Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 02:08 AM JST

PDB ID	:	9L5R / pdb_0000l5r
EMDB ID	:	EMD-62841
Title	:	Cryo-EM structure of the thermophile spliceosome (state ILS)
Authors	:	Li, Y.; Fischer, P.; Wang, M.; Yuan, R.; Meng, W.; Luehrmann, R.; Lau, B.; Hurt, E.; Cheng, J.
Deposited on	:	2024-12-23
Resolution	:	2.80 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:

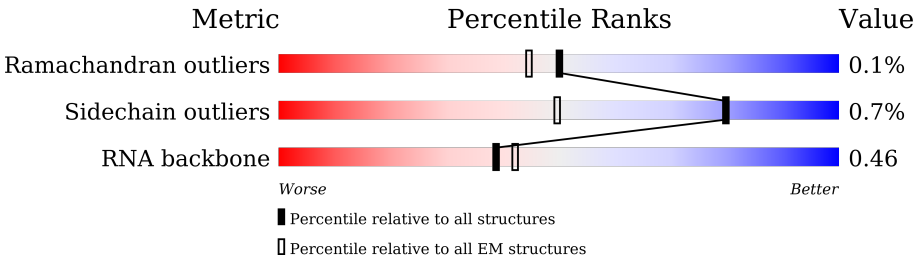
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	2	193	45% 9% • 45%
2	5	116	75% 20% • •
3	6	101	60% 36% • •
4	A	2463	81% • 19%
5	B	326	78% • 21%
6	C	1011	91% 9%
7	D	325	29% • 71%
8	E	352	87% • 12%
9	F	233	46% • 53%

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Mol	Chain	Length	Quality of chain
10	I	839	87% 12%
11	J	687	88% 11%
12	L	768	82% 17%
13	K	231	99%
14	q	480	29% 71%
14	r	480	29% 70%
14	s	480	29% 71%
14	t	480	29% 71%
15	N	148	97%
16	S	167	93% 6%
17	T	496	64% 34%
18	U	757	45% 54%
19	M	395	62% 37%
20	0	408	65% 32%
21	R	578	58% 41%
22	W	547	72% 27%
23	P	260	43% 56%
24	Y	1416	95% 5%
25	a	98	88% 12%
25	j	98	90% 10%
26	b	94	76% 24%
26	l	94	85% 14%
27	c	592	14% 86%
27	m	592	14% 85%
28	d	118	69% 31%

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Mol	Chain	Length	Quality of chain
28	o	118	72% 26%
29	e	211	37% 63%
29	p	211	48% 51%
30	f	114	74% 26%
30	u	114	79% 21%
31	g	82	88% 12%
31	k	82	88% 11%
32	h	242	50% 50%
33	i	201	51% 49%
34	CY	510	18% 82%
35	Cb	975	52% 48%
36	Cc	764	93% 7%
37	7	101	21% 74%
38	Ci	153	55% 45%
39	H	22	100%

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 104144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	106	2224	994	357	767	106	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	111	2343	1048	398	786	111	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	98	2090	935	379	678	98	0	0

- Molecule 4 is a protein called PRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	2006	16540	10628	2874	2976	62	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	258	2071	1273	388	405	5	0	0

- Molecule 6 is a protein called SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	922	7301	4668	1229	1368	36	0	0

- Molecule 7 is a protein called SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	95	Total	C	N	O	S	0	0
			786	477	150	154	5		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4-like WD40 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	310	Total	C	N	O	S	0	0
			2379	1493	414	462	10		

- Molecule 9 is a protein called CCDC12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	110	Total	C	N	O	S	0	0
			879	544	166	167	2		

- Molecule 10 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	738	Total	C	N	O	S	0	0
			6135	3924	1071	1112	28		

- Molecule 11 is a protein called Suppressor of forked domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	608	Total	C	N	O	S	0	0
			5176	3297	937	929	13		

- Molecule 12 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	637	Total	C	N	O	S	0	0
			5052	3111	952	974	15		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	231	Total	C	N	O	S	0	0
			1797	1122	317	354	4		

- Molecule 14 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	139	Total	C	N	O	S	0	0
			1110	699	195	214	2		
14	t	141	Total	C	N	O	S	0	0
			1122	707	197	216	2		
14	r	143	Total	C	N	O	S	0	0
			1132	713	199	218	2		
14	s	140	Total	C	N	O	S	0	0
			1115	702	196	215	2		

- Molecule 15 is a protein called Putative bud site selection protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	148	Total	C	N	O	S	0	0
			1200	755	213	220	12		

- Molecule 16 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	157	Total	C	N	O	S	0	0
			1209	763	217	223	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	328	Total	C	N	O	S	0	0
			2565	1621	461	469	14		

- Molecule 18 is a protein called Cell cycle control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	348	Total	C	N	O	S	0	0
			2821	1770	516	524	11		

- Molecule 19 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	248	Total	C	N	O	S	0	0
			1964	1238	355	354	17		

- Molecule 20 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	276	Total	C	N	O	S	0	0
			2224	1381	424	412	7		

- Molecule 21 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R	340	Total	C	N	O	P	S	0	0
			2686	1664	509	503	2	8		

- Molecule 22 is a protein called PRP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	397	Total	C	N	O	S	0	0
			2224	1336	444	440	4		

- Molecule 23 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	114	Total	C	N	O	S	0	0
			925	577	182	165	1		

- Molecule 24 is a protein called Pre-mRNA-splicing factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	1344	Total	C	N	O	S	0	0
			10819	6892	1900	2002	25		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	86	Total	C	N	O		0	0
			426	253	86	87			
25	j	88	Total	C	N	O	S	0	0
			704	456	121	126	1		

- Molecule 26 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	71	Total	C	N	O		0	0
			351	209	71	71			
26	l	81	Total	C	N	O	S	0	0
			649	412	114	120	3		

- Molecule 27 is a protein called Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	c	84	Total C N O 416 247 84 85	0	0
27	m	86	Total C N O S 678 427 129 118 4	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	d	81	Total C N O 401 239 81 81	0	0
28	o	87	Total C N O S 679 433 114 128 4	0	0

- Molecule 29 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	e	79	Total C N O 388 230 79 79	0	0
29	p	103	Total C N O S 788 490 148 145 5	0	0

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	f	84	Total C N O 414 246 84 84	0	0
30	u	90	Total C N O S 716 449 132 131 4	0	0

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	g	72	Total C N O 354 210 72 72	0	0
31	k	73	Total C N O S 577 369 101 105 2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	h	122	Total	C	N	O	0	0
			605	361	122	122		

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B'-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	i	102	Total	C	N	O	0	0
			504	300	102	102		

- Molecule 34 is a protein called Nineteen complex-related protein 2-domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	CY	91	Total	C	N	O	0	0
			444	262	91	91		

- Molecule 35 is a protein called G-patch domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Cb	505	Total	C	N	O	0	0
			2496	1486	505	505		

- Molecule 36 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Cc	714	Total	C	N	O	0	0
			3541	2112	714	715		

- Molecule 37 is a RNA chain called Unknown mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7	26	Total	C	N	O	P	0	0
			494	241	68	159	26		

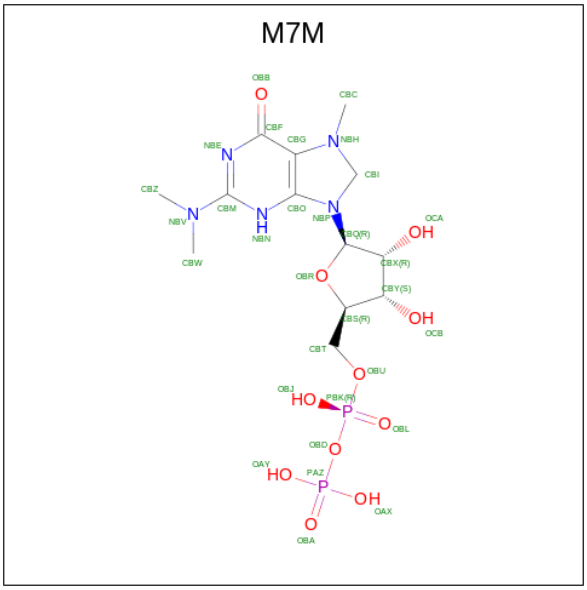
- Molecule 38 is a protein called Putative cyclophilin protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Ci	84	Total	C	N	O	0	0
			415	247	84	84		

- Molecule 39 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	H	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 40 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: $C_{13}H_{23}N_5O_{11}P_2$).

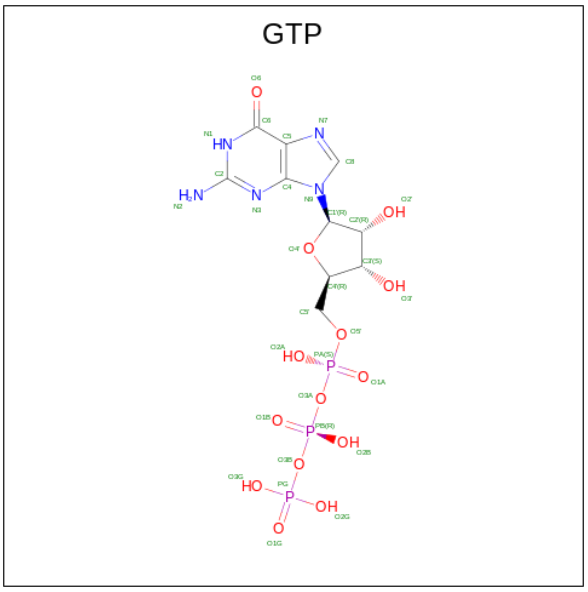


Mol	Chain	Residues	Atoms					AltConf
40	B	1	Total	C	N	O	P	0
			30	13	5	10	2	

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

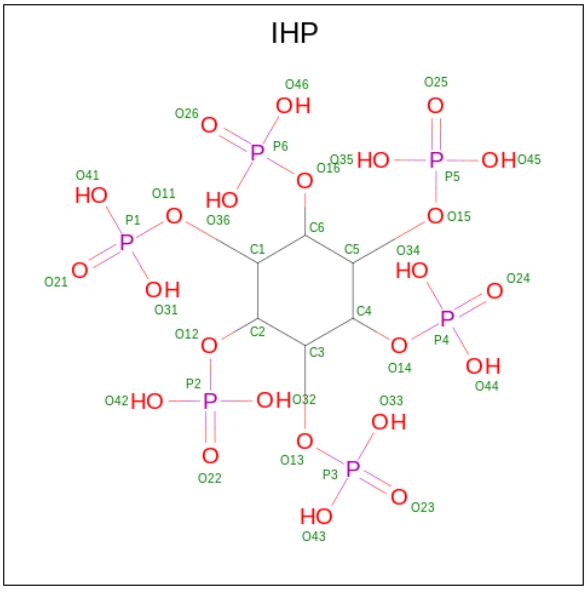
Mol	Chain	Residues	Atoms		AltConf
41	C	1	Total	Mg	0
			1	1	

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



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

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

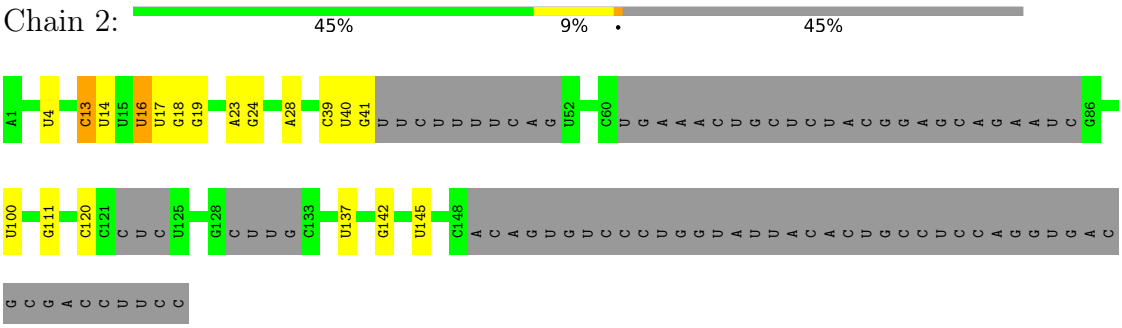
Mol	Chain	Residues	Atoms	AltConf
44	N	3	Total Zn 3 3	0
44	U	1	Total Zn 1 1	0
44	M	2	Total Zn 2 2	0

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

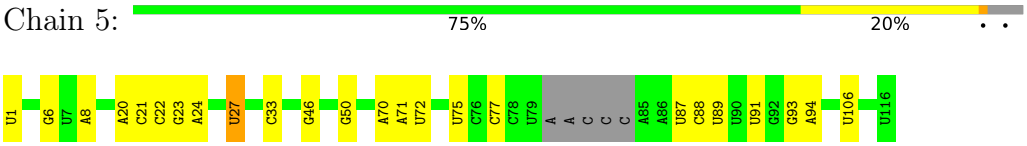
- Molecule 1: U2 snRNA

Chain 2:



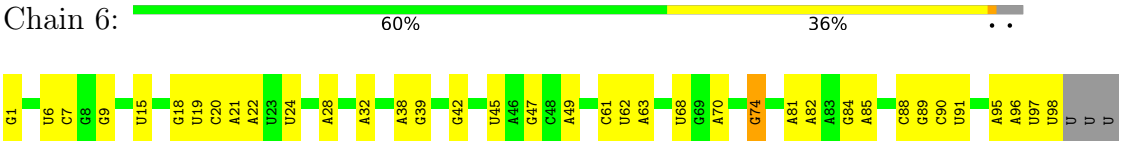
- Molecule 2: U5 snRNA

Chain 5:



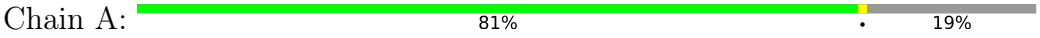
- Molecule 3: U6 snRNA

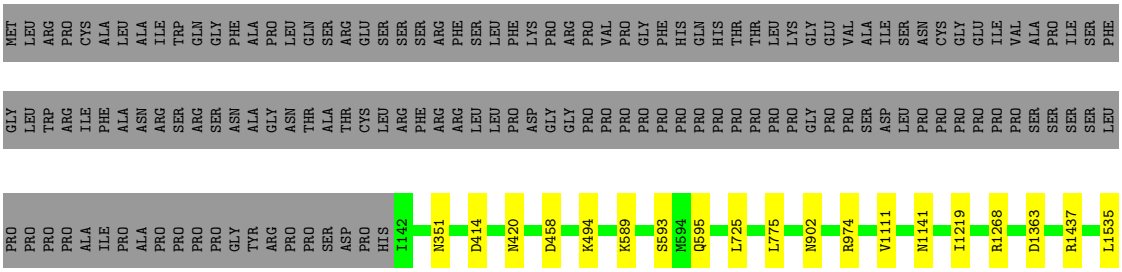
Chain 6:

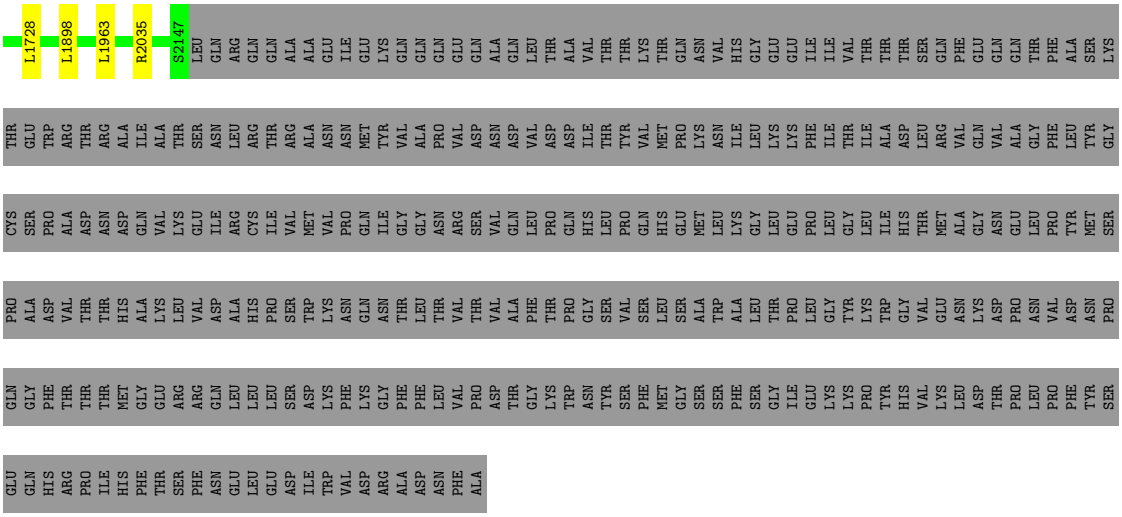


- Molecule 4: PRP8

Chain A:

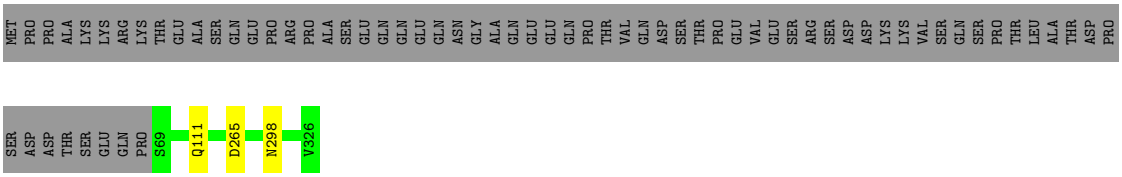






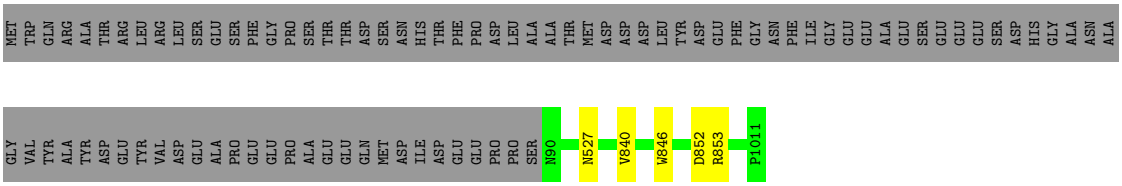
• Molecule 5: Pre-mRNA-splicing factor SYF2

Chain B:



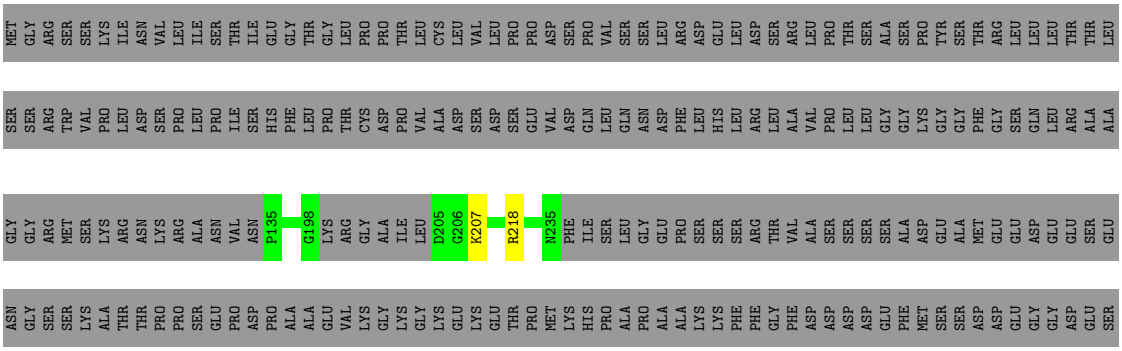
• Molecule 6: SNU114

Chain C:



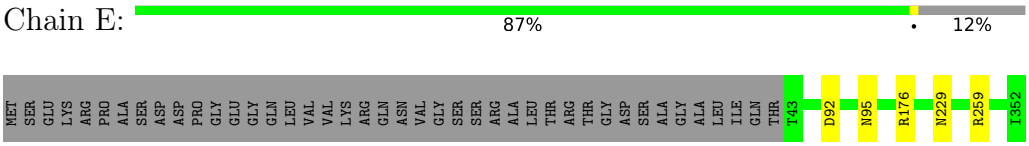
• Molecule 7: SDE2

Chain D:



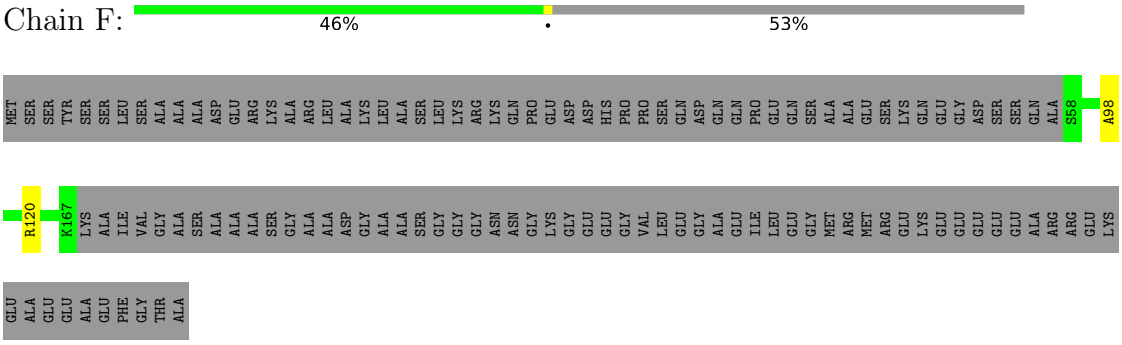
• Molecule 8: Anaphase-promoting complex subunit 4-like WD40 domain-containing protein

Chain E:



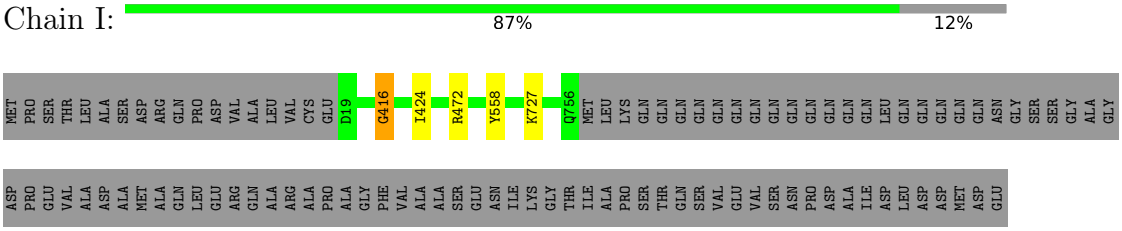
• Molecule 9: CCDC12

Chain F:



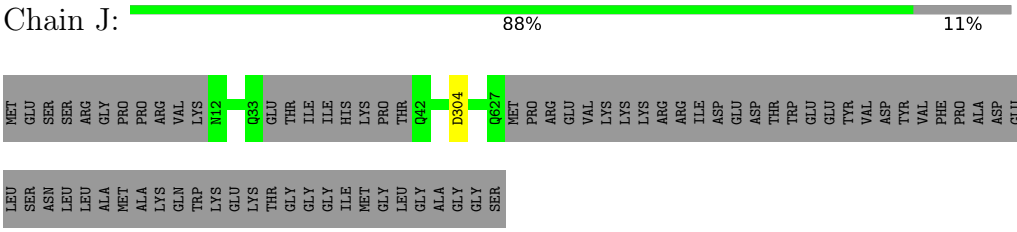
• Molecule 10: Putative pre-mRNA splicing protein

Chain I:



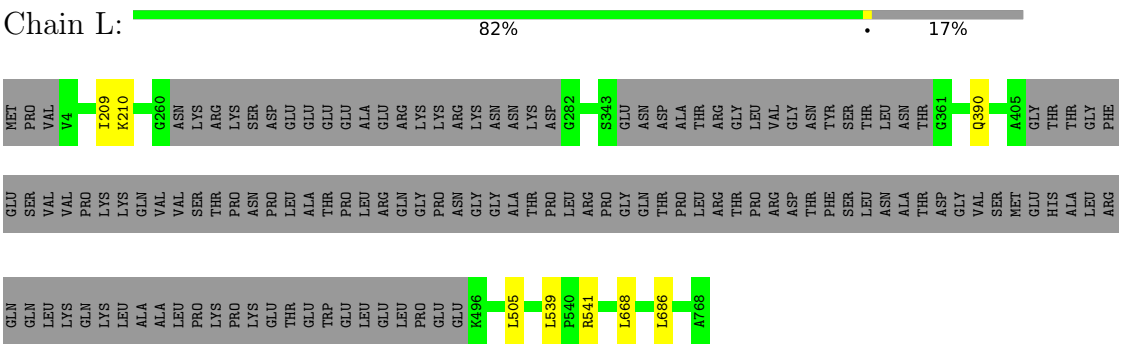
• Molecule 11: Suppressor of forked domain-containing protein

Chain J:



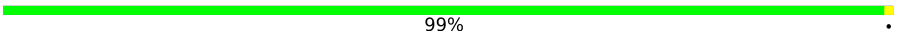
• Molecule 12: Putative pre-mRNA splicing protein

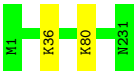
Chain L:



• Molecule 13: Pre-mRNA-splicing factor SPF27

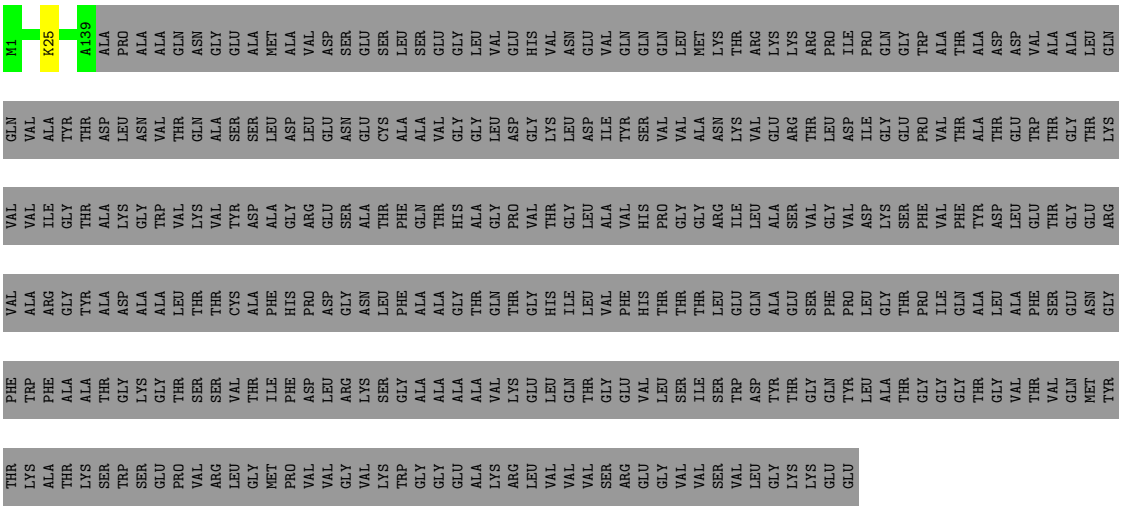
Chain K:





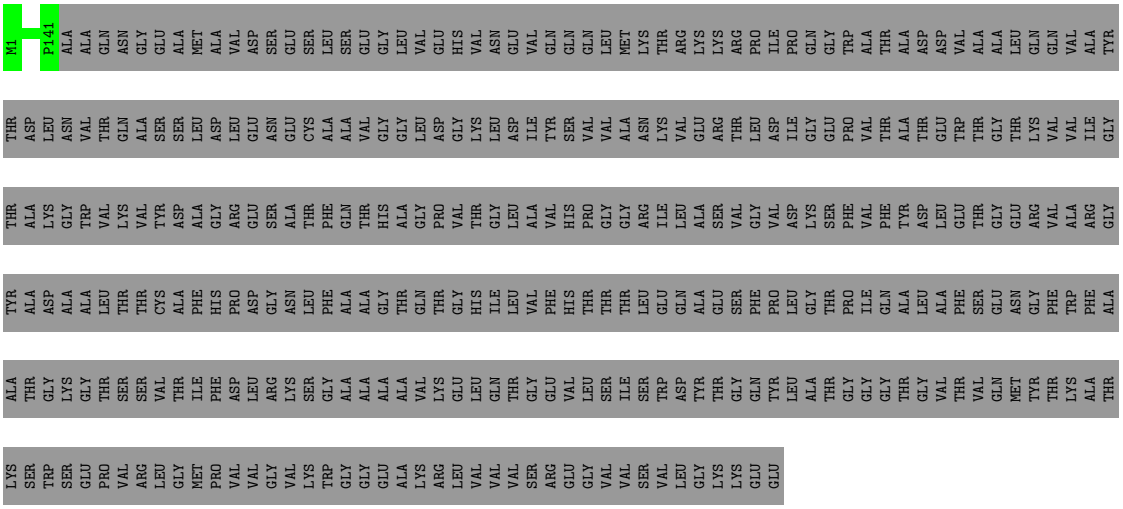
• Molecule 14: Pre-mRNA-processing factor 19

Chain q:



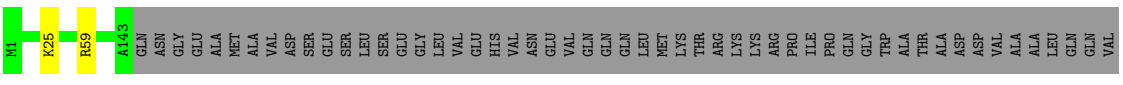
• Molecule 14: Pre-mRNA-processing factor 19

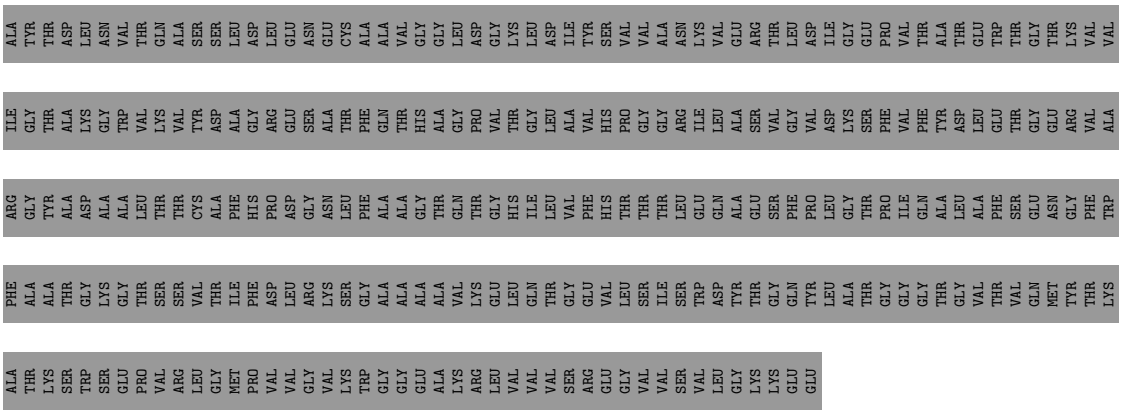
Chain t:



• Molecule 14: Pre-mRNA-processing factor 19

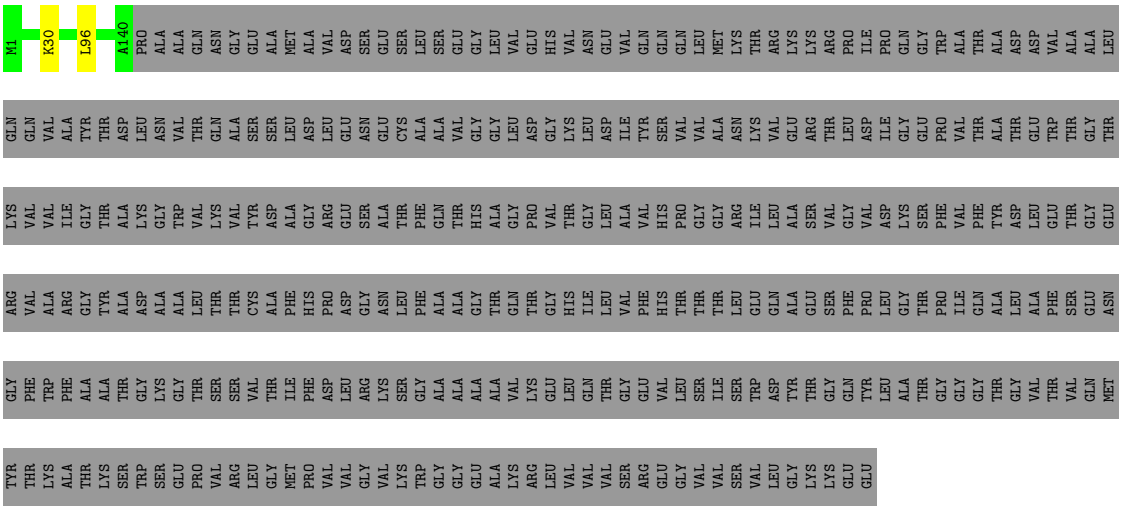
Chain r:





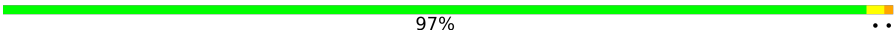
• Molecule 14: Pre-mRNA-processing factor 19

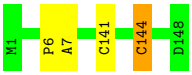
Chain s:



• Molecule 15: Putative bud site selection protein

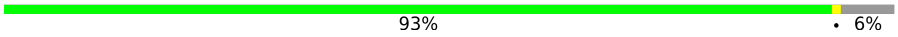
Chain N:

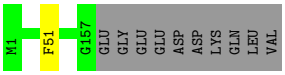




• Molecule 16: Peptidyl-prolyl cis-trans isomerase

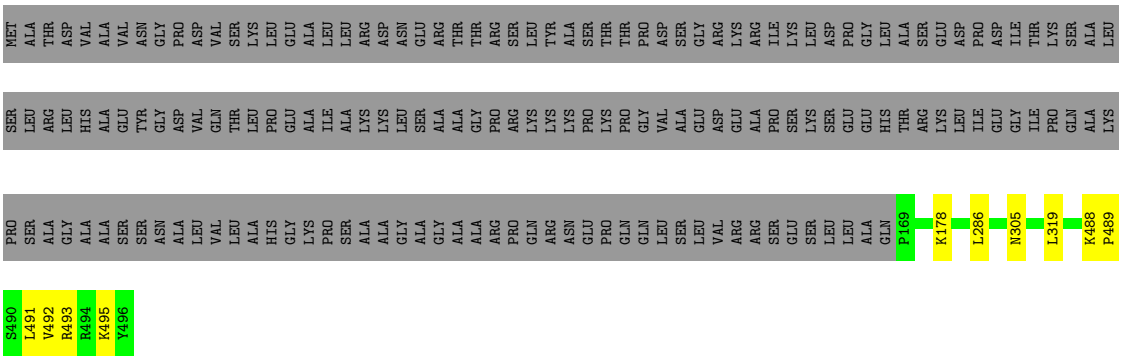
Chain S:





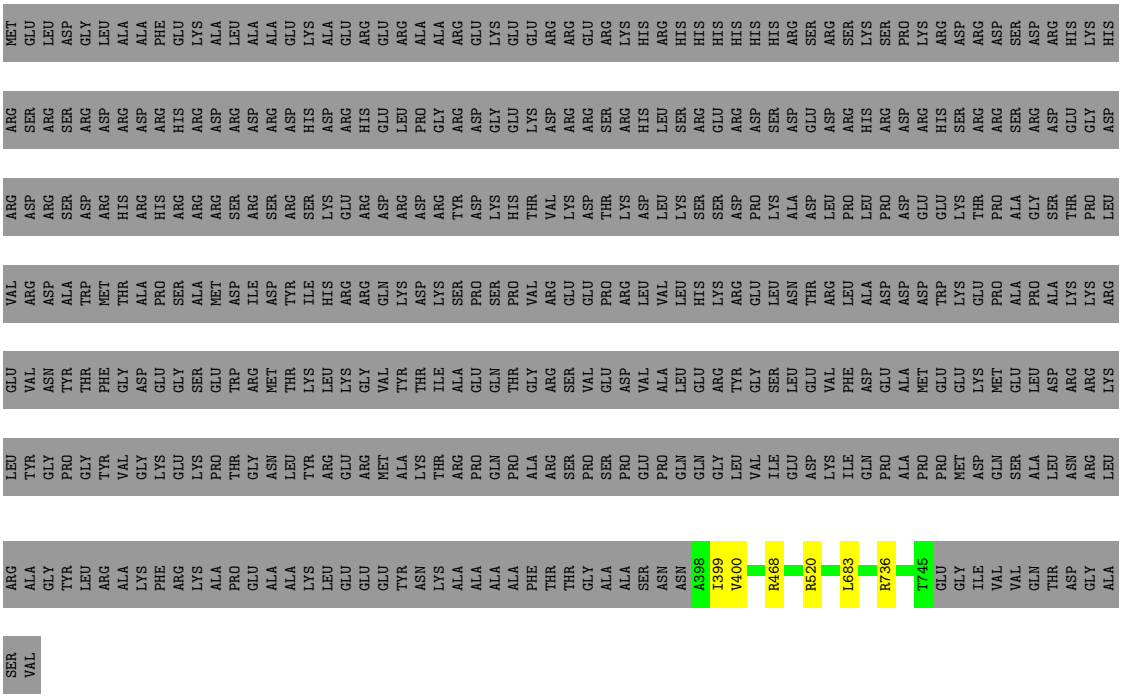
• Molecule 17: Pre-mRNA-splicing factor PRP46

Chain T:



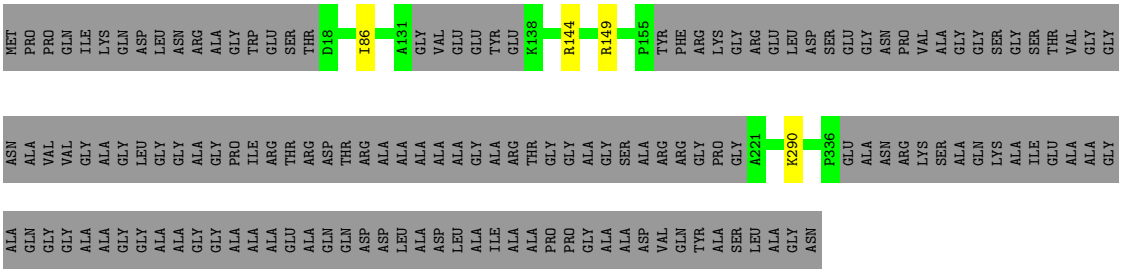
• Molecule 18: Cell cycle control protein

Chain U:



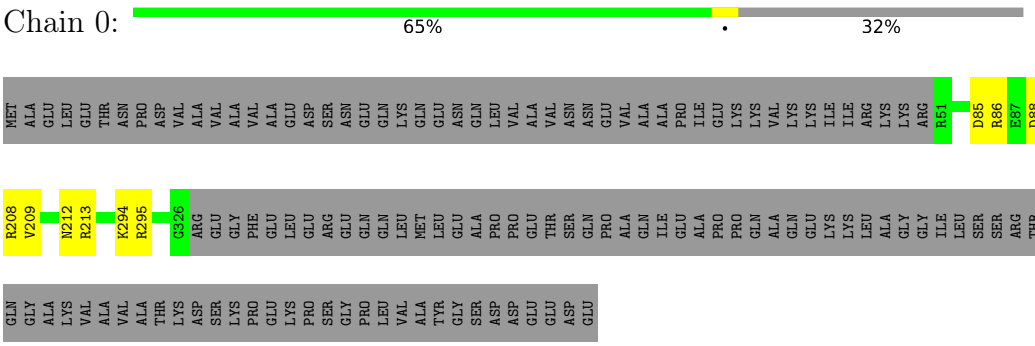
• Molecule 19: Putative pre-mRNA splicing protein

Chain M:



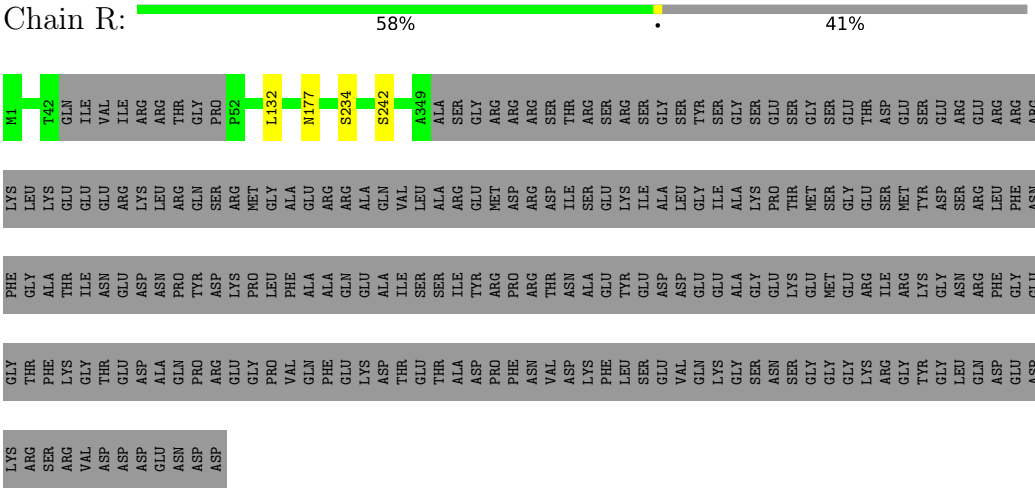
• Molecule 20: Putative pre-mRNA splicing protein

Chain 0:



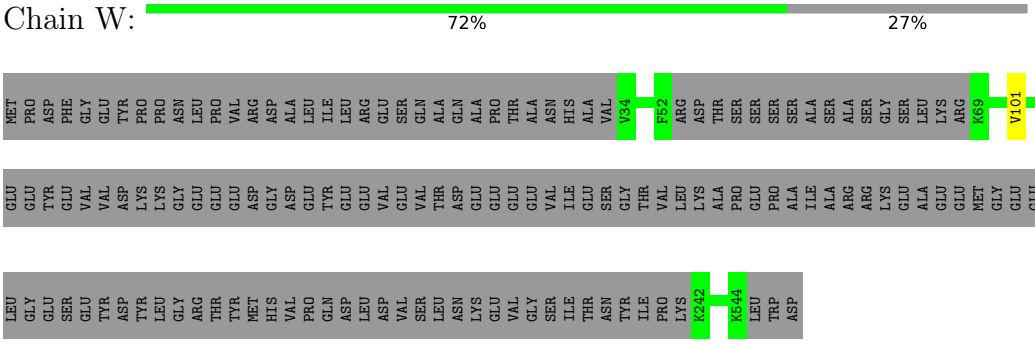
• Molecule 21: Pre-mRNA-processing protein 45

Chain R:



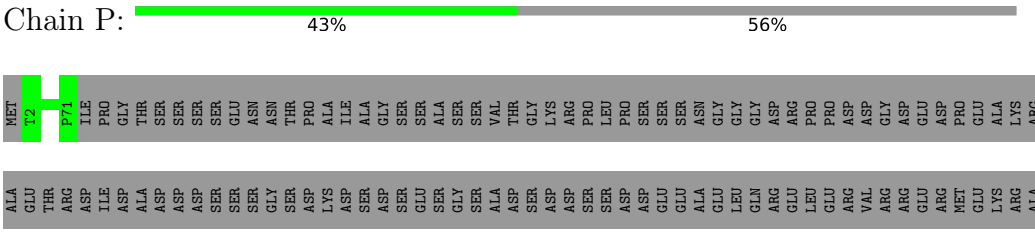
• Molecule 22: PRP17

Chain W:



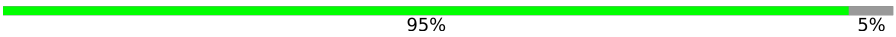
• Molecule 23: Putative pre-mRNA splicing protein

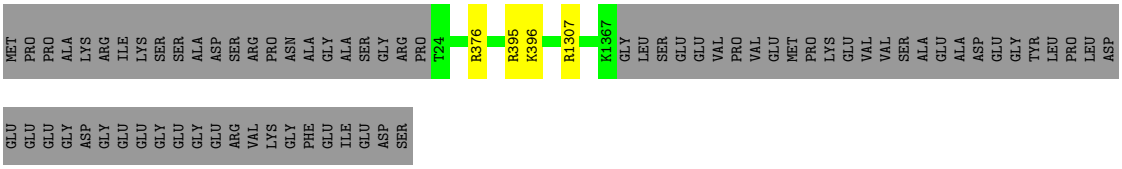
Chain P:



• Molecule 24: Pre-mRNA-splicing factor

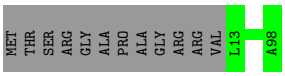
Chain Y:





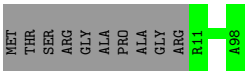
• Molecule 25: Small nuclear ribonucleoprotein E

Chain a:



• Molecule 25: Small nuclear ribonucleoprotein E

Chain j:



• Molecule 26: Sm protein F

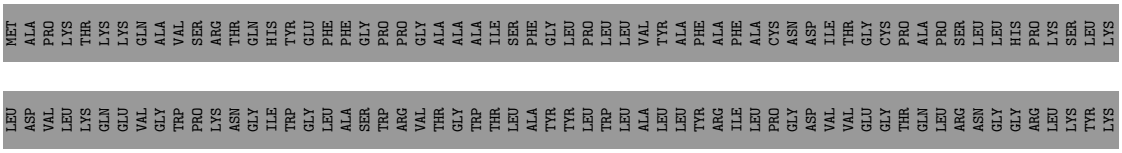
Chain b:

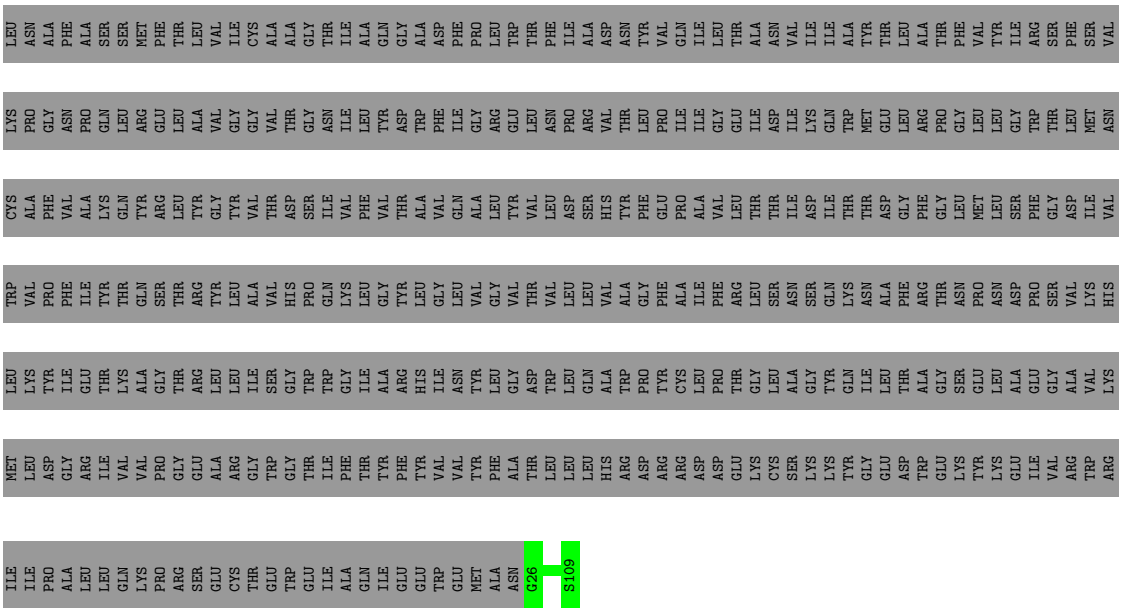
• Molecule 26: Sm protein F

Chain l:

• Molecule 27: Delta(14)-sterol reductase

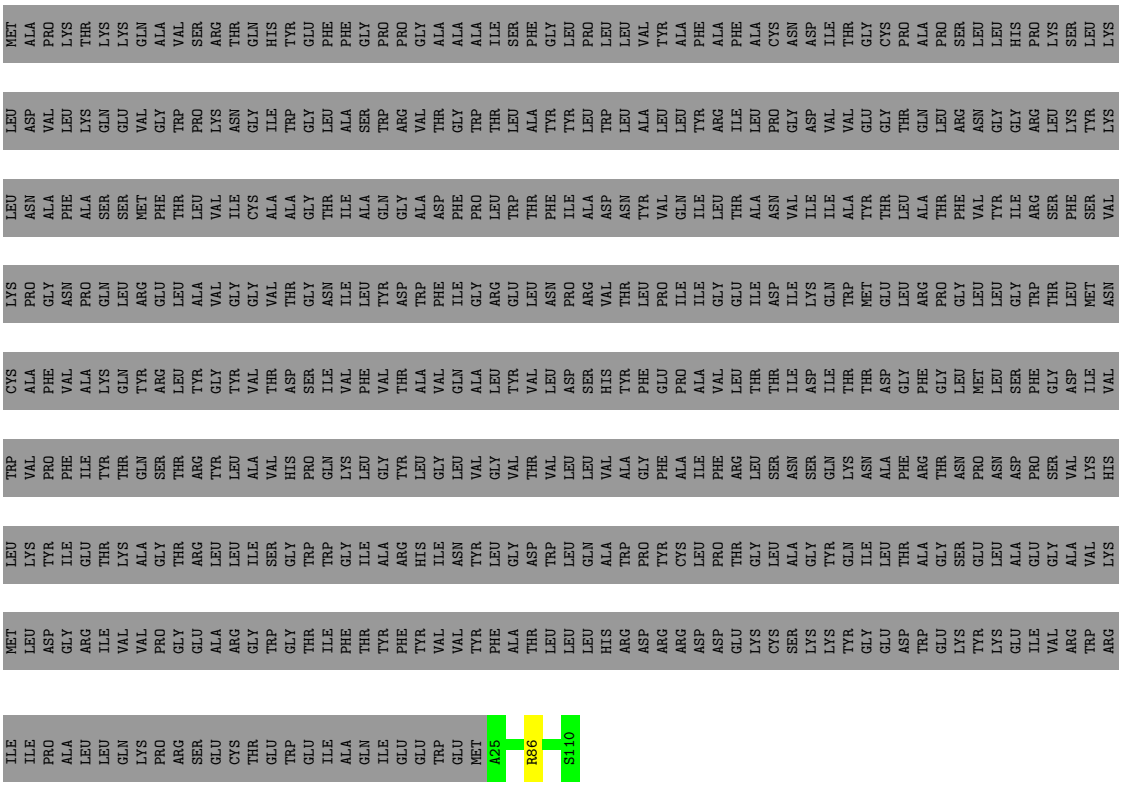
Chain c:





• Molecule 27: Delta(14)-sterol reductase

Chain m:



• Molecule 28: Small nuclear ribonucleoprotein Sm D1

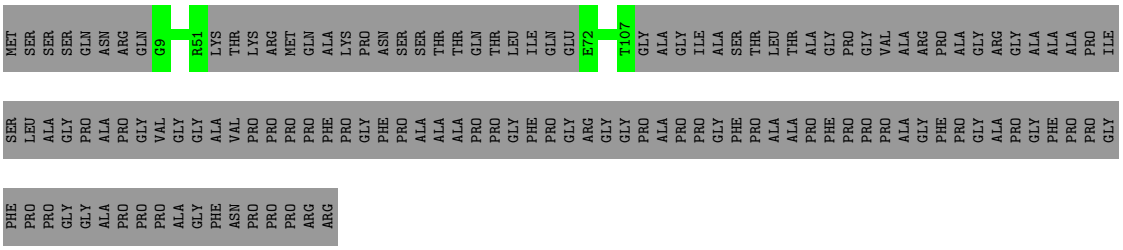
Chain d:

• Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain o:

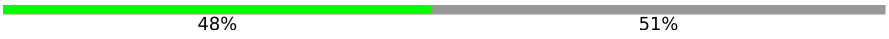
• Molecule 29: Sm protein B

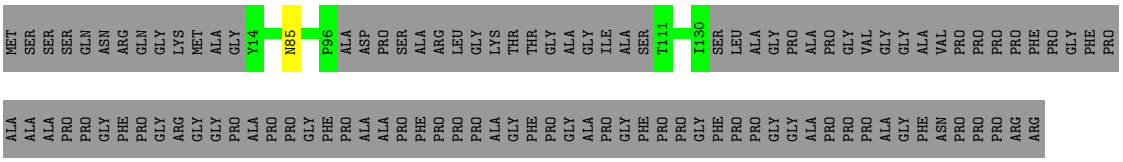
Chain e:



• Molecule 29: Sm protein B

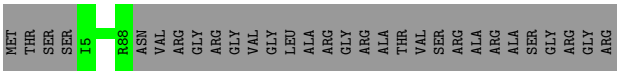
Chain p:





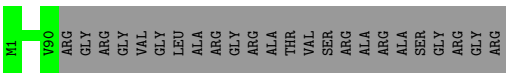
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain f:



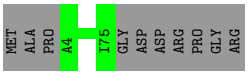
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain u:



• Molecule 31: Small nuclear ribonucleoprotein G

Chain g:

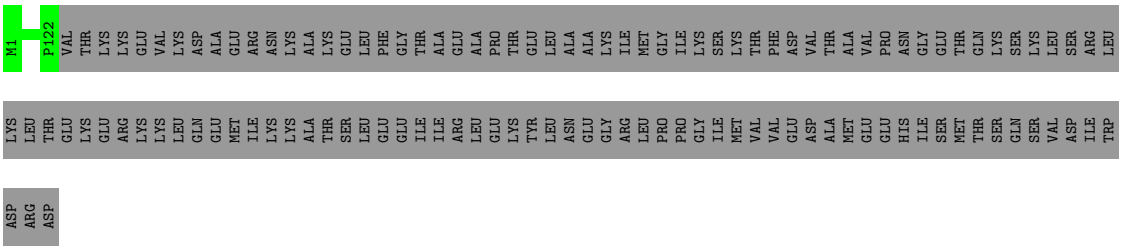


• Molecule 31: Small nuclear ribonucleoprotein G

Chain k:

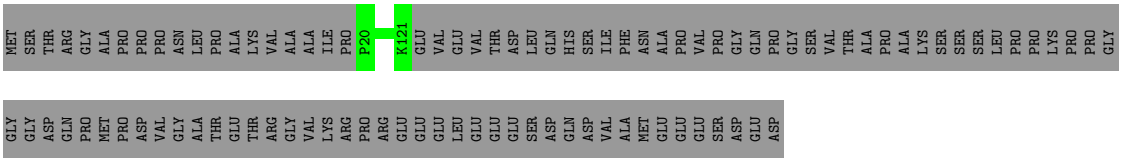
• Molecule 32: U2 small nuclear ribonucleoprotein A'

Chain h:



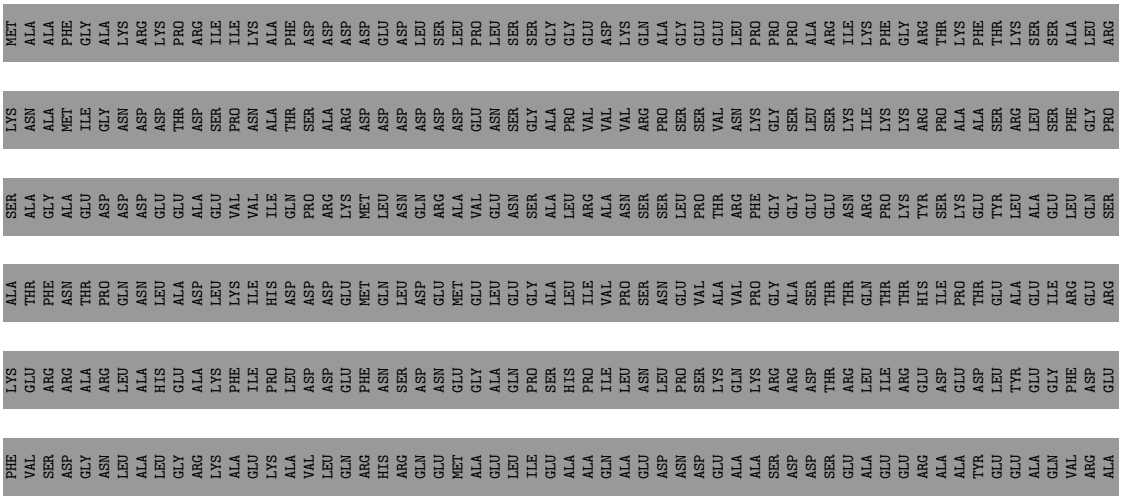
• Molecule 33: U2 small nuclear ribonucleoprotein B'-like protein

Chain i:



• Molecule 34: Nineteen complex-related protein 2-domain-containing protein

Chain CY:



ALA MET ASP GLY LEU ARG GLY LYS TYR ARG GLU GLU HIS LEU GLU ARG GLY GLY GLY ALA D381 G471 GLN SER PRO LEU ARG PRO PHE PRO PRO GLY LEU ALA ARG GLU MET PRO THR GLU ARG GLY LEU GLU SER TYR GLY ALA THR PRO ILE ARG ARG TYR GLY GLY GLU GLU ASP

ASP GLY

- Molecule 35: G-patch domain-containing protein

Chain Cb: 52% 48%

MET ALA ARG LEU ASP ASP LEU GLN PHE ASP PRO ALA ARG LEU LYS ASN SER SER VAL ASP ALA TYR SER SER SER ASP SER ASP GLY ASP SER ASP SER ASP ASP TYR VAL ILE PRO SER ARG ASN PRO HIS ASP ASP GLU PHE ALA ASP TYR ASN PRO ARG LYS ARG ARG ARG THR GLY

ARG ASP PRO LYS GLU SER ALA ALA LEU GLY ILE PHE ALA GLU ASP SER ASP GLU ASP GLU GLY PRO ALA ARG ARG TRP LYS HIS LYS PRO LEU ARG ASN ARG GLY VAL ASN PHE VAL SER GLY GLY GLN GLN LYS GLU GLU ASP SER SER GLU SER ASP GLU GLU GLU SER ASN ASP

ASP GLU ARG LYS GLN GLN GLU ALA VAL ASP ASN GLU TYR ASP ASP ASP PRO GLY GLY VAL PRO ALA ALA LEU THR GLU ASP ASP VAL ASP GLU ASP GLU ASP ASP GLU MET GLY GLY VAL GLY LEU GLY PHE LYS PRO SER SER THR SER ALA THR SER GLN PRO GLN GLY GLY LEU

GLY TRP THR LEU PRO THR GLN GLN GLU THR THR THR LYS LYS PRO PRO PRO PHE GLN ARG PHE VAL LYS SER LYS ILE ASP PRO SER ASN PRO LEU GLY PRO GLY PHE THR PRO THR SER ALA ARG ALA PRO THR LEU LEU ALA ARG ASN ASP GLU PRO THR PRO PRO R237 A299 VAL

LYS GLU LYS THR LYS GLN GLU ARG GLU GLU GLU LYS ARG GLN ALA ARG LEU ARG GLY GLU GLU VAL ILE ASP SER SER GLU GLU ARG LYS LYS LYS ALA ALA LYS LYS LYS LYS GLY LEU ALA GLY LYS ILE GLY SER GLY SER GLY SER GLY ALA SER THR PRO ARG PRO GLN LYS

PRO LYS TYR LEU THR MET GLU GLU ILE LYS LYS VAL ALA PRO GLY LEU HIS ILE PRO GLU ALA PHE THR PRO ILE LEU ASP MET THR GLY PRO GLU LYS LYS LEU LEU THR SER THR SER GLY LEU MET THR PRO THR GLY T409 E850 LEU LYS PRO PRO GLU ARG GLY PRO ALA

LEU ARG THR GLY ARG GLU GLU ARG ARG ARG THR GLU LYS GLU ARG GLU ARG GLU ARG GLU ARG GLU LYS LYS GLU LYS GLU ARG ALA THR VAL GLY LYS PRO PRO GLU GLU ILE THR PHE ARG GLN VAL LEU GLU GLU TRP CYS GLN GLU HIS ASP LEU GLN PHE MET PRO GLU ARG ASN LYS

ILE HIS ALA GLU GLY PRO LEU TYR ARG ILE SER GLY PRO ASP GLY LYS LYS GLY VAL SER VAL TYR PHE LYS GLY ASN SER VAL PHE VAL LEU MET LYS ASP ARG LYS PRO LEU GLU PHE ARG ARG ASP ASP GLU ALA GLU TRP GLY ILE LEU LEU ASP MET VAL TYR

- Molecule 36: RNA helicase

Chain Cc: 93% 7%

MET ALA ASP ILE THR LYS GLY THR LYS ARG LEU SER GLY GLU ALA GLU GLY SER GLN ASP SER LYS ARG VAL LYS THR ASN GLY ASP LYS MET ASP ALA LYS ASN PRO TYR LEU ALA HIS LEU GLU GLU LYS PRO GLU ALA ASP PHE GLU S51 A764

- Molecule 37: Unknown mRNA

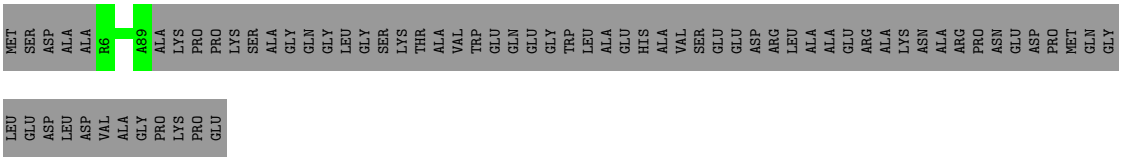
Chain 7: • 21% • 74%

G1 U2 A3 Y5P4 A5 Y5P6 A7 Y5P8 N Y5P10 Y5P11 Y5P12 Y5P13 Y5P14 N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N N

N N N N N N N N N N N N N N N N N N N N N N N N N N N N Y5P89 Y5P90 A91 Y5P92 A93 Y5P94 Y5P95 Y5P96 A97 Y5P98 Y5P99 Y5P100 Y5P101

- Molecule 38: Putative cyclophilin protein

Chain Ci: 55% 45%



• Molecule 39: Unknown protein

Chain H: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, SEP, P5P, ZN, M7M, IHP, MG, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.43	0/2471	0.82	2/3832 (0.1%)
2	5	0.73	1/2612 (0.0%)	0.90	3/4059 (0.1%)
3	6	0.86	1/2338 (0.0%)	0.96	3/3639 (0.1%)
4	A	0.46	1/16969 (0.0%)	0.62	11/23006 (0.0%)
5	B	0.41	0/2099	0.63	1/2806 (0.0%)
6	C	0.40	0/7464	0.59	1/10117 (0.0%)
7	D	0.33	0/793	0.66	0/1051
8	E	0.35	0/2428	0.66	0/3295
9	F	0.31	0/891	0.66	0/1201
10	I	0.32	0/6282	0.59	1/8491 (0.0%)
11	J	0.42	0/5301	0.60	1/7149 (0.0%)
12	L	0.35	0/5120	0.63	2/6882 (0.0%)
13	K	0.29	0/1833	0.57	0/2493
14	q	0.27	0/1128	0.61	0/1533
14	r	0.27	0/1151	0.58	0/1566
14	s	0.26	0/1133	0.58	1/1540 (0.1%)
14	t	0.25	0/1141	0.56	0/1552
15	N	0.52	0/1227	0.66	1/1655 (0.1%)
16	S	0.36	0/1235	0.66	0/1671
17	T	0.56	0/2635	0.76	3/3582 (0.1%)
18	U	0.34	0/2883	0.62	1/3895 (0.0%)
19	M	0.39	0/2006	0.67	1/2703 (0.0%)
20	0	0.39	0/2278	0.61	0/3081
21	R	0.44	0/2724	0.63	0/3675
22	W	0.32	0/2237	0.57	1/3068 (0.0%)
23	P	0.46	0/945	0.66	0/1264
24	Y	0.25	0/11057	0.49	0/14995
25	a	0.24	0/425	0.43	0/589
25	j	0.26	0/716	0.60	0/969
26	b	0.24	0/350	0.47	0/486
26	l	0.26	0/661	0.63	0/898
27	c	0.24	0/415	0.45	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	m	0.27	0/687	0.61	0/922
28	d	0.24	0/400	0.44	0/556
28	o	0.29	0/691	0.61	0/940
29	e	0.25	0/386	0.47	0/533
29	p	0.29	0/799	0.72	0/1079
30	f	0.24	0/413	0.48	0/573
30	u	0.30	0/726	0.72	0/979
31	g	0.24	0/353	0.47	0/489
31	k	0.28	0/584	0.76	1/787 (0.1%)
32	h	0.24	0/604	0.44	0/841
33	i	0.24	0/503	0.40	0/699
34	CY	0.24	0/443	0.34	0/612
35	Cb	0.24	0/2494	0.35	0/3471
36	Cc	0.24	0/3540	0.39	0/4935
37	7	0.73	0/71	1.48	1/106 (0.9%)
38	Ci	0.25	0/414	0.42	0/575
All	All	0.40	3/106056 (0.0%)	0.62	35/145415 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
8	E	0	1
10	I	0	1
12	L	0	2
16	S	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	1	G	OP3-P	-10.80	1.48	1.61
2	5	1	U	OP3-P	-10.61	1.48	1.61
4	A	1111	VAL	CB-CG1	-6.05	1.40	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	725	LEU	CB-CG-CD1	-8.57	96.42	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	108	MET	CA-CB-CG	8.11	127.08	113.30
10	I	424	ILE	CG1-CB-CG2	-7.69	94.49	111.40
3	6	74	G	C4-C5-N7	7.67	113.87	110.80
15	N	144	CYS	CB-CA-C	-7.66	95.08	110.40
31	k	37	LEU	CA-CB-CG	7.52	132.59	115.30
17	T	319	LEU	CA-CB-CG	7.26	132.00	115.30
4	A	725	LEU	CA-CB-CG	7.21	131.89	115.30
2	5	27	U	N3-C2-O2	-7.16	117.19	122.20
4	A	458	ASP	CB-CG-OD1	6.82	124.44	118.30
11	J	304	ASP	CB-CG-OD1	6.68	124.31	118.30
5	B	265	ASP	CB-CG-OD1	6.67	124.31	118.30
4	A	1728	LEU	CA-CB-CG	6.58	130.43	115.30
2	5	46	G	O4'-C1'-N9	6.36	113.29	108.20
4	A	1898	LEU	CA-CB-CG	6.32	129.82	115.30
3	6	74	G	C6-C5-N7	-6.12	126.73	130.40
18	U	683	LEU	CA-CB-CG	6.06	129.23	115.30
19	M	86	ILE	CG1-CB-CG2	-5.84	98.56	111.40
4	A	1363	ASP	CB-CG-OD2	-5.81	113.07	118.30
12	L	668	LEU	CA-CB-CG	5.75	128.53	115.30
2	5	27	U	N1-C2-O2	5.70	126.79	122.80
1	2	13	C	P-O3'-C3'	5.69	126.53	119.70
4	A	775	LEU	CA-CB-CG	5.62	128.22	115.30
6	C	852	ASP	CB-CG-OD1	5.57	123.31	118.30
4	A	414	ASP	CB-CG-OD1	5.53	123.27	118.30
14	s	96	LEU	CA-CB-CG	5.39	127.69	115.30
4	A	1963	LEU	CA-CB-CG	5.34	127.58	115.30
17	T	286	LEU	CA-CB-CG	5.24	127.35	115.30
4	A	1111	VAL	CG1-CB-CG2	-5.19	102.60	110.90
3	6	74	G	N9-C4-C5	-5.14	103.34	105.40
12	L	686	LEU	CA-CB-CG	5.13	127.11	115.30
4	A	1535	LEU	CB-CG-CD1	5.09	119.65	111.00
1	2	16	U	C5-C6-N1	5.07	125.23	122.70
17	T	286	LEU	CB-CG-CD1	-5.07	102.39	111.00
37	7	97	A	C4-N9-C1'	5.02	135.33	126.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1437	ARG	Peptide
8	E	92	ASP	Peptide
10	I	416	GLY	Peptide

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Mol	Chain	Res	Type	Group
12	L	505	LEU	Peptide
12	L	539	LEU	Peptide
16	S	51	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	2004/2463 (81%)	1911 (95%)	90 (4%)	3 (0%)	48 77
5	B	256/326 (78%)	249 (97%)	6 (2%)	1 (0%)	30 61
6	C	920/1011 (91%)	889 (97%)	29 (3%)	2 (0%)	44 73
7	D	91/325 (28%)	90 (99%)	1 (1%)	0	100 100
8	E	308/352 (88%)	285 (92%)	23 (8%)	0	100 100
9	F	108/233 (46%)	104 (96%)	3 (3%)	1 (1%)	14 42
10	I	736/839 (88%)	705 (96%)	29 (4%)	2 (0%)	37 67
11	J	604/687 (88%)	592 (98%)	12 (2%)	0	100 100
12	L	629/768 (82%)	602 (96%)	26 (4%)	1 (0%)	44 73
13	K	229/231 (99%)	224 (98%)	5 (2%)	0	100 100
14	q	137/480 (28%)	135 (98%)	2 (2%)	0	100 100
14	r	141/480 (29%)	140 (99%)	1 (1%)	0	100 100
14	s	138/480 (29%)	137 (99%)	1 (1%)	0	100 100
14	t	139/480 (29%)	136 (98%)	3 (2%)	0	100 100
15	N	146/148 (99%)	136 (93%)	8 (6%)	2 (1%)	9 30
16	S	155/167 (93%)	148 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	326/496 (66%)	311 (95%)	14 (4%)	1 (0%)	37	67
18	U	346/757 (46%)	321 (93%)	23 (7%)	2 (1%)	22	51
19	M	242/395 (61%)	225 (93%)	17 (7%)	0	100	100
20	0	274/408 (67%)	261 (95%)	13 (5%)	0	100	100
21	R	334/578 (58%)	312 (93%)	21 (6%)	1 (0%)	37	67
22	W	391/547 (72%)	376 (96%)	14 (4%)	1 (0%)	37	67
23	P	110/260 (42%)	102 (93%)	8 (7%)	0	100	100
24	Y	1342/1416 (95%)	1315 (98%)	27 (2%)	0	100	100
25	a	84/98 (86%)	83 (99%)	1 (1%)	0	100	100
25	j	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
26	b	69/94 (73%)	69 (100%)	0	0	100	100
26	l	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
27	c	82/592 (14%)	80 (98%)	2 (2%)	0	100	100
27	m	84/592 (14%)	80 (95%)	4 (5%)	0	100	100
28	d	79/118 (67%)	76 (96%)	3 (4%)	0	100	100
28	o	85/118 (72%)	78 (92%)	7 (8%)	0	100	100
29	e	75/211 (36%)	73 (97%)	2 (3%)	0	100	100
29	p	99/211 (47%)	92 (93%)	7 (7%)	0	100	100
30	f	82/114 (72%)	79 (96%)	3 (4%)	0	100	100
30	u	88/114 (77%)	83 (94%)	5 (6%)	0	100	100
31	g	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
31	k	71/82 (87%)	68 (96%)	3 (4%)	0	100	100
32	h	120/242 (50%)	117 (98%)	3 (2%)	0	100	100
33	i	100/201 (50%)	100 (100%)	0	0	100	100
34	CY	89/510 (18%)	88 (99%)	1 (1%)	0	100	100
35	Cb	501/975 (51%)	495 (99%)	6 (1%)	0	100	100
36	Cc	712/764 (93%)	694 (98%)	18 (2%)	0	100	100
38	Ci	82/153 (54%)	82 (100%)	0	0	100	100
All	All	12843/19790 (65%)	12373 (96%)	453 (4%)	17 (0%)	50	77

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	494	LYS
4	A	1219	ILE
5	B	111	GLN
6	C	840	VAL
9	F	98	ALA
15	N	7	ALA
18	U	400	VAL
21	R	177	ASN
4	A	595	GLN
12	L	390	GLN
6	C	846	TRP
10	I	558	TYR
22	W	101	VAL
18	U	399	ILE
15	N	6	PRO
10	I	416	GLY
17	T	489	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1813/2212 (82%)	1804 (100%)	9 (0%)	86 95
5	B	208/270 (77%)	207 (100%)	1 (0%)	86 95
6	C	809/884 (92%)	807 (100%)	2 (0%)	92 97
7	D	80/276 (29%)	78 (98%)	2 (2%)	42 75
8	E	254/287 (88%)	250 (98%)	4 (2%)	58 85
9	F	92/179 (51%)	91 (99%)	1 (1%)	70 90
10	I	646/729 (89%)	644 (100%)	2 (0%)	91 97
11	J	525/592 (89%)	525 (100%)	0	100 100
12	L	520/635 (82%)	517 (99%)	3 (1%)	84 95
13	K	186/186 (100%)	184 (99%)	2 (1%)	70 90
14	q	122/385 (32%)	121 (99%)	1 (1%)	79 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	r	123/385 (32%)	121 (98%)	2 (2%)	58 85
14	s	122/385 (32%)	121 (99%)	1 (1%)	79 93
14	t	123/385 (32%)	123 (100%)	0	100 100
15	N	131/131 (100%)	129 (98%)	2 (2%)	60 86
16	S	126/135 (93%)	126 (100%)	0	100 100
17	T	276/408 (68%)	269 (98%)	7 (2%)	42 75
18	U	294/649 (45%)	291 (99%)	3 (1%)	73 91
19	M	210/293 (72%)	207 (99%)	3 (1%)	62 87
20	0	227/335 (68%)	216 (95%)	11 (5%)	21 53
21	R	278/476 (58%)	277 (100%)	1 (0%)	89 96
22	W	73/459 (16%)	73 (100%)	0	100 100
23	P	91/213 (43%)	90 (99%)	1 (1%)	70 90
24	Y	1173/1231 (95%)	1169 (100%)	4 (0%)	91 97
25	j	79/85 (93%)	79 (100%)	0	100 100
26	l	72/84 (86%)	71 (99%)	1 (1%)	62 87
27	m	77/497 (16%)	76 (99%)	1 (1%)	65 88
28	o	78/95 (82%)	76 (97%)	2 (3%)	41 75
29	p	84/152 (55%)	83 (99%)	1 (1%)	67 89
30	u	80/94 (85%)	80 (100%)	0	100 100
31	k	64/71 (90%)	64 (100%)	0	100 100
All	All	9036/13198 (68%)	8969 (99%)	67 (1%)	80 94

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	351	ASN
4	A	420	ASN
4	A	589	LYS
4	A	593	SER
4	A	902	ASN
4	A	974	ARG
4	A	1141	ASN
4	A	1268	ARG
4	A	2035	ARG
5	B	298	ASN

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Mol	Chain	Res	Type
6	C	527	ASN
6	C	853	ARG
7	D	207	LYS
7	D	218	ARG
8	E	95	ASN
8	E	176	ARG
8	E	229	ASN
8	E	259	ARG
9	F	120	ARG
10	I	472	ARG
10	I	727	LYS
12	L	209	ILE
12	L	210	LYS
12	L	541	ARG
13	K	36	LYS
13	K	80	LYS
14	q	25	LYS
14	r	25	LYS
14	r	59	ARG
14	s	30	LYS
15	N	141	CYS
15	N	144	CYS
17	T	178	LYS
17	T	305	ASN
17	T	488	LYS
17	T	491	LEU
17	T	492	VAL
17	T	493	ARG
17	T	495	LYS
18	U	468	ARG
18	U	520	ARG
18	U	736	ARG
19	M	144	ARG
19	M	149	ARG
19	M	290	LYS
20	0	85	ASP
20	0	86	ARG
20	0	88	ASP
20	0	89	LYS
20	0	91	LEU
20	0	208	ARG
20	0	209	VAL

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Mol	Chain	Res	Type
20	0	212	ASN
20	0	213	ARG
20	0	294	LYS
20	0	295	ARG
21	R	132	LEU
23	P	238	ARG
24	Y	376	ARG
24	Y	395	ARG
24	Y	396	LYS
24	Y	1307	ARG
26	l	25	ARG
27	m	86	ARG
28	o	9	LYS
28	o	44	ARG
29	p	85	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	834	ASN
4	A	1141	ASN
4	A	1525	GLN
4	A	1737	GLN
14	q	110	HIS
17	T	220	GLN
17	T	305	ASN
20	0	212	ASN
24	Y	683	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	101/193 (52%)	18 (17%)	2 (1%)
2	5	109/116 (93%)	21 (19%)	1 (0%)
3	6	97/101 (96%)	36 (37%)	2 (2%)
37	7	2/101 (1%)	2 (100%)	0
All	All	309/511 (60%)	77 (24%)	5 (1%)

All (77) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	U
1	2	14	U
1	2	16	U
1	2	17	U
1	2	18	G
1	2	19	G
1	2	23	A
1	2	24	G
1	2	28	A
1	2	39	C
1	2	40	U
1	2	41	G
1	2	100	U
1	2	111	G
1	2	120	C
1	2	137	U
1	2	142	G
1	2	145	U
2	5	6	G
2	5	8	A
2	5	20	A
2	5	21	C
2	5	22	C
2	5	23	G
2	5	24	A
2	5	27	U
2	5	33	C
2	5	50	G
2	5	71	A
2	5	72	U
2	5	75	U
2	5	77	C
2	5	87	U
2	5	88	C
2	5	89	U
2	5	91	U
2	5	93	G
2	5	94	A
2	5	106	U
3	6	6	U
3	6	7	C
3	6	9	G
3	6	15	U

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Mol	Chain	Res	Type
3	6	18	G
3	6	19	U
3	6	20	C
3	6	21	A
3	6	22	A
3	6	24	U
3	6	28	A
3	6	32	A
3	6	38	A
3	6	39	G
3	6	42	G
3	6	45	U
3	6	47	G
3	6	49	A
3	6	61	C
3	6	62	U
3	6	63	A
3	6	68	U
3	6	70	A
3	6	74	G
3	6	81	A
3	6	82	A
3	6	84	G
3	6	85	A
3	6	88	C
3	6	89	G
3	6	90	C
3	6	91	U
3	6	95	A
3	6	96	A
3	6	97	U
3	6	98	U
37	7	2	U
37	7	97	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	13	C
1	2	23	A
2	5	70	A
3	6	15	U

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Mol	Chain	Res	Type
3	6	38	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	Y5P	7	14	37	14,19,20	2.35	1 (7%)	18,26,29	1.02	1 (5%)
37	Y5P	7	4	37	14,19,20	2.42	1 (7%)	18,26,29	1.11	1 (5%)
37	Y5P	7	13	37	14,19,20	2.41	1 (7%)	18,26,29	1.00	1 (5%)
37	P5P	7	3	37,3	16,23,24	0.80	0	14,33,36	0.75	0
37	Y5P	7	95	37	14,19,20	2.34	1 (7%)	18,26,29	0.99	1 (5%)
37	Y5P	7	8	37	14,19,20	3.67	1 (7%)	18,26,29	0.81	1 (5%)
21	SEP	R	242	21	8,9,10	0.68	0	8,12,14	1.20	1 (12%)
37	Y5P	7	101	37	14,19,20	2.30	1 (7%)	18,26,29	1.03	1 (5%)
37	Y5P	7	99	37	14,19,20	3.84	1 (7%)	18,26,29	0.79	0
37	P5P	7	93	37,1	16,23,24	0.79	0	14,33,36	0.76	0
37	Y5P	7	98	37	14,19,20	2.43	1 (7%)	18,26,29	0.98	1 (5%)
37	Y5P	7	90	37	14,19,20	3.73	1 (7%)	18,26,29	0.78	1 (5%)
37	Y5P	7	6	37	14,19,20	2.37	1 (7%)	18,26,29	0.94	1 (5%)
37	P5P	7	7	37,3	16,23,24	1.28	2 (12%)	14,33,36	1.96	2 (14%)
37	Y5P	7	96	37	14,19,20	2.48	1 (7%)	18,26,29	1.02	1 (5%)
37	Y5P	7	94	37	14,19,20	3.78	1 (7%)	18,26,29	0.77	1 (5%)
37	Y5P	7	92	37	14,19,20	2.35	1 (7%)	18,26,29	0.96	1 (5%)
37	Y5P	7	100	37	14,19,20	3.75	1 (7%)	18,26,29	0.79	1 (5%)
21	SEP	R	234	21	8,9,10	1.37	1 (12%)	8,12,14	0.95	0
37	P5P	7	91	37,1	16,23,24	0.77	0	14,33,36	0.73	0
37	P5P	7	5	37	16,23,24	1.33	2 (12%)	14,33,36	1.95	2 (14%)
37	Y5P	7	12	37	14,19,20	2.43	1 (7%)	18,26,29	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	Y5P	7	11	37	14,19,20	2.39	1 (7%)	18,26,29	0.99	1 (5%)
37	Y5P	7	89	37	14,19,20	2.36	1 (7%)	18,26,29	0.96	1 (5%)
37	Y5P	7	10	37	14,19,20	2.41	1 (7%)	18,26,29	0.99	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	Y5P	7	14	37	-	2/7/33/34	0/2/2/2
37	Y5P	7	4	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	13	37	-	1/7/33/34	0/2/2/2
37	P5P	7	3	37,3	-	2/3/25/26	0/3/3/3
37	Y5P	7	95	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	8	37	-	1/7/33/34	0/2/2/2
21	SEP	R	242	21	-	2/5/8/10	-
37	Y5P	7	101	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	99	37	-	1/7/33/34	0/2/2/2
37	P5P	7	93	37,1	-	1/3/25/26	0/3/3/3
37	Y5P	7	98	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	90	37	-	2/7/33/34	0/2/2/2
37	Y5P	7	6	37	-	1/7/33/34	0/2/2/2
37	P5P	7	7	37,3	-	2/3/25/26	0/3/3/3
37	Y5P	7	96	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	94	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	92	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	100	37	-	1/7/33/34	0/2/2/2
21	SEP	R	234	21	-	1/5/8/10	-
37	P5P	7	91	37,1	-	0/3/25/26	0/3/3/3
37	P5P	7	5	37	-	0/3/25/26	0/3/3/3
37	Y5P	7	12	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	11	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	89	37	-	3/7/33/34	0/2/2/2
37	Y5P	7	10	37	-	3/7/33/34	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	99	Y5P	C4-N3	-14.20	1.33	1.46
37	7	94	Y5P	C4-N3	-13.97	1.33	1.46
37	7	100	Y5P	C4-N3	-13.85	1.33	1.46
37	7	90	Y5P	C4-N3	-13.72	1.33	1.46
37	7	8	Y5P	C4-N3	-13.53	1.33	1.46
37	7	96	Y5P	C4-N3	-9.10	1.37	1.46
37	7	12	Y5P	C4-N3	-8.99	1.38	1.46
37	7	98	Y5P	C4-N3	-8.93	1.38	1.46
37	7	13	Y5P	C4-N3	-8.91	1.38	1.46
37	7	10	Y5P	C4-N3	-8.89	1.38	1.46
37	7	4	Y5P	C4-N3	-8.88	1.38	1.46
37	7	11	Y5P	C4-N3	-8.86	1.38	1.46
37	7	14	Y5P	C4-N3	-8.72	1.38	1.46
37	7	6	Y5P	C4-N3	-8.68	1.38	1.46
37	7	89	Y5P	C4-N3	-8.65	1.38	1.46
37	7	92	Y5P	C4-N3	-8.56	1.38	1.46
37	7	95	Y5P	C4-N3	-8.55	1.38	1.46
37	7	101	Y5P	C4-N3	-8.48	1.38	1.46
37	7	5	P5P	C6-N1	3.80	1.39	1.32
37	7	7	P5P	C6-N1	3.72	1.39	1.32
21	R	234	SEP	P-O1P	3.04	1.60	1.50
37	7	5	P5P	C8-N7	-2.43	1.30	1.34
37	7	7	P5P	C8-N7	-2.32	1.30	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	7	P5P	C6-N1-C2	6.43	125.06	115.84
37	7	5	P5P	C6-N1-C2	6.36	124.94	115.84
37	7	101	Y5P	N1-C2-N3	-3.67	114.56	125.33
37	7	10	Y5P	N1-C2-N3	-3.60	114.76	125.33
37	7	11	Y5P	N1-C2-N3	-3.59	114.79	125.33
37	7	12	Y5P	N1-C2-N3	-3.59	114.80	125.33
37	7	4	Y5P	N1-C2-N3	-3.59	114.81	125.33
37	7	95	Y5P	N1-C2-N3	-3.59	114.81	125.33
37	7	13	Y5P	N1-C2-N3	-3.58	114.84	125.33
37	7	14	Y5P	N1-C2-N3	-3.58	114.84	125.33
37	7	98	Y5P	N1-C2-N3	-3.51	115.03	125.33
37	7	89	Y5P	N1-C2-N3	-3.50	115.07	125.33
37	7	92	Y5P	N1-C2-N3	-3.50	115.07	125.33
37	7	6	Y5P	N1-C2-N3	-3.43	115.26	125.33
37	7	96	Y5P	N1-C2-N3	-3.39	115.40	125.33
37	7	7	P5P	N1-C2-N3	-2.95	123.88	127.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	5	P5P	N1-C2-N3	-2.84	124.02	127.65
21	R	242	SEP	OG-CB-CA	2.74	110.81	108.14
37	7	8	Y5P	N1-C2-N3	-2.20	118.88	125.33
37	7	100	Y5P	N1-C2-N3	-2.05	119.31	125.33
37	7	90	Y5P	N1-C2-N3	-2.03	119.37	125.33
37	7	94	Y5P	N1-C2-N3	-2.02	119.40	125.33

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	234	SEP	N-CA-CB-OG
37	7	6	Y5P	O4'-C1'-N1-C2
37	7	11	Y5P	O4'-C1'-N1-C2
37	7	89	Y5P	O4'-C1'-N1-C2
37	7	94	Y5P	O4'-C1'-N1-C2
37	7	96	Y5P	O4'-C1'-N1-C2
37	7	98	Y5P	O4'-C1'-N1-C2
37	7	99	Y5P	O4'-C1'-N1-C2
37	7	100	Y5P	O4'-C1'-N1-C2
37	7	4	Y5P	O4'-C1'-N1-C2
37	7	8	Y5P	O4'-C1'-N1-C2
37	7	10	Y5P	O4'-C1'-N1-C2
37	7	14	Y5P	O4'-C1'-N1-C2
37	7	90	Y5P	O4'-C1'-N1-C2
37	7	92	Y5P	O4'-C1'-N1-C2
37	7	95	Y5P	O4'-C1'-N1-C2
37	7	89	Y5P	C4'-C5'-O5'-P
37	7	3	P5P	C3'-C4'-C5'-O5'
37	7	11	Y5P	O4'-C4'-C5'-O5'
37	7	11	Y5P	C3'-C4'-C5'-O5'
37	7	12	Y5P	C2'-C1'-N1-C2
37	7	12	Y5P	C2'-C1'-N1-C6
37	7	3	P5P	O4'-C4'-C5'-O5'
37	7	95	Y5P	C3'-C4'-C5'-O5'
37	7	12	Y5P	O4'-C1'-N1-C6
37	7	93	P5P	C4'-C5'-O5'-P
37	7	12	Y5P	O4'-C1'-N1-C2
37	7	10	Y5P	C4'-C5'-O5'-P
37	7	7	P5P	C3'-C4'-C5'-O5'
37	7	13	Y5P	O4'-C1'-N1-C2
37	7	11	Y5P	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
37	7	95	Y5P	C4'-C5'-O5'-P
37	7	95	Y5P	O4'-C4'-C5'-O5'
21	R	242	SEP	N-CA-CB-OG
21	R	242	SEP	CB-OG-P-O1P
37	7	14	Y5P	C4'-C5'-O5'-P
37	7	10	Y5P	O4'-C4'-C5'-O5'
37	7	101	Y5P	O4'-C1'-N1-C2
37	7	89	Y5P	O4'-C4'-C5'-O5'
37	7	7	P5P	O4'-C4'-C5'-O5'
37	7	90	Y5P	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	IHP	J	1001	-	36,36,36	1.47	6 (16%)	54,60,60	0.98	3 (5%)
42	GTP	C	1102	41	26,34,34	1.38	3 (11%)	32,54,54	1.54	6 (18%)
40	M7M	B	401	-	27,32,33	4.11	15 (55%)	33,49,52	1.31	4 (12%)

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
43	IHP	J	1001	-	-	9/30/54/54	0/1/1/1
42	GTP	C	1102	41	-	6/18/38/38	0/3/3/3
40	M7M	B	401	-	-	2/17/47/48	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	401	M7M	CBI-NBP	8.02	1.50	1.46
40	B	401	M7M	CBG-NBH	7.81	1.44	1.35
40	B	401	M7M	CBY-CBS	-7.10	1.34	1.53
40	B	401	M7M	OBR-CBS	6.91	1.60	1.45
40	B	401	M7M	CBO-NBP	6.25	1.44	1.35
40	B	401	M7M	CBM-NBE	5.34	1.45	1.32
40	B	401	M7M	OBR-CBQ	-5.25	1.29	1.42
40	B	401	M7M	CBO-NBN	5.21	1.46	1.37
40	B	401	M7M	CBM-NBV	5.20	1.45	1.35
40	B	401	M7M	CBM-NBN	4.48	1.47	1.36
42	C	1102	GTP	C5-C6	-4.43	1.38	1.47
43	J	1001	IHP	P4-O14	3.57	1.66	1.59
40	B	401	M7M	OBB-CBF	-3.30	1.18	1.23
40	B	401	M7M	OCB-CBY	3.23	1.50	1.43
40	B	401	M7M	OCA-CBX	-3.16	1.35	1.43
43	J	1001	IHP	P3-O13	3.15	1.65	1.59
43	J	1001	IHP	P5-O15	3.11	1.65	1.59
40	B	401	M7M	CBF-NBE	3.10	1.43	1.38
40	B	401	M7M	CBG-CBO	3.06	1.43	1.37
43	J	1001	IHP	P1-O11	2.98	1.64	1.59
43	J	1001	IHP	P2-O12	2.92	1.64	1.59
43	J	1001	IHP	P6-O16	2.91	1.64	1.59
42	C	1102	GTP	C5-C4	-2.08	1.37	1.43
42	C	1102	GTP	O4'-C4'	-2.07	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	401	M7M	CBO-CBG-NBH	4.35	109.30	106.71
43	J	1001	IHP	C5-C4-C3	-3.73	102.25	110.41
42	C	1102	GTP	PB-O3B-PG	-3.69	120.15	132.83
42	C	1102	GTP	C5-C6-N1	3.38	119.91	113.95
42	C	1102	GTP	C8-N7-C5	3.07	108.85	102.99
43	J	1001	IHP	O15-C5-C4	3.06	115.91	108.69
42	C	1102	GTP	C2-N1-C6	-3.04	119.50	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	C	1102	GTP	O2G-PG-O3B	2.38	112.60	104.64
40	B	401	M7M	NBP-CBI-NBH	2.33	106.71	103.38
40	B	401	M7M	CBY-CBX-CBQ	2.24	105.68	101.43
42	C	1102	GTP	C3'-C2'-C1'	2.11	104.16	100.98
40	B	401	M7M	CBG-CBO-NBN	-2.11	120.28	124.00
43	J	1001	IHP	C6-C1-C2	2.07	114.94	110.41

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	C	1102	GTP	C5'-O5'-PA-O1A
42	C	1102	GTP	C5'-O5'-PA-O2A
43	J	1001	IHP	C4-C5-O15-P5
43	J	1001	IHP	C3-O13-P3-O23
43	J	1001	IHP	C5-O15-P5-O35
42	C	1102	GTP	PA-O3A-PB-O1B
40	B	401	M7M	OBR-CBS-CBT-OBU
43	J	1001	IHP	C6-C5-O15-P5
43	J	1001	IHP	C4-O14-P4-O44
42	C	1102	GTP	PB-O3A-PA-O2A
43	J	1001	IHP	C1-O11-P1-O21
42	C	1102	GTP	C5'-O5'-PA-O3A
43	J	1001	IHP	C1-O11-P1-O31
43	J	1001	IHP	C1-O11-P1-O41
43	J	1001	IHP	C3-O13-P3-O43
42	C	1102	GTP	PB-O3A-PA-O1A
40	B	401	M7M	CBT-OBU-PBK-OBL

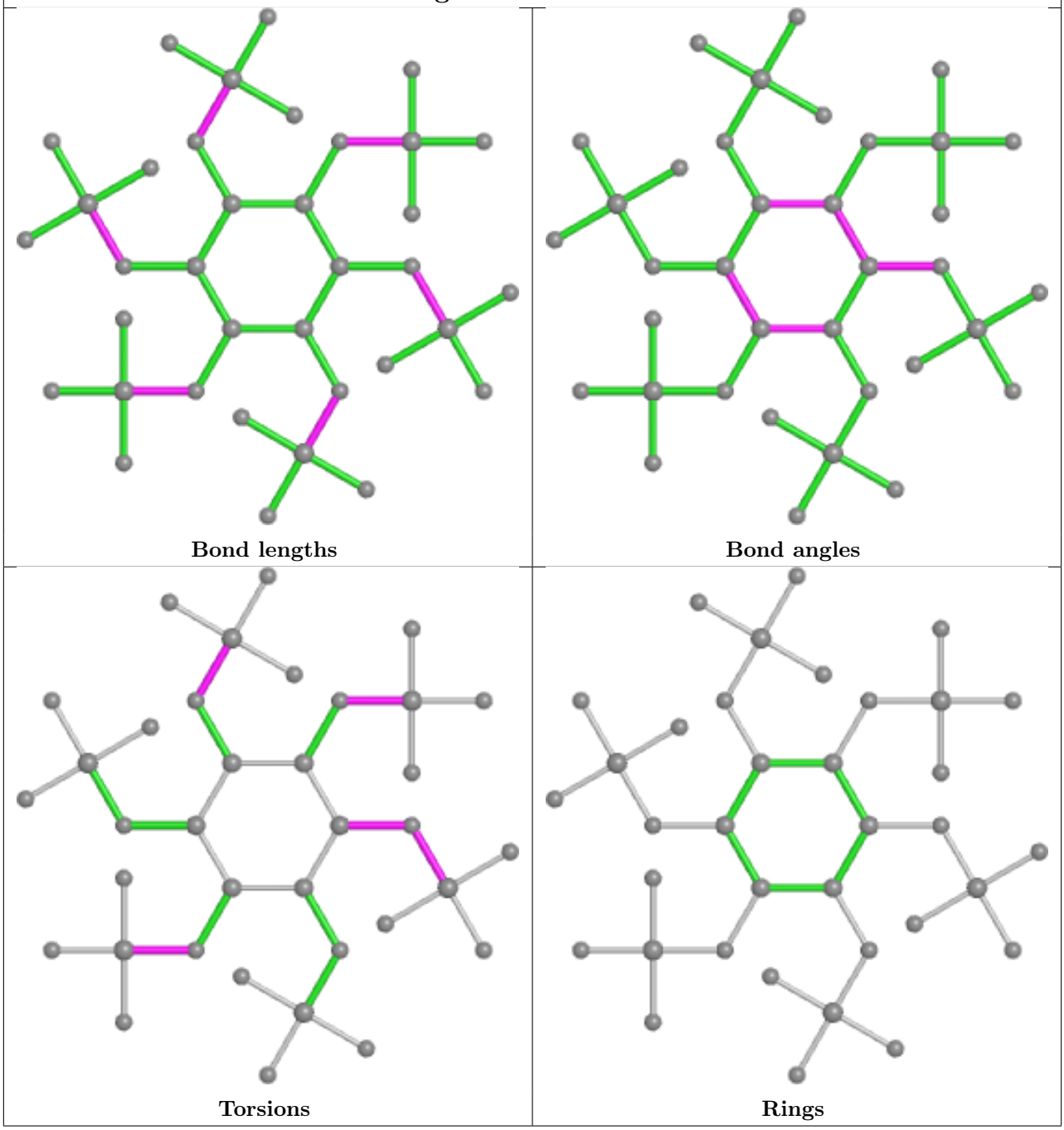
There are no ring outliers.

No monomer is involved in short contacts.

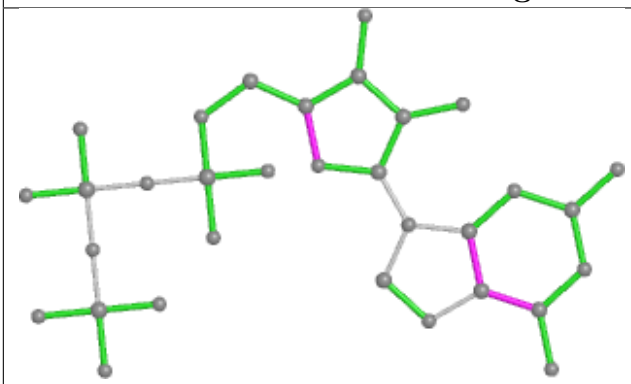
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

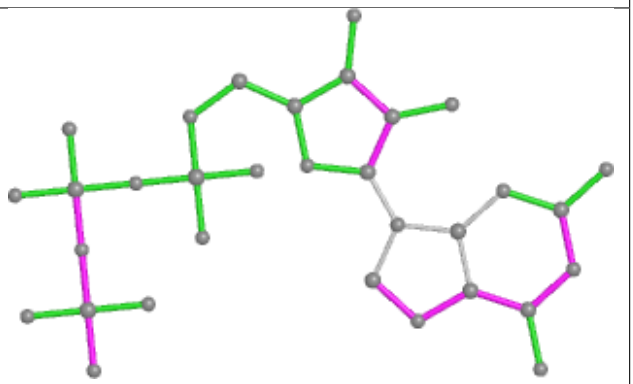
Ligand IHP J 1001



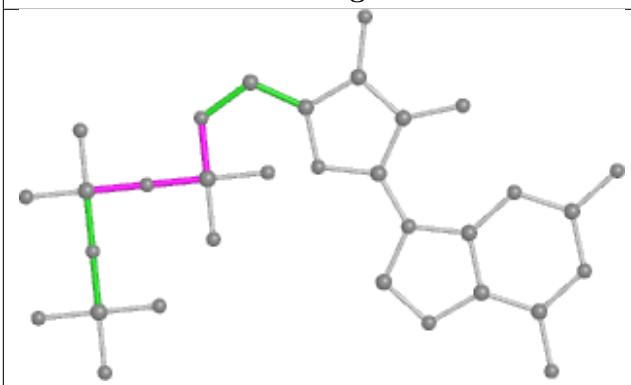
Ligand GTP C 1102



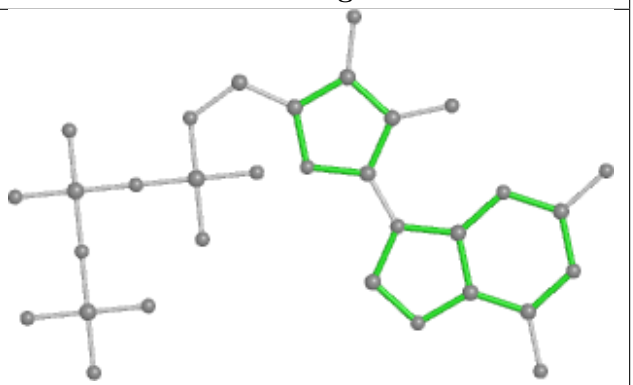
Bond lengths



Bond angles

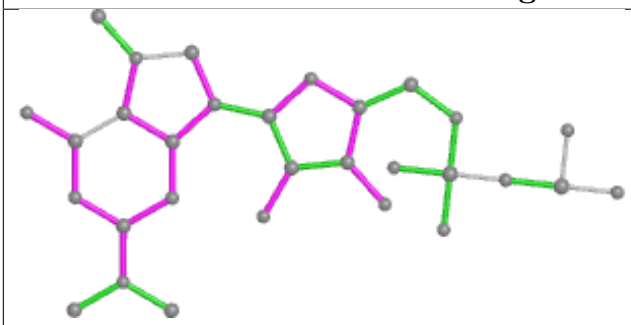


Torsions

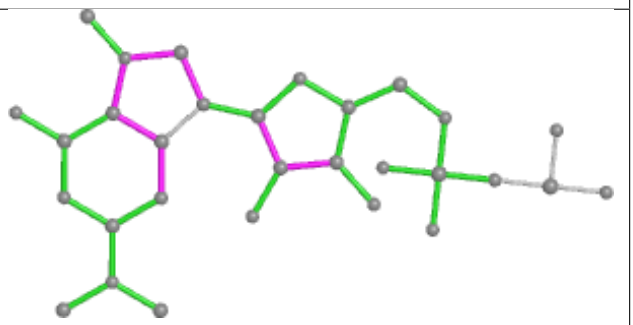


Rings

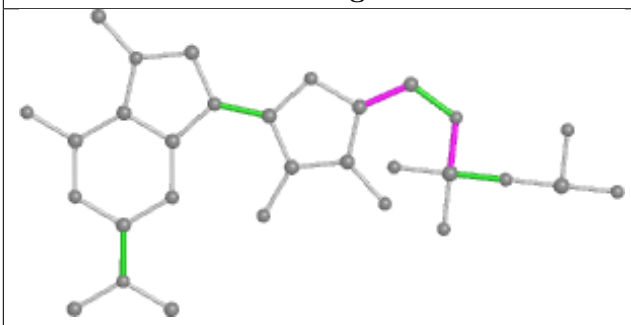
Ligand M7M B 401



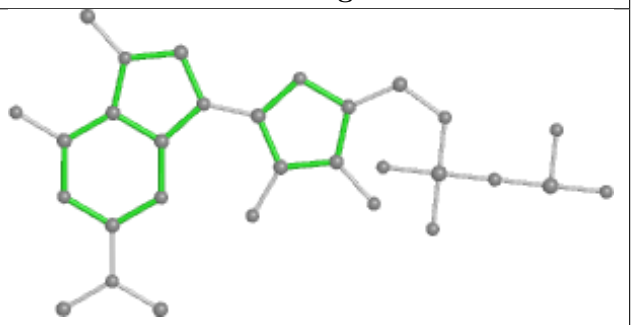
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.