
F	 0.5400	 0.4790
G	 0.6930	 0.5240
H	 0.5260	 0.5260
I	 0.7560	 0.5480
K	 0.3800	 0.4500
L	 0.4030	 0.3920
M	 0.5040	 0.5000
N	 0.5580	 0.4770
O	 0.4720	 0.4870
P	 0.1570	 0.3460
R	 0.6000	 0.5230
S	 0.7020	 0.5300
T	 0.5060	 0.4260
U	 0.0770	 0.2040
X	 0.4060	 0.4340
Y	 0.3380	 0.3790
a	 0.0000	 0.0440
b	 0.0000	 0.0190
c	 0.0000	 0.0250
d	 0.0000	 0.0920
e	 0.4160	 0.4330
f	 0.0000	 0.0780
g	 0.0000	 0.1650
h	 0.0000	 0.0050
i	 0.4260	 0.3650
k	 0.0000	 0.0040
l	 0.0000	 0.0130



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Chain	Atom inclusion	Q-score
m	 0.0000	 0.0240
n	 0.0000	 0.0090
o	 0.0000	 0.0240
p	 0.0000	 0.0100
q	 0.0000	 0.0120
r	 0.0000	 0.0330
s	 0.0000	 0.0040
u	 0.0000	 -0.0080
v	 0.0000	 -0.0290
w	 0.0000	 -0.0040
x	 0.0000	 -0.0220
y	 0.0000	 -0.0290