



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:37 PM BST

PDB ID : 4V8Y
EMDB ID: : EMD-2421
Title : Cryo-EM reconstruction of the 80S-eIF5B-Met-itRNAMet Eukaryotic Translation Initiation Complex
Authors : Fernandez, I.S.; Bai, X.C.; Hussain, T.; Kelley, A.C.; Lorsch, J.R.; Ramakrishnan, V.; Scheres, S.H.W.
Deposited on : 2013-07-20
Resolution : 4.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

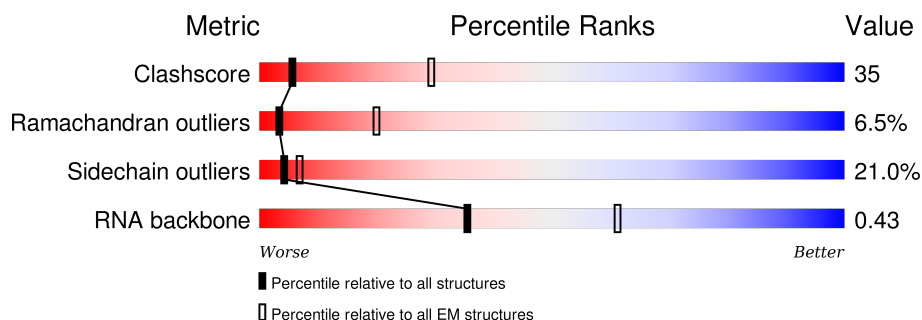
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.



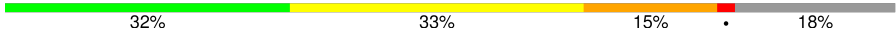


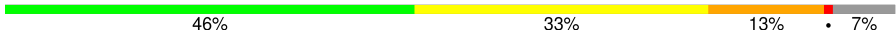
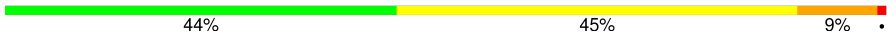
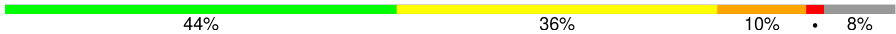
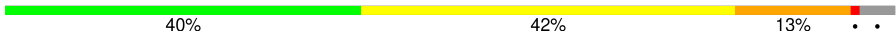
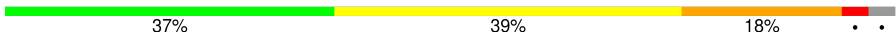
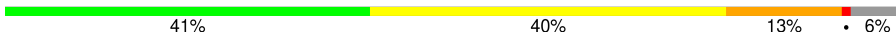
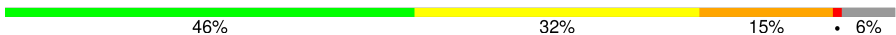
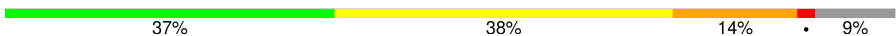
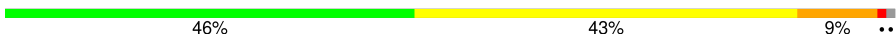
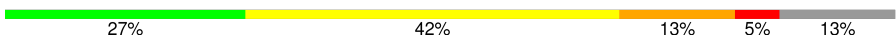







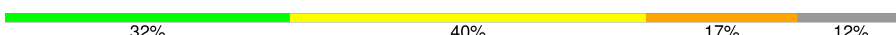




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A0	119	
2	A1	82	
3	A2	67	
4	A3	56	
5	A4	63	
6	A5	152	
7	A6	319	
8	A7	273	









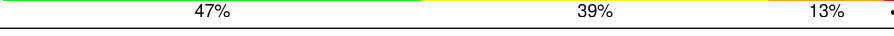

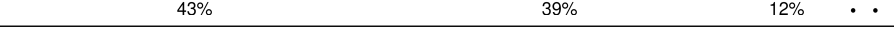
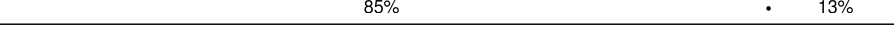

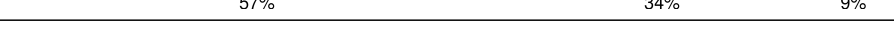


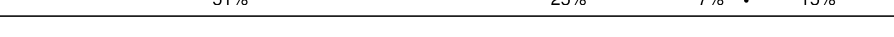

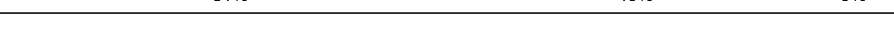






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Mol	Chain	Length	Quality of chain
9	AA	252	
10	AB	255	
11	AC	254	
12	AD	240	
13	AE	261	
14	AF	225	
15	AG	236	
16	AH	190	
17	AI	200	
18	AJ	197	
19	AK	105	
20	AL	156	
21	AM	143	
22	AN	151	
23	AO	137	
24	AP	142	
25	AQ	143	
26	AR	136	
27	AS	146	
28	AT	144	
29	AU	121	
30	AV	87	
31	AW	130	
32	AX	145	
33	AY	135	

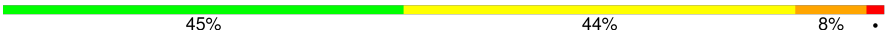









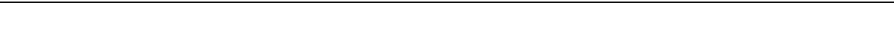

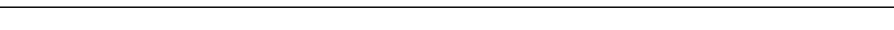
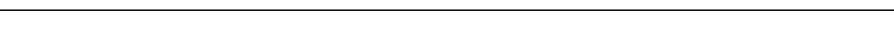





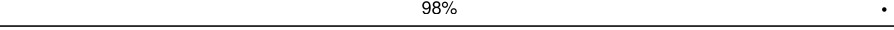
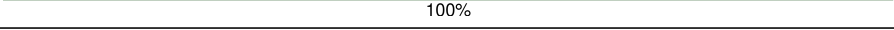



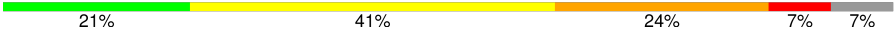
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Mol	Chain	Length	Quality of chain
34	AZ	108	
35	BA	253	
36	BB	386	
37	BC	361	
38	BD	296	
39	BE	175	
40	BF	243	
41	BG	255	
42	BH	191	
43	BI	220	
44	BJ	173	
45	BK	174	
46	BL	198	
47	BM	137	
48	BN	203	
49	BO	218	
50	BP	183	
51	BQ	185	
52	BR	188	
53	BS	172	
54	BT	159	
55	BU	120	
56	BV	136	
57	BW	155	
58	BX	141	

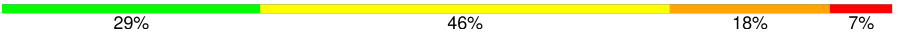



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Mol	Chain	Length	Quality of chain
59	BY	126	
60	BZ	135	
61	Ba	148	
62	Bb	58	
63	Bc	104	
64	Bd	112	
65	Be	129	
66	Bf	106	
67	Bg	120	
68	Bh	119	
69	Bi	99	
70	Bj	87	
71	Bk	77	
72	Bl	50	
73	Bm	128	
74	Bn	25	
75	Bo	105	
76	Bq	312	
77	Br	47	
78	Bs	46	
79	By	229	
79	CL	229	
80	B2	1800	
81	B5	3396	
82	B7	121	

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Mol	Chain	Length	Quality of chain
83	B8	158	
84	CN	87	
85	CP	339	
86	CW	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	OHX	A3	102	-	-	X	-
89	OHX	AC	301	-	-	X	-
89	OHX	AL	201	-	-	X	-
89	OHX	B2	1907	-	-	X	-
89	OHX	B2	1915	-	-	X	-
89	OHX	B2	1918	-	-	X	-
89	OHX	B2	1921	-	-	X	-
89	OHX	B2	1922	-	-	X	-
89	OHX	B2	1940	-	-	X	-
89	OHX	B2	1954	-	-	X	-
89	OHX	B2	1961	-	-	X	-
89	OHX	B2	1963	-	-	X	-
89	OHX	B2	1964	-	-	X	-
89	OHX	B2	1968	-	-	X	-
89	OHX	B2	1969	-	-	X	-
89	OHX	B2	1974	-	-	X	-
89	OHX	B2	1977	-	-	X	-
89	OHX	B2	1982	-	-	X	-
89	OHX	B2	1988	-	-	X	-
89	OHX	B2	1996	-	-	X	-
89	OHX	B2	2013	-	-	X	-
89	OHX	B2	2016	-	-	X	-
89	OHX	B2	2027	-	-	X	-
89	OHX	B2	2046	-	-	X	-
89	OHX	B2	2050	-	-	X	-
89	OHX	B2	2064	-	-	X	-
89	OHX	B2	2068	-	-	X	-
89	OHX	B2	2071	-	-	X	-
89	OHX	B2	2073	-	-	X	-
89	OHX	B2	2079	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	OHX	B2	2083	-	-	X	-
89	OHX	BR	201	-	-	X	-
90	GCP	CP	401	-	-	X	-

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 222555 atoms, of which 8300 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 protein called 40S RIBOSOMAL PROTEIN S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 6 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	82	UNK	LYS	SEE REMARK 999	UNP P05759
A5	83	UNK	LYS	SEE REMARK 999	UNP P05759
A5	84	UNK	VAL	SEE REMARK 999	UNP P05759
A5	85	UNK	TYR	SEE REMARK 999	UNP P05759
A5	86	UNK	THR	SEE REMARK 999	UNP P05759
A5	87	UNK	THR	SEE REMARK 999	UNP P05759
A5	88	UNK	PRO	SEE REMARK 999	UNP P05759
A5	89	UNK	LYS	SEE REMARK 999	UNP P05759
A5	90	UNK	LYS	SEE REMARK 999	UNP P05759
A5	91	UNK	ILE	SEE REMARK 999	UNP P05759
A5	92	UNK	LYS	SEE REMARK 999	UNP P05759
A5	93	UNK	HIS	SEE REMARK 999	UNP P05759
A5	94	UNK	LYS	SEE REMARK 999	UNP P05759
A5	95	UNK	HIS	SEE REMARK 999	UNP P05759
A5	96	UNK	LYS	SEE REMARK 999	UNP P05759
A5	97	UNK	LYS	SEE REMARK 999	UNP P05759
A5	98	UNK	VAL	SEE REMARK 999	UNP P05759
A5	99	UNK	LYS	SEE REMARK 999	UNP P05759
A5	100	UNK	LEU	SEE REMARK 999	UNP P05759
A5	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 7 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 8 is a protein called SUPPRESSOR PROTEIN STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A7	159	Total	C	N	O	0	0
			1105	653	221	231		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	9	UNK	GLY	SEE REMARK 999	UNP P39015
A7	10	UNK	ASN	SEE REMARK 999	UNP P39015
A7	11	UNK	ASP	SEE REMARK 999	UNP P39015
A7	12	UNK	VAL	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
A7	13	UNK	GLU	SEE REMARK 999	UNP P39015
A7	14	UNK	ASP	SEE REMARK 999	UNP P39015
A7	15	UNK	ALA	SEE REMARK 999	UNP P39015
A7	16	UNK	ASP	SEE REMARK 999	UNP P39015
A7	17	UNK	VAL	SEE REMARK 999	UNP P39015
A7	18	UNK	VAL	SEE REMARK 999	UNP P39015
A7	19	UNK	VAL	SEE REMARK 999	UNP P39015
A7	20	UNK	LEU	SEE REMARK 999	UNP P39015
A7	151	UNK	LEU	SEE REMARK 999	UNP P39015
A7	152	UNK	GLN	SEE REMARK 999	UNP P39015
A7	153	UNK	ASP	SEE REMARK 999	UNP P39015
A7	154	UNK	TYR	SEE REMARK 999	UNP P39015
A7	155	UNK	LEU	SEE REMARK 999	UNP P39015
A7	156	UNK	ASN	SEE REMARK 999	UNP P39015
A7	157	UNK	GLN	SEE REMARK 999	UNP P39015
A7	158	UNK	GLN	SEE REMARK 999	UNP P39015
A7	159	UNK	ALA	SEE REMARK 999	UNP P39015
A7	160	UNK	ASN	SEE REMARK 999	UNP P39015
A7	161	UNK	ASN	SEE REMARK 999	UNP P39015
A7	162	UNK	GLN	SEE REMARK 999	UNP P39015
A7	163	UNK	PHE	SEE REMARK 999	UNP P39015
A7	164	UNK	ASN	SEE REMARK 999	UNP P39015
A7	165	UNK	LYS	SEE REMARK 999	UNP P39015
A7	166	UNK	VAL	SEE REMARK 999	UNP P39015
A7	167	UNK	PRO	SEE REMARK 999	UNP P39015
A7	168	UNK	GLU	SEE REMARK 999	UNP P39015
A7	169	UNK	ALA	SEE REMARK 999	UNP P39015
A7	170	UNK	LYS	SEE REMARK 999	UNP P39015
A7	171	UNK	LYS	SEE REMARK 999	UNP P39015
A7	172	UNK	VAL	SEE REMARK 999	UNP P39015
A7	173	UNK	GLU	SEE REMARK 999	UNP P39015
A7	174	UNK	LEU	SEE REMARK 999	UNP P39015
A7	175	UNK	ASP	SEE REMARK 999	UNP P39015

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AH	184	Total	C	N	O		0	0
			1481	951	265	265			

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AO	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AP	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AR	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AZ	70	Total	C	N	O		0	0
			563	360	104	99			

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	151	Total	C	H	N	O	0	1
			1507	450	756	151	150		

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 47 is a protein called 60S RIBOSOMAL PROTEIN L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	89	ALA	GLY	CONFLICT	UNP P38754

- Molecule 48 is a protein called 60S RIBOSOMAL PROTEIN L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 49 is a protein called 60S RIBOSOMAL PROTEIN L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	197	Total	C	N	O	S	197	0
			3119	2008	581	528	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	3	VAL	SER	MICROHETEROGENEITY	UNP P26784
BO	4	GLU	GLN	MICROHETEROGENEITY	UNP P26784
BO	11	GLY	ALA	MICROHETEROGENEITY	UNP P26784
BO	13	GLY	ASP	MICROHETEROGENEITY	UNP P26784
BO	16	VAL	LEU	MICROHETEROGENEITY	UNP P26784
BO	22	VAL	THR	MICROHETEROGENEITY	UNP P26784
BO	23	VAL	ILE	MICROHETEROGENEITY	UNP P26784

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Chain	Residue	Modelled	Actual	Comment	Reference
BO	27	LEU	VAL	MICROHETEROGENEITY	UNP P26784
BO	40	GLU	ALA	MICROHETEROGENEITY	UNP P26784
BO	80	PHE	LEU	MICROHETEROGENEITY	UNP P26784
BO	84	LEU	ILE	MICROHETEROGENEITY	UNP P26784
BO	104	VAL	ILE	MICROHETEROGENEITY	UNP P26784
BO	158	ALA	ASP	MICROHETEROGENEITY	UNP P26784
BO	163	SER	ARG	MICROHETEROGENEITY	UNP P26784
BO	179	ALA	SER	MICROHETEROGENEITY	UNP P26784
BO	182	ASN	SER	MICROHETEROGENEITY	UNP P26784
BO	184	THR	ALA	MICROHETEROGENEITY	UNP P26784
BO	186	ALA	SER	MICROHETEROGENEITY	UNP P26784
BO	196	ALA	SER	MICROHETEROGENEITY	UNP P26784
BO	197	LEU	PHE	MICROHETEROGENEITY	UNP P26784

- Molecule 50 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	155	Total	C	N	O	0	0
			1227	764	238	225		

- Molecule 51 is a protein called 60S RIBOSOMAL PROTEIN L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 52 is a protein called 60S RIBOSOMAL PROTEIN L19-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 53 is a protein called 60S RIBOSOMAL PROTEIN L20-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 54 is a protein called 60S RIBOSOMAL PROTEIN L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 55 is a protein called 60S RIBOSOMAL PROTEIN L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 56 is a protein called 60S RIBOSOMAL PROTEIN L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 57 is a protein called 60S RIBOSOMAL PROTEIN L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	135	Total	C	N	O	S	0	0
			1038	651	206	180	1		

- Molecule 58 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 59 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BY	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 60 is a protein called 60S RIBOSOMAL PROTEIN L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BZ	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 61 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ba	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 62 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bb	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 63 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 64 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bd	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 65 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Be	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 66 is a protein called 60S RIBOSOMAL PROTEIN L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 67 is a protein called 60S RIBOSOMAL PROTEIN L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 68 is a protein called 60S RIBOSOMAL PROTEIN L35-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 69 is a protein called 60S RIBOSOMAL PROTEIN L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bi	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 70 is a protein called 60S RIBOSOMAL PROTEIN L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 71 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 72 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 73 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 74 is a protein called 60S RIBOSOMAL PROTEIN L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 75 is a protein called 60S RIBOSOMAL PROTEIN L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 76 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace	
76	Bq	143	Total	C	H	N	O	S	0	0
			2187	687	1110	192	195	3		

- Molecule 77 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Br	47	Total	C	H	N	O	0	0
			473	141	237	47	48		

- Molecule 78 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bs	46	Total	C	H	N	O	0	0
			463	138	232	46	47		

- Molecule 79 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	By	225	Total	C	H	N	O	S	0	0
			3492	1086	1773	315	316	2		
79	CL	225	Total	C	N	O	S		0	0
			1719	1086	315	316	2			

- Molecule 80 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	B2	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 81 is a RNA chain called 25S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	B5	3147	Total	C	H	N	O	P	0	0
			67972	30066	664	12132	21965	3145		

- Molecule 82 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 83 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	B8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 84 is a RNA chain called EUKARYOTIC RIBOSOMAL L1_RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CN	87	Total	C	N	O	P	0	0
			1875	832	347	609	87		

- Molecule 85 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
85	CP	339	Total	C	H	N	O	S	0	0
			5380	1679	2725	457	507	12		

- Molecule 86 is a RNA chain called EUKARYOTIC RIBOSOMAL P_E TRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	CW	74	Total	C	H	N	O	P	0	0
			2379	705	803	285	514	72		

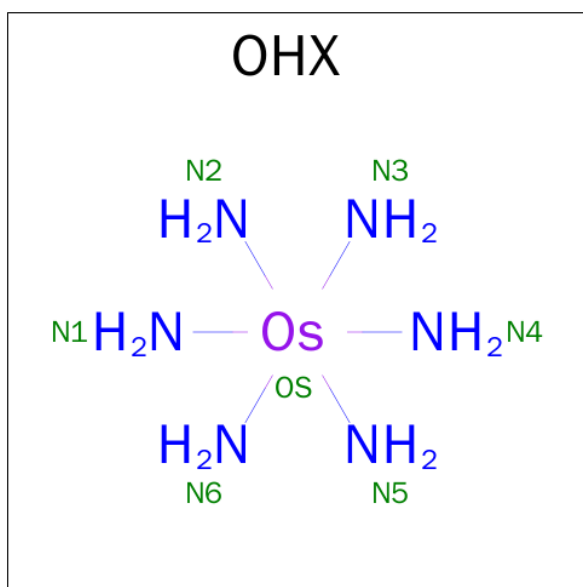
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	A0	1	Total	Zn	0
			1	1	
87	A1	1	Total	Zn	0
			1	1	
87	Bm	1	Total	Zn	0
			1	1	
87	A5	1	Total	Zn	0
			1	1	
87	Bj	1	Total	Zn	0
			1	1	
87	A3	1	Total	Zn	0
			1	1	

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A0	2	Total 2	Mg 2	0
88	AG	1	Total 1	Mg 1	0
88	AJ	1	Total 1	Mg 1	0
88	AE	1	Total 1	Mg 1	0
88	AB	1	Total 1	Mg 1	0
88	AI	1	Total 1	Mg 1	0
88	AC	2	Total 2	Mg 2	0
88	AS	1	Total 1	Mg 1	0
88	B2	169	Total 169	Mg 169	0
88	B5	3	Total 3	Mg 3	0
88	AU	1	Total 1	Mg 1	0
88	AN	1	Total 1	Mg 1	0
88	A5	1	Total 1	Mg 1	0
88	AL	2	Total 2	Mg 2	0
88	A3	3	Total 3	Mg 3	0
88	AP	1	Total 1	Mg 1	0

- Molecule 89 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			AltConf
89	A3	1	Total	N	Os	0
			7	6	1	
89	A6	1	Total	N	Os	0
			7	6	1	
89	AC	1	Total	N	Os	0
			7	6	1	
89	AI	1	Total	N	Os	0
			14	12	2	
89	AI	1	Total	N	Os	0
			14	12	2	
89	AL	1	Total	N	Os	0
			7	6	1	
89	AN	1	Total	N	Os	0
			7	6	1	
89	AP	1	Total	N	Os	0
			7	6	1	
89	BR	1	Total	N	Os	0
			7	6	1	
89	Bn	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	

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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	

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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	

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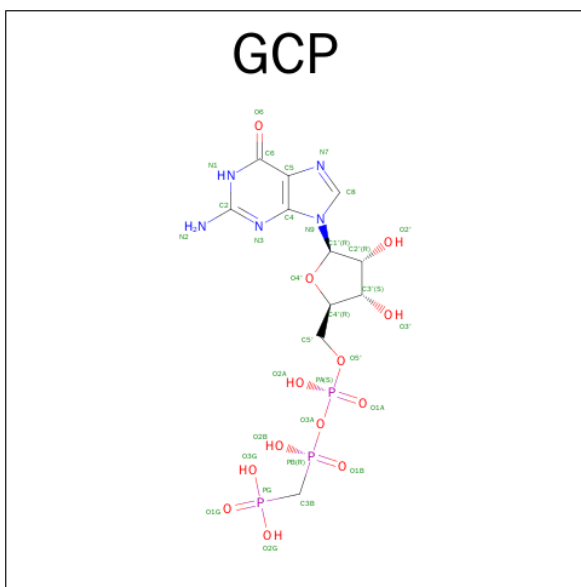
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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B5	1	Total	N	Os	0
			21	18	3	
89	B5	1	Total	N	Os	0
			21	18	3	
89	B5	1	Total	N	Os	0
			21	18	3	

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

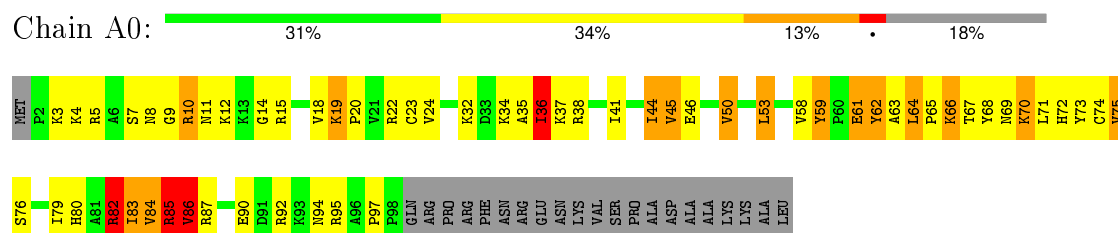


Mol	Chain	Residues	Atoms					AltConf
90	CP	1	Total	C	N	O	P	0
			32	11	5	13	3	

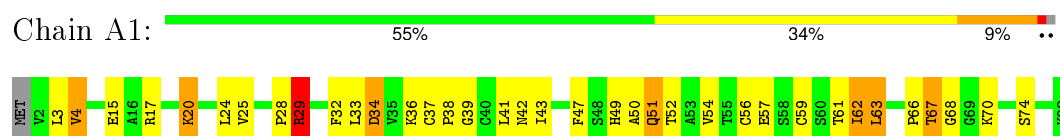
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

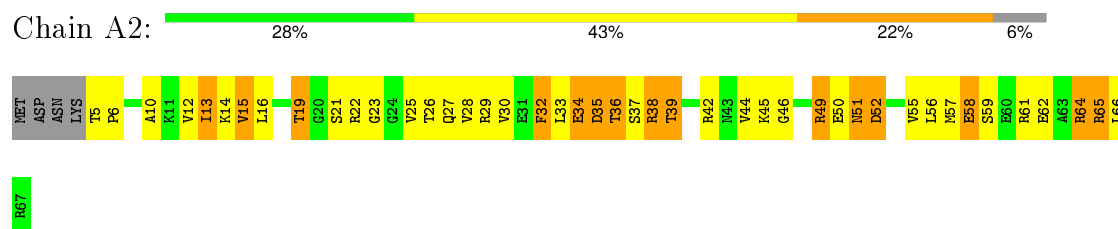
- Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



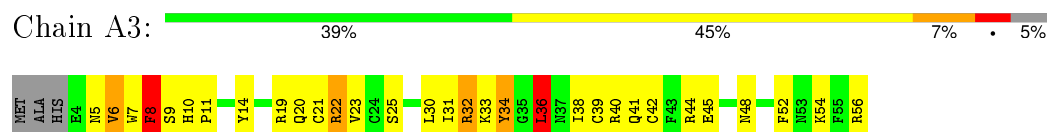
- Molecule 2: 40S RIBOSOMAL PROTEIN S27-A



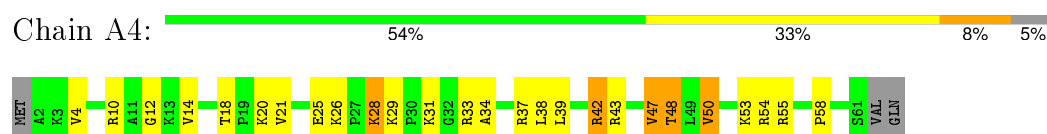
- Molecule 3: 40S RIBOSOMAL PROTEIN S28-A



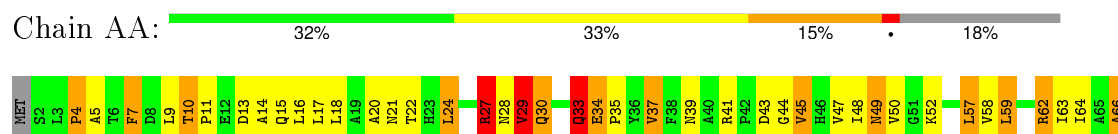
- Molecule 4: 40S RIBOSOMAL PROTEIN S29-A

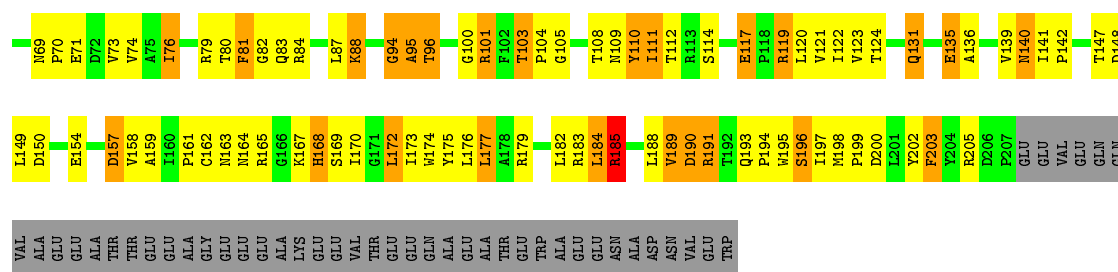


- Molecule 5: 40S RIBOSOMAL PROTEIN S30-A



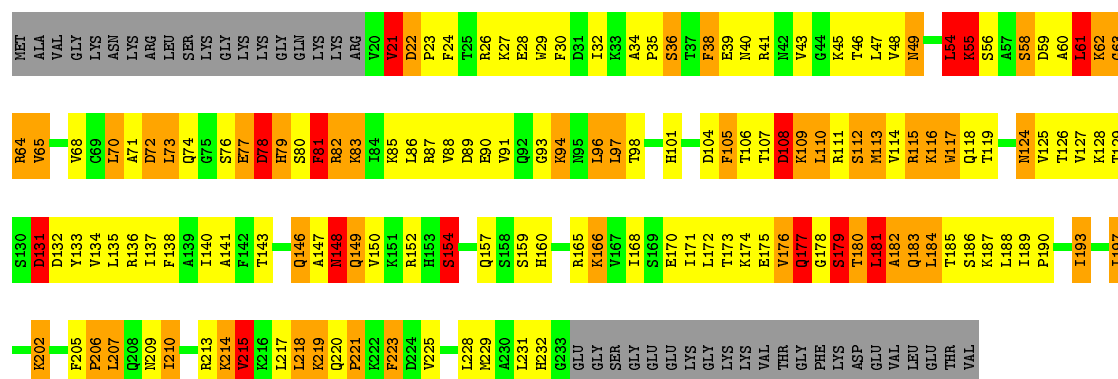
- Molecule 6: UBIQUITIN-40S RIBOSOMAL PROTEIN S31





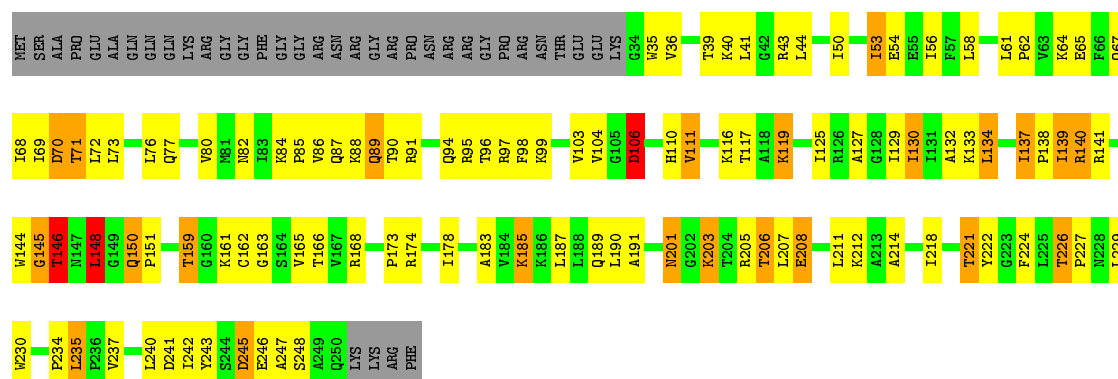
• Molecule 10: 40S RIBOSOMAL PROTEIN S1-A

Chain AB: 25% 35% 18% 5% 16%



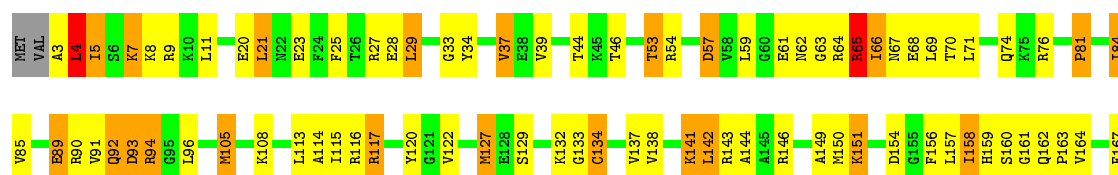
• Molecule 11: 40S RIBOSOMAL PROTEIN S2

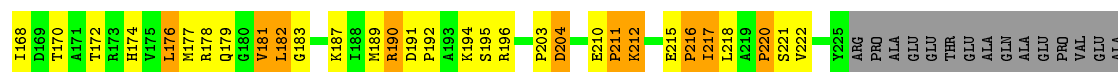
Chain AC: 42% 33% 9% 15%



• Molecule 12: 40S RIBOSOMAL PROTEIN S3

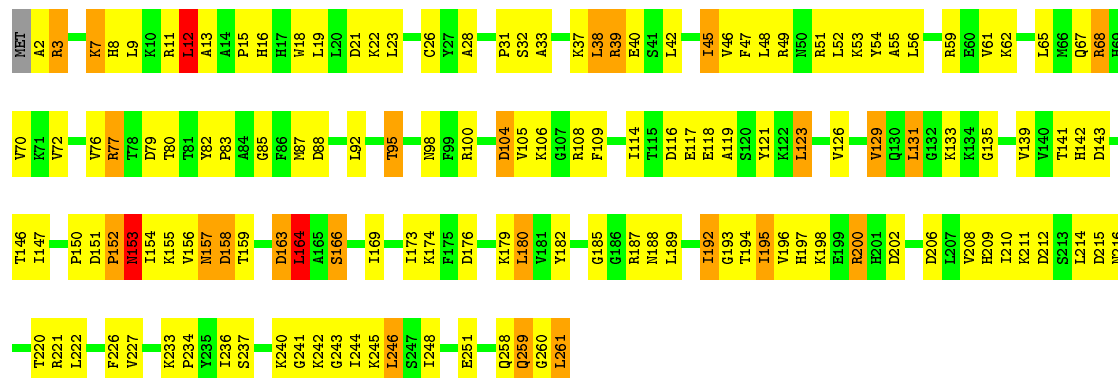
Chain AD: 46% 33% 13% 7%





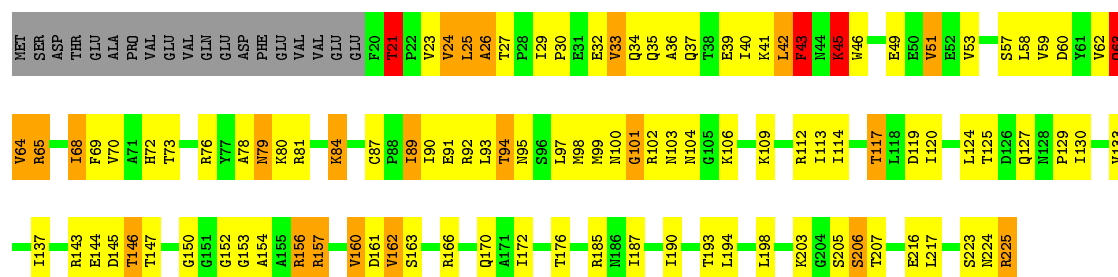
• Molecule 13: 40S RIBOSOMAL PROTEIN S4-A

Chain AE: 44% 45% 9%



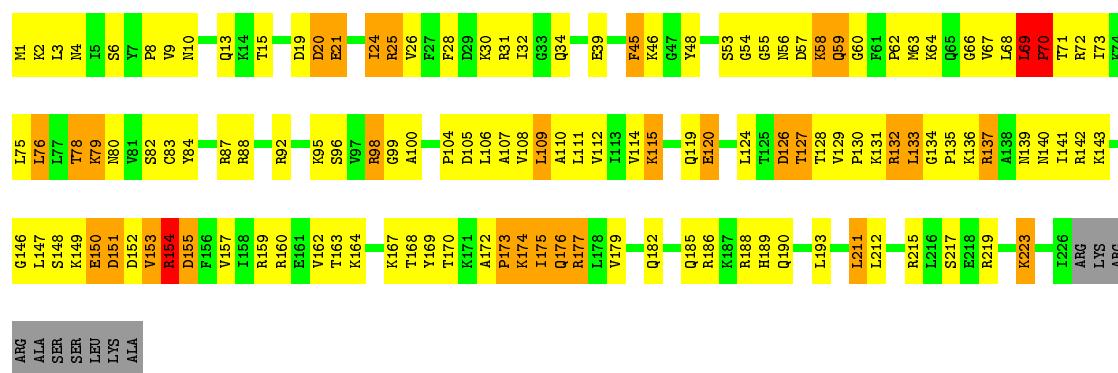
• Molecule 14: 40S RIBOSOMAL PROTEIN S5

Chain AF: 44% 36% 10% 8%



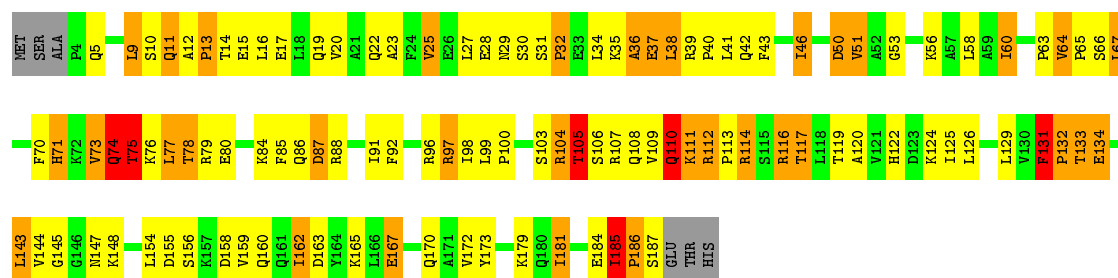
• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A

Chain AG: 40% 42% 13%



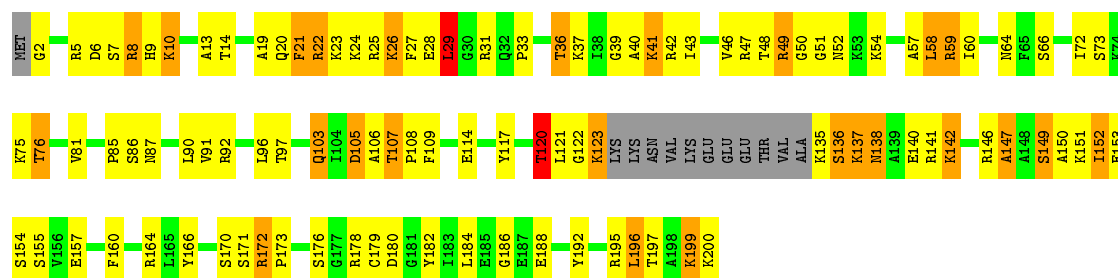
• Molecule 16: 40S RIBOSOMAL PROTEIN S7-A

Chain AH: 37% 39% 18%



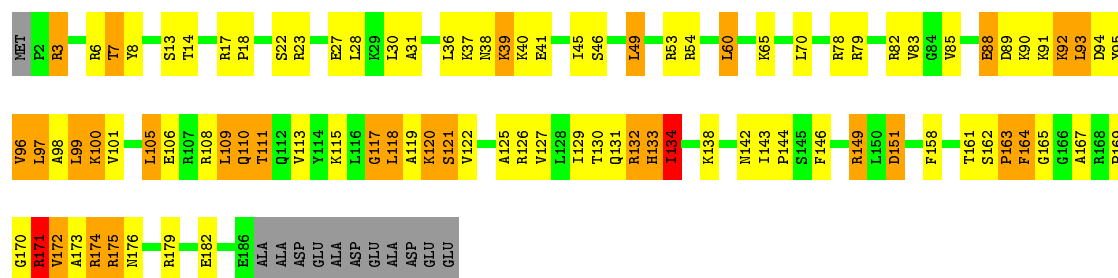
• Molecule 17: 40S RIBOSOMAL PROTEIN S8-A

Chain AI: 41% 40% 13% 6%



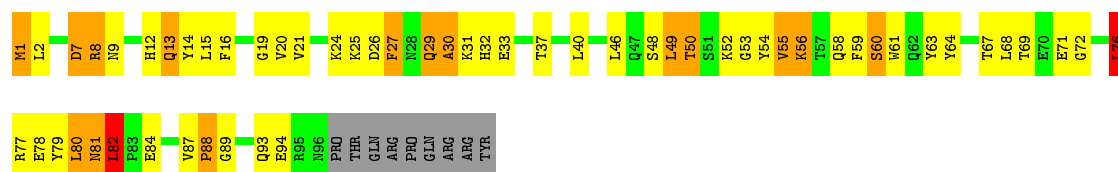
• Molecule 18: 40S RIBOSOMAL PROTEIN S9-A

Chain AJ: 46% 32% 15% 6%



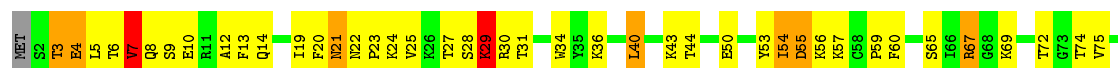
• Molecule 19: 40S RIBOSOMAL PROTEIN S10-A

Chain AK: 37% 38% 14% 9%

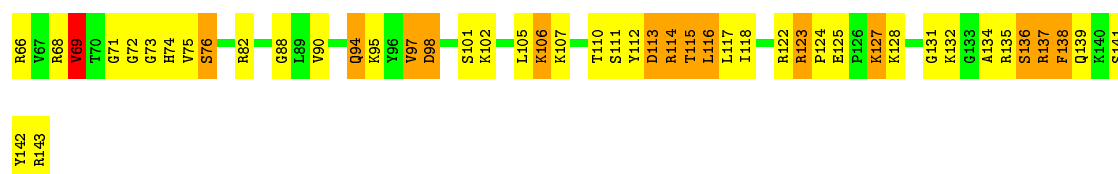


• Molecule 20: 40S RIBOSOMAL PROTEIN S11-A

Chain AL: 46% 43% 9% ..

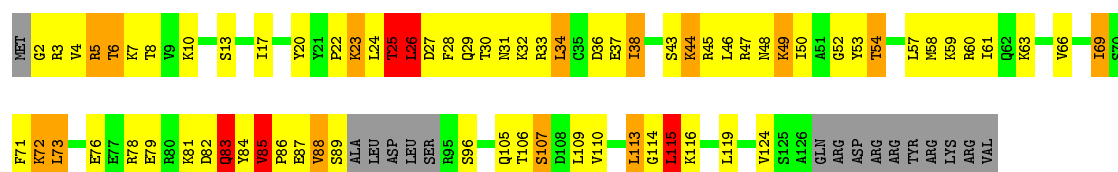






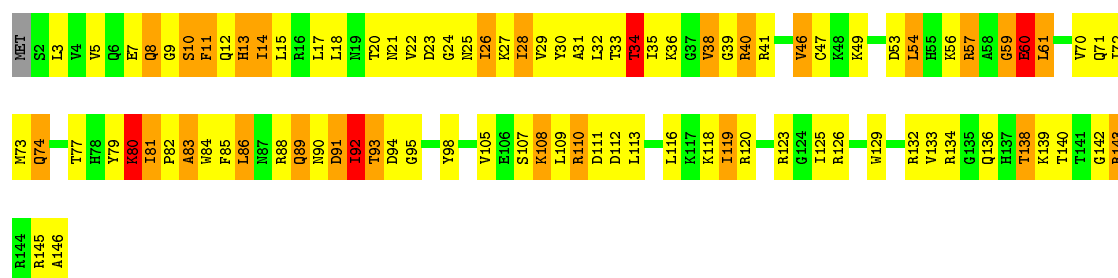
• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A

Chain AR: 35% 40% 10% 12%



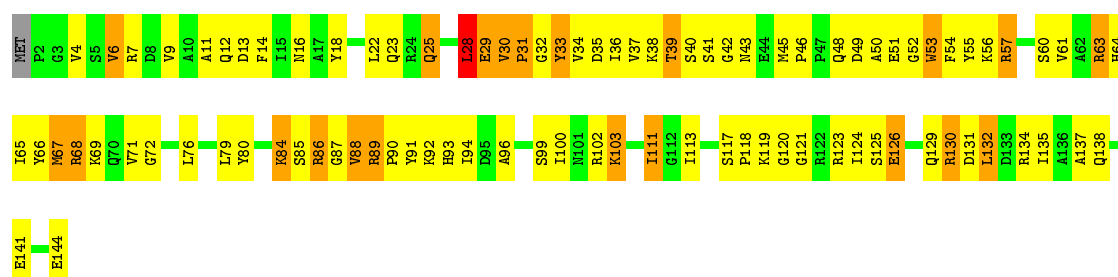
• Molecule 27: 40S RIBOSOMAL PROTEIN S18-A

Chain AS: 35% 44% 18%



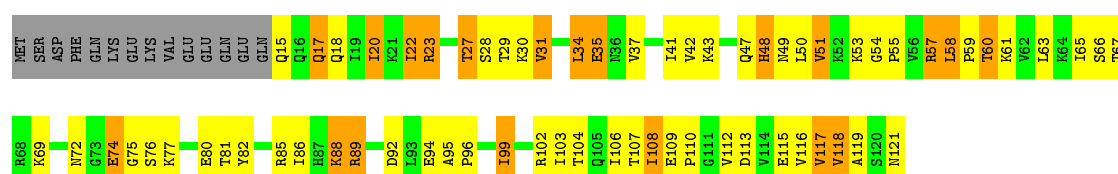
• Molecule 28: 40S RIBOSOMAL PROTEIN S19-A

Chain AT: 35% 49% 15%

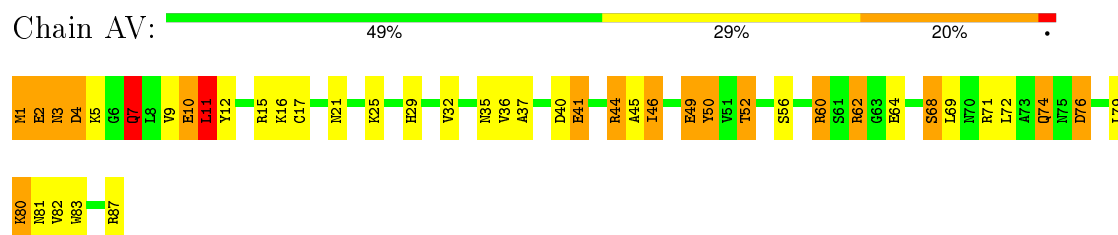


• Molecule 29: 40S RIBOSOMAL PROTEIN S20

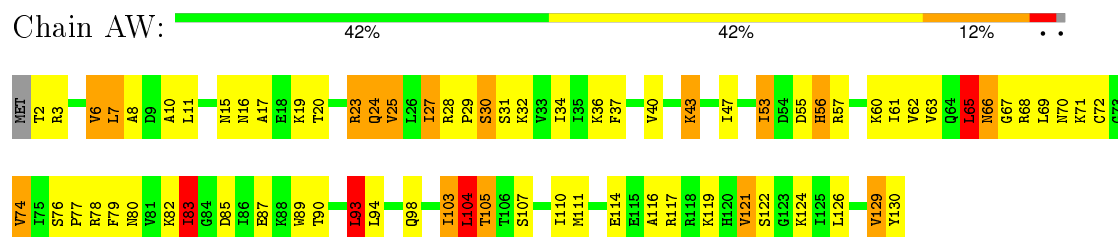
Chain AU: 32% 40% 17% 12%



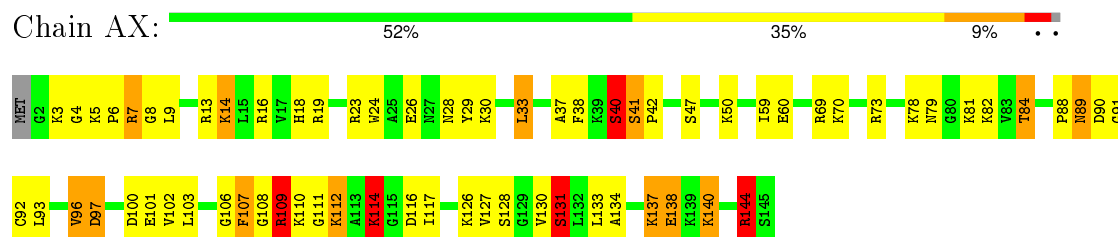
- Molecule 30: 40S RIBOSOMAL PROTEIN S21-A



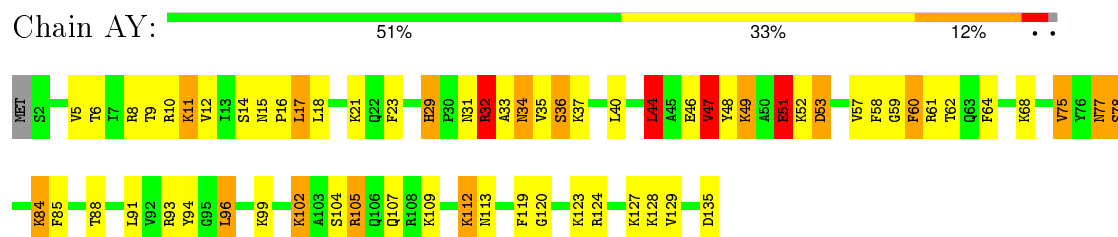
- Molecule 31: 40S RIBOSOMAL PROTEIN S22-A



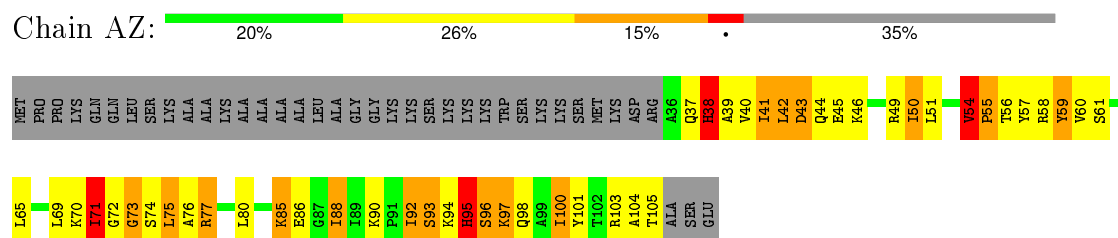
- Molecule 32: 40S RIBOSOMAL PROTEIN S23-A



- Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

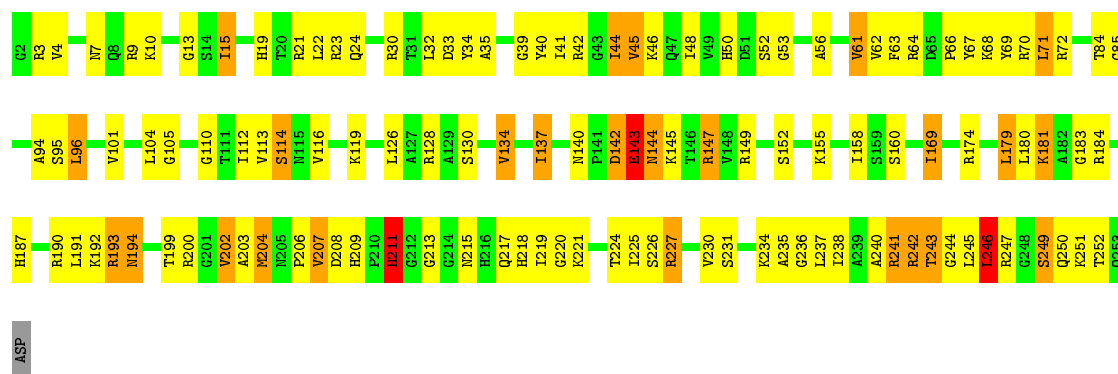


- Molecule 34: 40S RIBOSOMAL PROTEIN S25-A



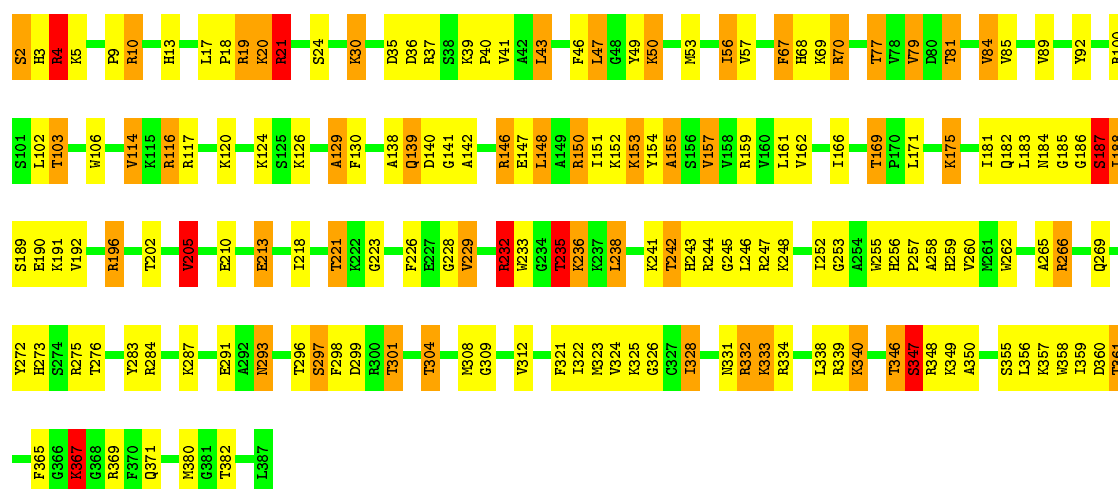
- Molecule 35: 60S RIBOSOMAL PROTEIN L2-B





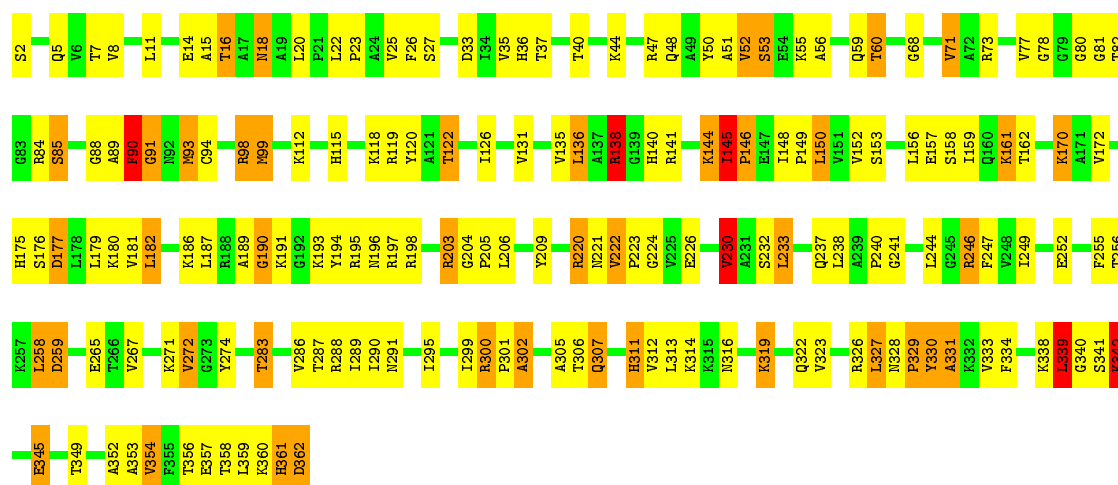
• Molecule 36: 60S RIBOSOMAL PROTEIN L3

Chain BB: 56% 30% 12%

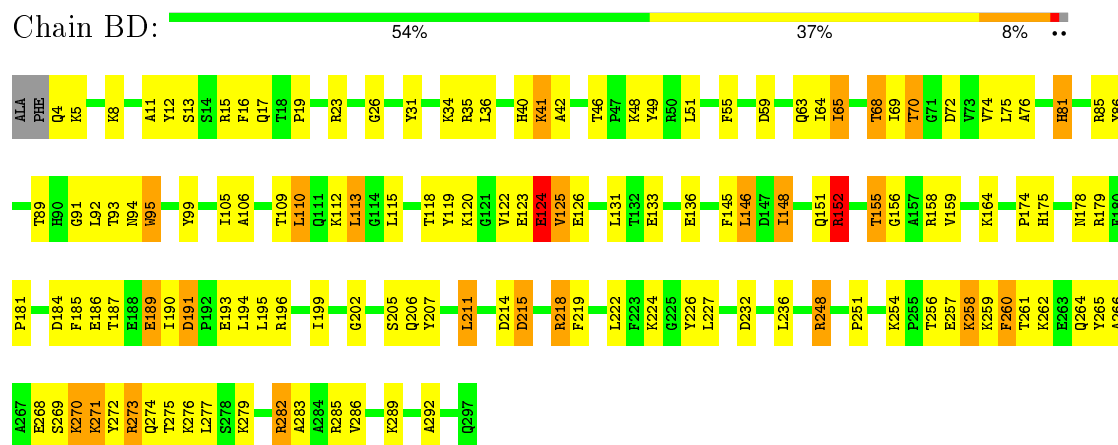


• Molecule 37: 60S RIBOSOMAL PROTEIN L4-A

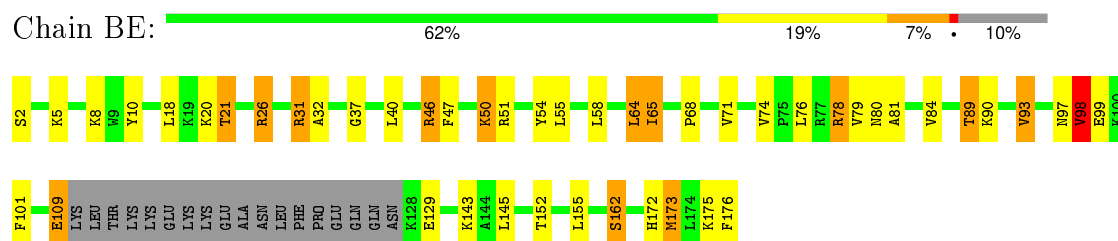
Chain BC: 51% 35% 12%



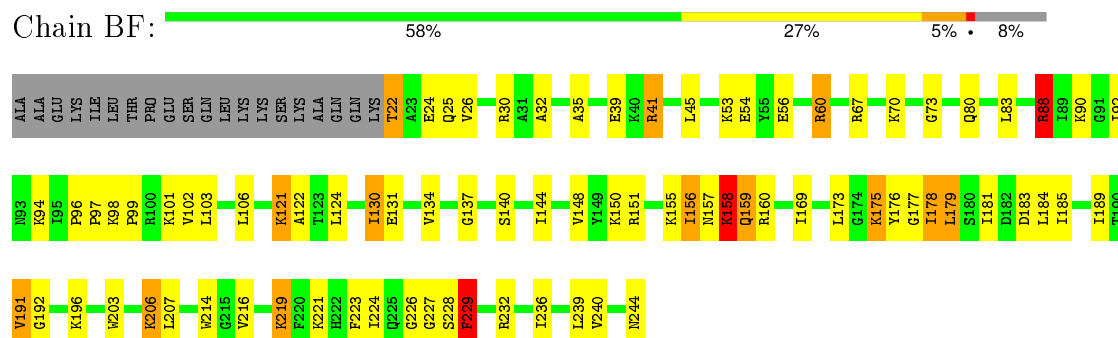
• Molecule 38: 60S RIBOSOMAL PROTEIN L5



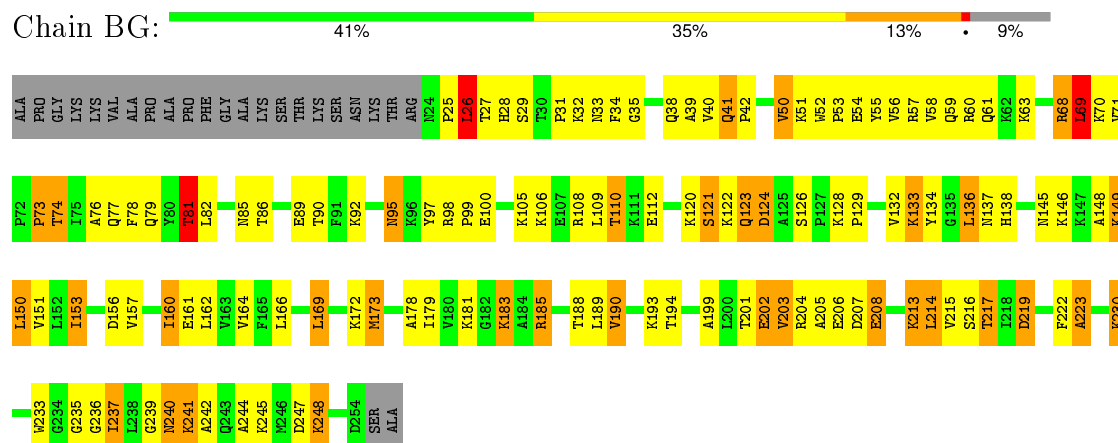
• Molecule 39: 60S RIBOSOMAL PROTEIN L6-A



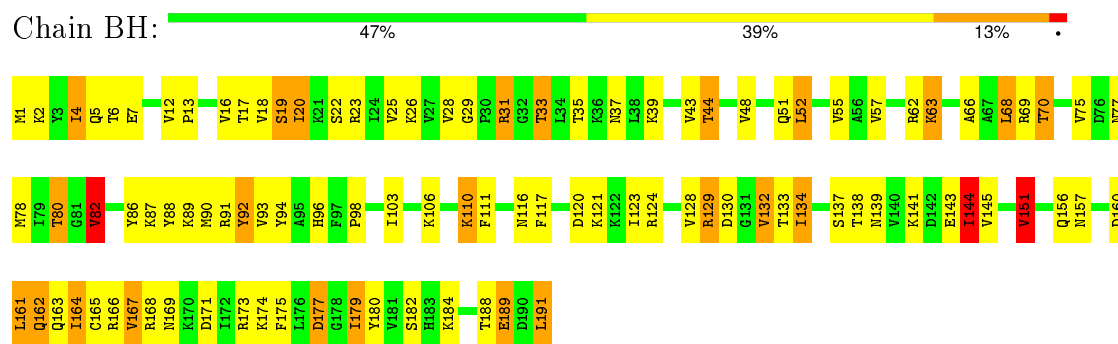
• Molecule 40: 60S RIBOSOMAL PROTEIN L7-A



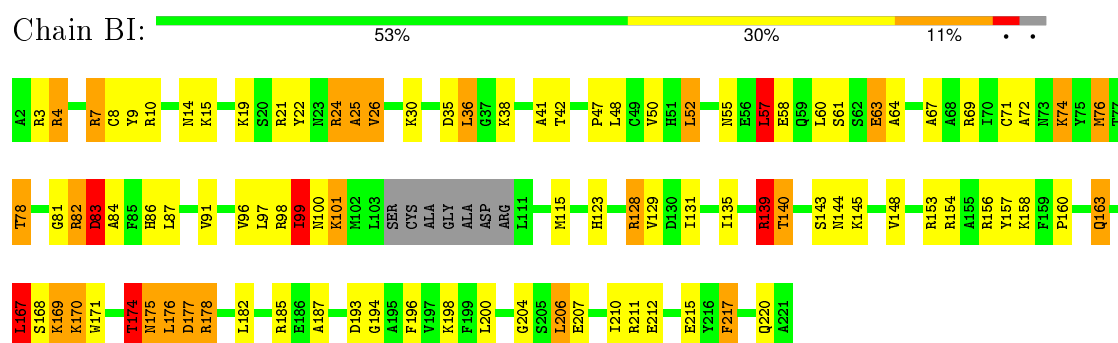
• Molecule 41: 60S RIBOSOMAL PROTEIN L8-A



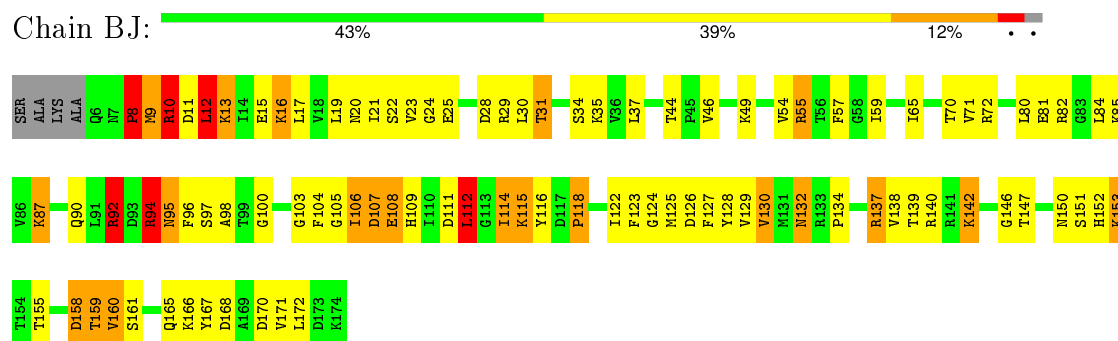
- Molecule 42: 60S RIBOSOMAL PROTEIN L9-A



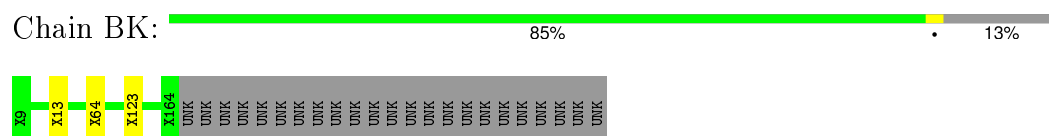
- Molecule 43: 60S RIBOSOMAL PROTEIN L10



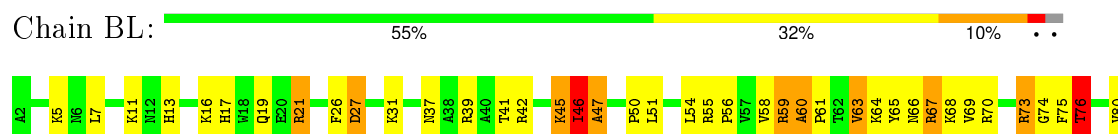
- Molecule 44: 60S RIBOSOMAL PROTEIN L11-A

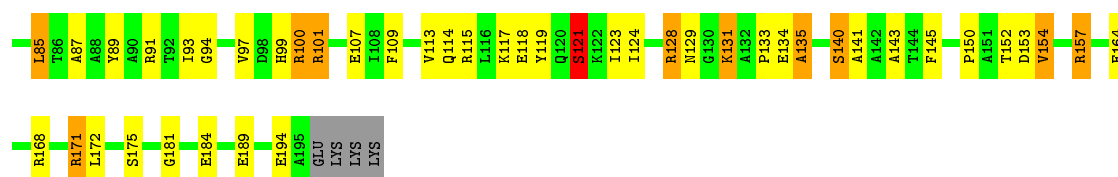


- Molecule 45: 60S RIBOSOMAL PROTEIN L11-A



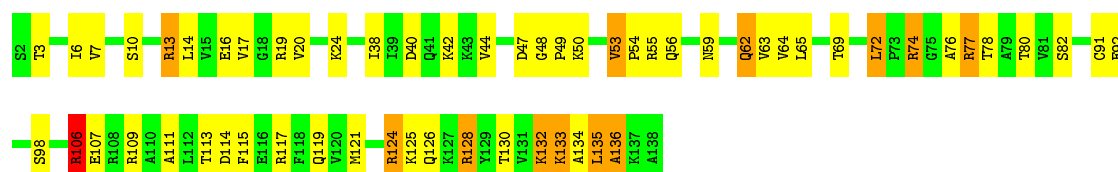
- Molecule 46: 60S RIBOSOMAL PROTEIN L13-A





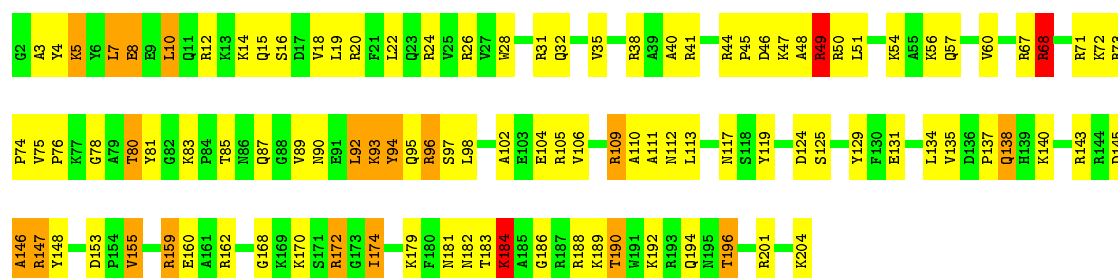
• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

Chain BM: 57% 34% 9% •



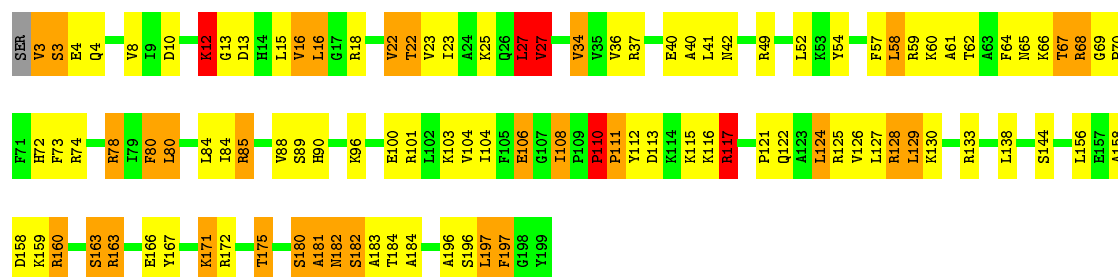
• Molecule 48: 60S RIBOSOMAL PROTEIN L15-A

Chain BN: 48% 41% 9% •



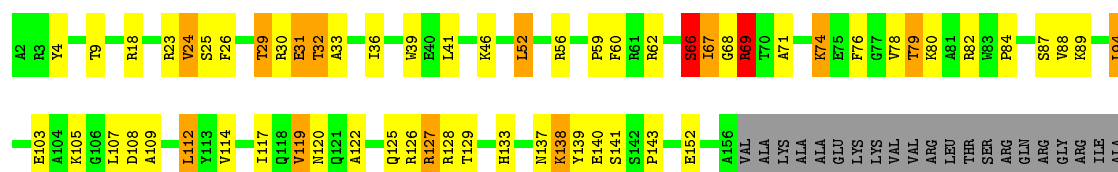
• Molecule 49: 60S RIBOSOMAL PROTEIN L16-A

Chain BO: 51% 32% 14% •



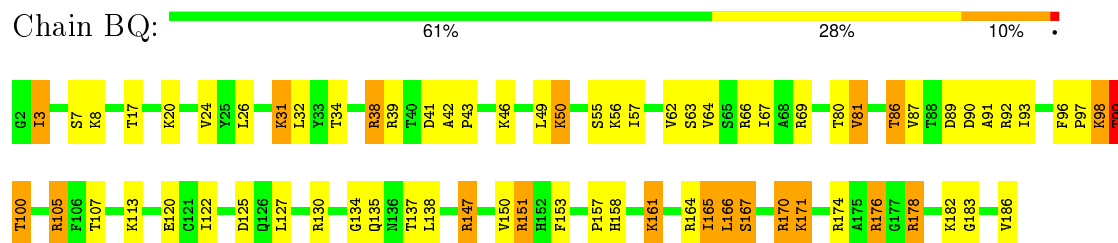
• Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

Chain BP: 51% 25% 7% • 15%

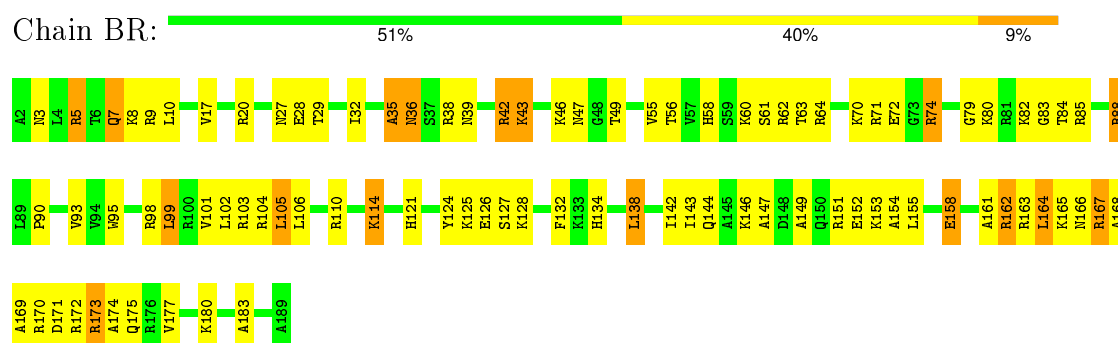


ALA
GLN
LYS
ARG
ILE
ALA
ALA

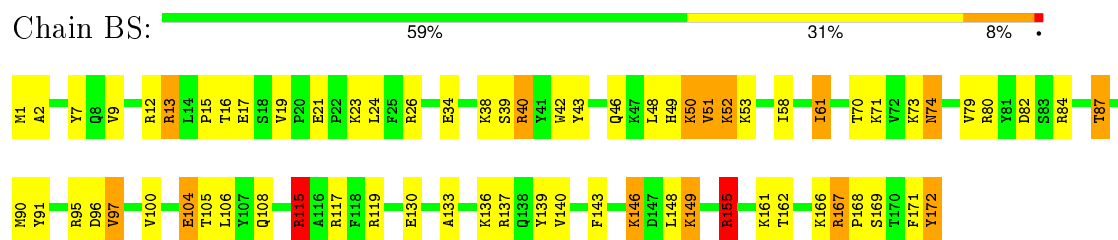
• Molecule 51: 60S RIBOSOMAL PROTEIN L18-A



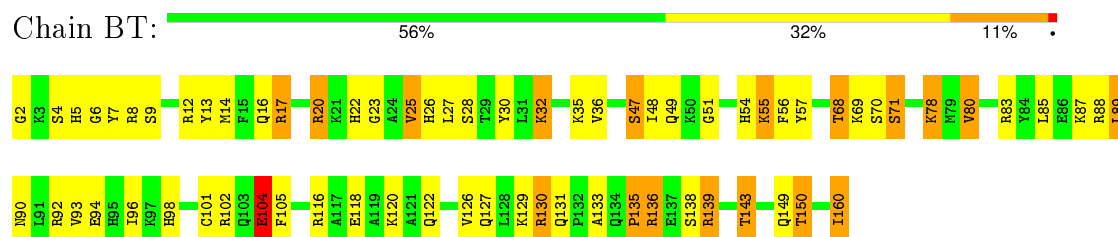
• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B



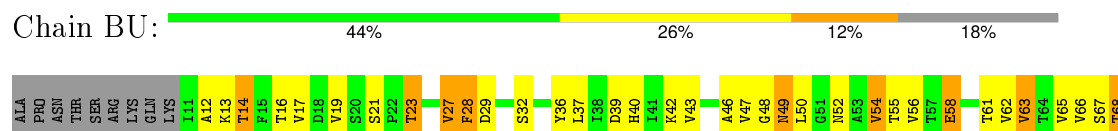
• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B



• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A



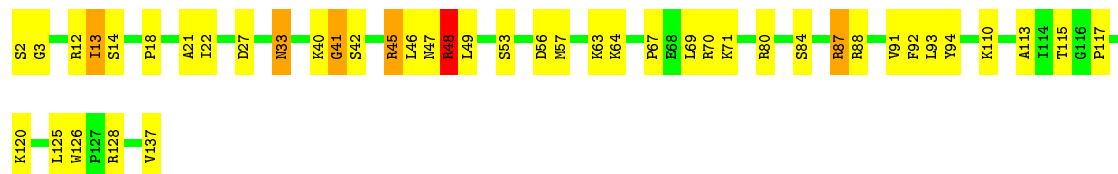
• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A





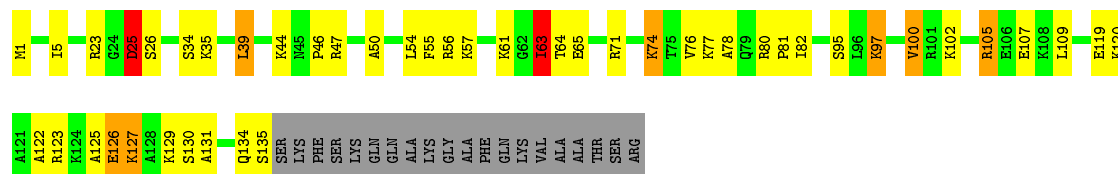
• Molecule 56: 60S RIBOSOMAL PROTEIN L23-A

Chain BV: 68% 28%



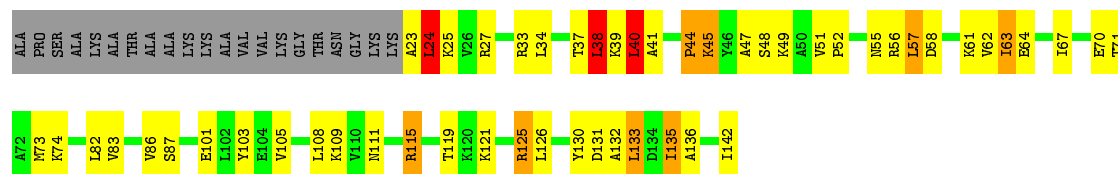
• Molecule 57: 60S RIBOSOMAL PROTEIN L24-A

Chain BW: 57% 25% 5% 13%



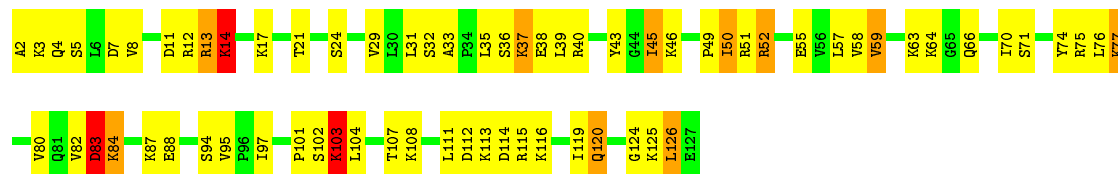
• Molecule 58: 60S RIBOSOMAL PROTEIN L25

Chain BX: 48% 30% 6% 15%



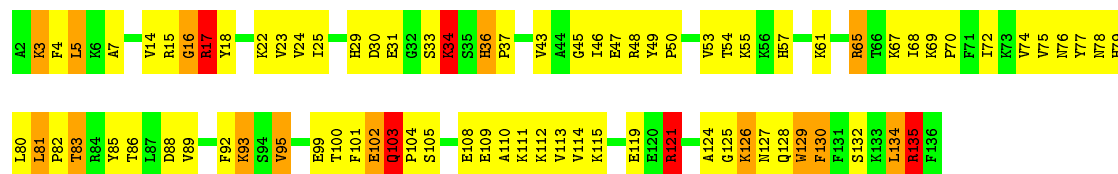
• Molecule 59: 60S RIBOSOMAL PROTEIN L26-A

Chain BY: 45% 44% 8%

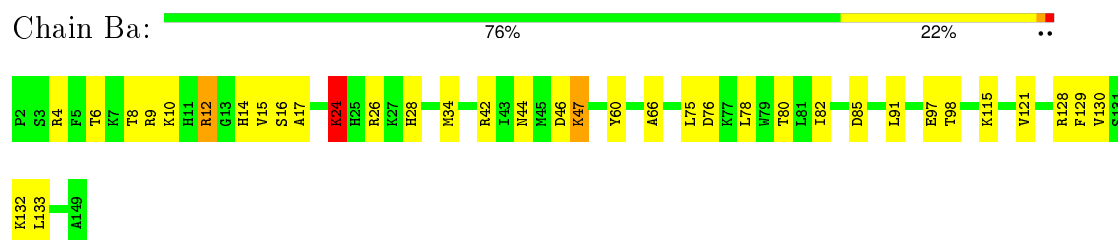


• Molecule 60: 60S RIBOSOMAL PROTEIN L27-A

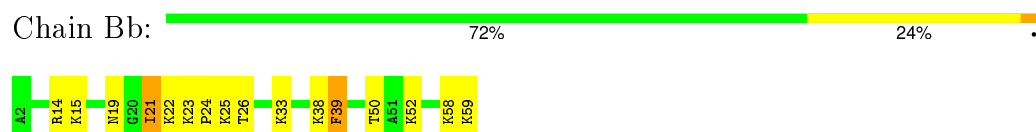
Chain BZ: 39% 47% 10%



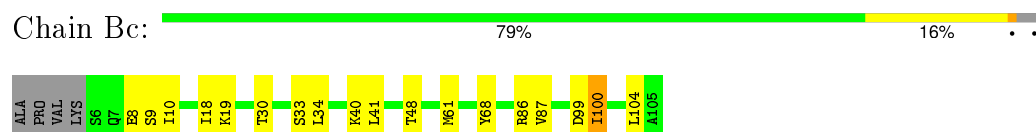
- Molecule 61: 60S RIBOSOMAL PROTEIN L28



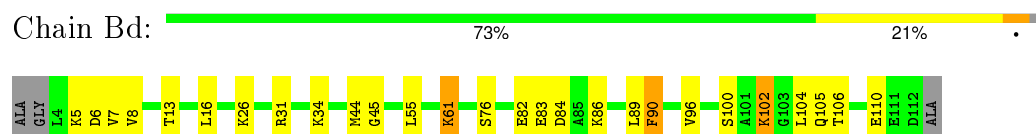
- Molecule 62: 60S RIBOSOMAL PROTEIN L29



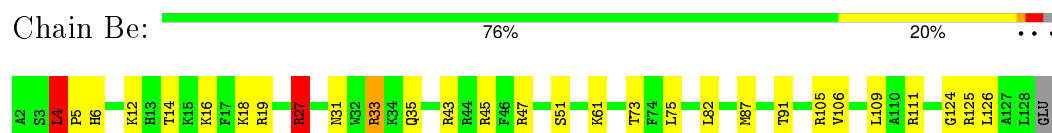
- Molecule 63: 60S RIBOSOMAL PROTEIN L30



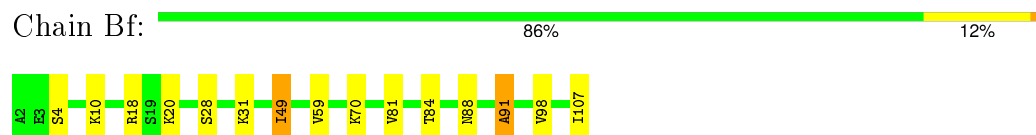
- Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



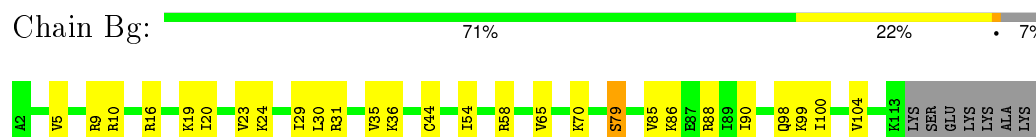
- Molecule 65: 60S RIBOSOMAL PROTEIN L32



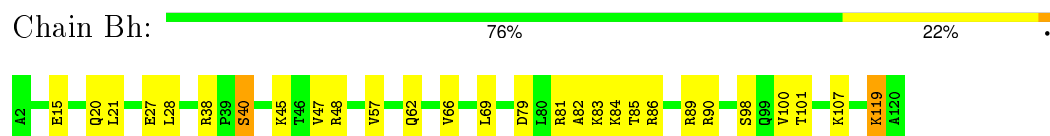
- Molecule 66: 60S RIBOSOMAL PROTEIN L33-A



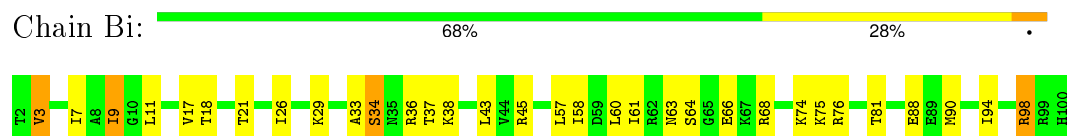
- Molecule 67: 60S RIBOSOMAL PROTEIN L34-A



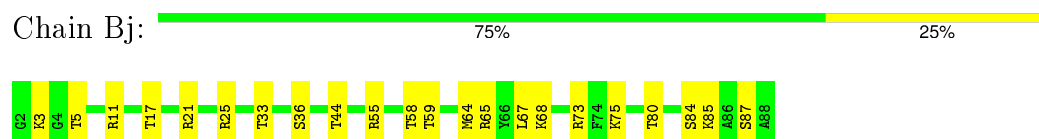
- Molecule 68: 60S RIBOSOMAL PROTEIN L35-B



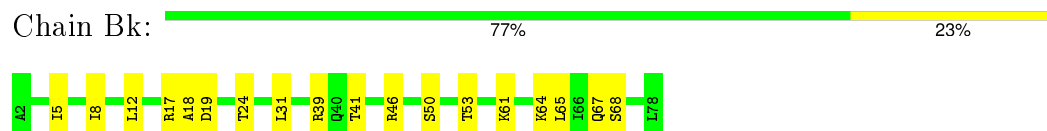
- Molecule 69: 60S RIBOSOMAL PROTEIN L36-A



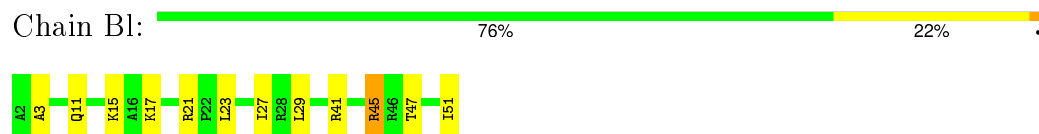
- Molecule 70: 60S RIBOSOMAL PROTEIN L37-A



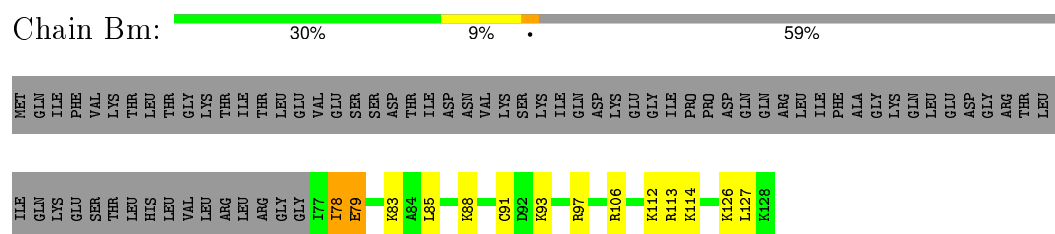
- Molecule 71: 60S RIBOSOMAL PROTEIN L38



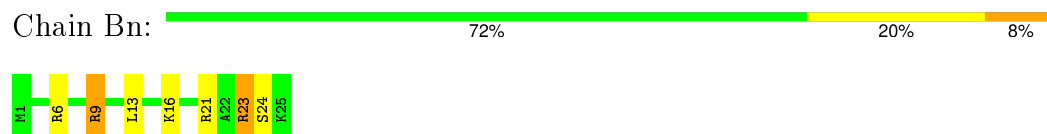
- Molecule 72: 60S RIBOSOMAL PROTEIN L39




- Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

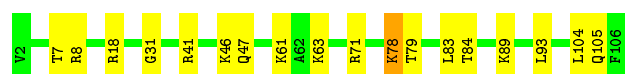


- Molecule 74: 60S RIBOSOMAL PROTEIN L41-B

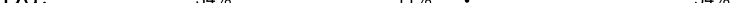


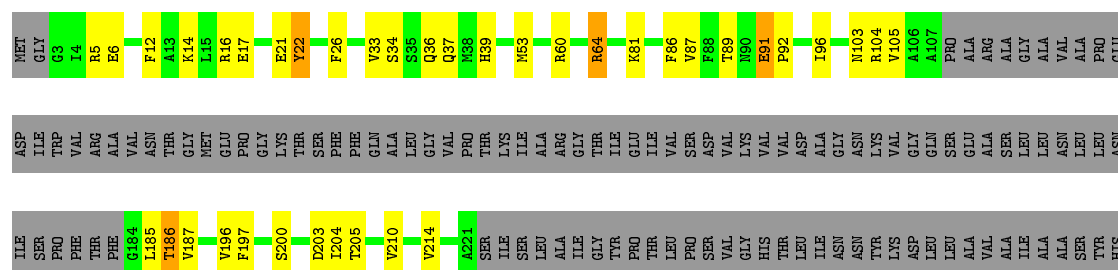
- Molecule 75: 60S RIBOSOMAL PROTEIN L42-A

Chain Bo:  83% 16%



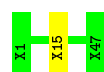
- Molecule 76: 60S ACIDIC RIBOSOMAL PROTEIN P0

Chain Bq:  34% 11% 54%



- Molecule 77: 60S ACIDIC RIBOSOMAL PROTEIN P1

Chain Br: 98%




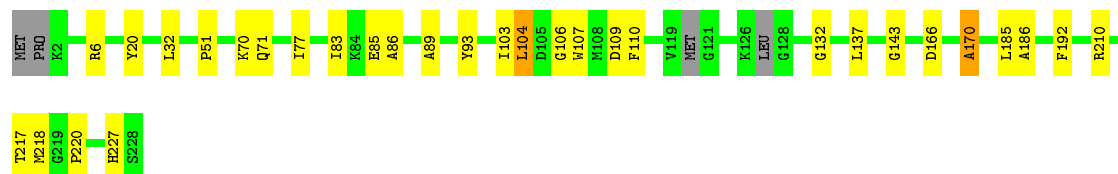
- Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2

Chain Bs: 100%

There are no outlier residues recorded for this chain.

- Molecule 79: 50S RIBOSOMAL PROTEIN L1

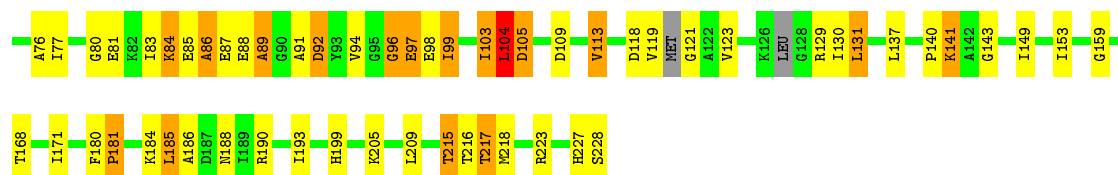
Chain By: 



- Molecule 79: 50S RIBOSOMAL PROTEIN L1

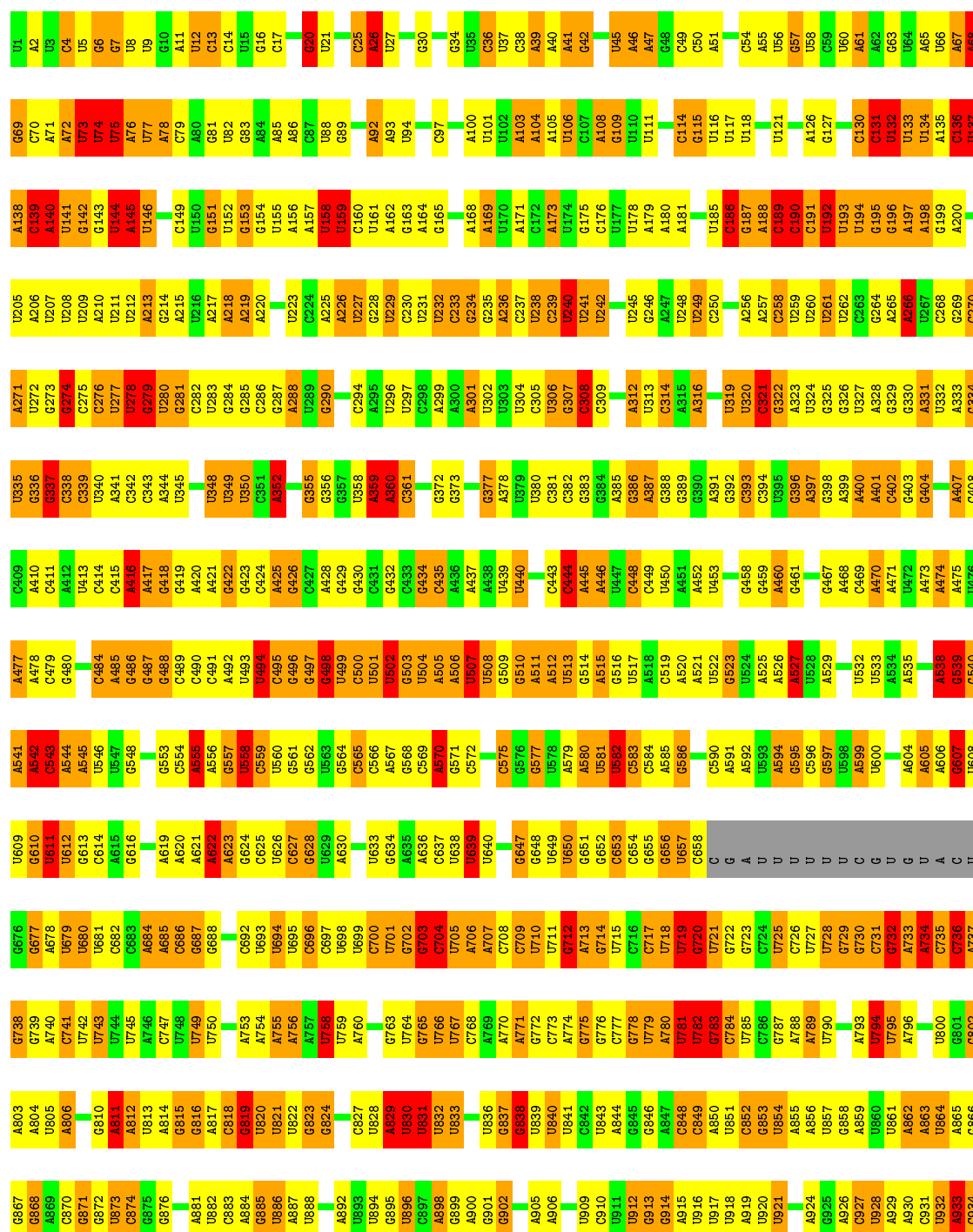
Chain CL: 57% 31% 10%

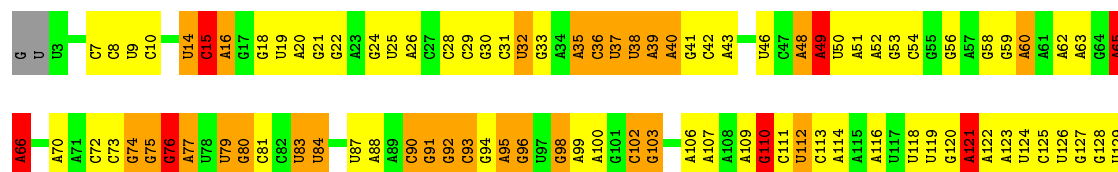




• Molecule 80: 18S RIBOSOMAL RNA

Chain B2: 26% 40% 26% 7%



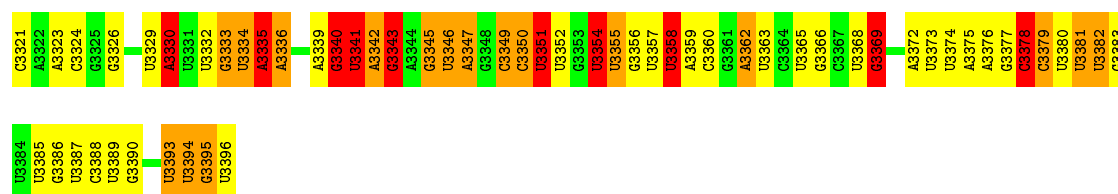


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A1182	U133	A201	U270	C340	G400	C	A522	A589	A653	G721	U796	C861	C923	U985	C1049	U1122	U1182
C1183	U134	C205	G272	G341	U401	U	A523	G590	A654	G722	U797	C862	G924	U986	U1050	U1123	U1183
A1184	C135		C271	A342	A402	C	U524	G591	C655		G798	C863	A925	U987		U1124	U1184
	G136			U343	C403	C	C525	A592	A656	G725	G799	C864	A926	U990	A1054	U1125	C1187
	G137	C208	U275	A344	G404	U	C526	G593	A657	G726	G800	U865	C927	U991	A1055	U1126	U1185
	G138	A209	U276	G345	U405	U	A527	U594	G658	G727	G801	A866	C928	U992	U1056	U1127	U1186
	U139	U210	U277	C346	G406	G	U528	G595	G659	G728	C802	A867	A929	U993	U1057	U1128	C1189
	G139	A211	U278	G347	U407	U	A529	C599	A660	G729	C803	C868	U930	U994		U1129	A1190
	C140	G212	U279	A348	A408	G	G530	G600	G661	U730	G804	U871	C931	G995	U1060	A1130	C1191
	C141	A213	U280	A349	U409	G	G531	U601	U662	G731	G805	U872	U932	U996	A1061	A1131	C1192
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	U147	U217	A284	G353	U413	G	U536		A666	A735	G809	A875	A936	G1000	A1065	C1196	C1196
	G148	C225	G285	U354	U414	G	A537	A607	C667	U736	A810	A876	G937	G1001		A1135	C1197
	U149	A219	U286	A355	G415	G	G538	A608	G668	G737	U811	C877	C938	G1002	U1070	U1136	C1198
	C150	G220	G287	C356	G416	G	G540	G609	U669		G812	G878	U939	G1003	U1071	U1137	C1199
	A151	A221	C288	A357	U417	A	U541	G610	U670	U741	G813	U879	G940	A1004	U1072	U1138	A1200
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	U153	C224	A289	U359	U419	U	G543	A612	U672	G743	U815	C881	U942		U1077	U1141	A1202
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	C156	C227	U292	A361	G420	U	U545	G614	U674	G745	A817	A883	C944	U1008	U1079	A1143	A1204
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	U167	A238	A306	U370	U431	A	A554	U623	U683	A755	A828	C893	U954	G1017	G1087	G1152	G1213
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	G173	G245	A313	G376	A436	C496	G560	U629	A692	C765	G834	U899	U960	C1023	G1097	A1158	A1221
	C175	U246	U314	A377	G437	C497	C561	A630	A693	U766	U835	G900	C961	G1024	A1098	A1159	G
		C247	U316	C379	A438	U498	C562	U631	C694	U767	G836	G901	A962	A1025	A1099	C1160	A
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			A317	U380	U440	C500	G564	C633	C696	G769	G838	U903	G964	A1027	G1101	U1162	A1225
	U178	U248	A318	U381	U441	A501		C634			C839	A904	A965	U1028	A1102	A1163	G1226
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	U187	G258	U329	G390	G	G511	G579	U643	A709	A784	A848	A913	G974		A1112	U1172	U1235
	G188	C259	U391	A391	U	G514	C580	G644	A710	G785		A914	C975	A1040	G1113	G1173	G1236
	U189	G260	U392	A392	G	U515	U581	A645	A711	A786	C851	A915	U976	U1041	U1114	G1174	C1237
	U190	U261	G333	U393	C	C516	G582	A646	G712	G787	U852	G916	U977	U1042	G1115	C1175	C1238
	C192	U262	A334	G394	C	A516	G583	A647		C788		A917	U978	C1043	U1116	C1176	C1239
		A266	G335	A395	C	G517	G584	C648	A713		G856	G918	U979	U1044	G1117	G1177	A1240
	G197	A268	A336	A396	U	G518	A585	A649	A714	G792	G857	U919	U980	U1045	G1118	U1178	U1241
			G337	A397	C	A519	C586	G650	A715	U793	C858	U920	U981	A1046	C1119	A1179	G1242
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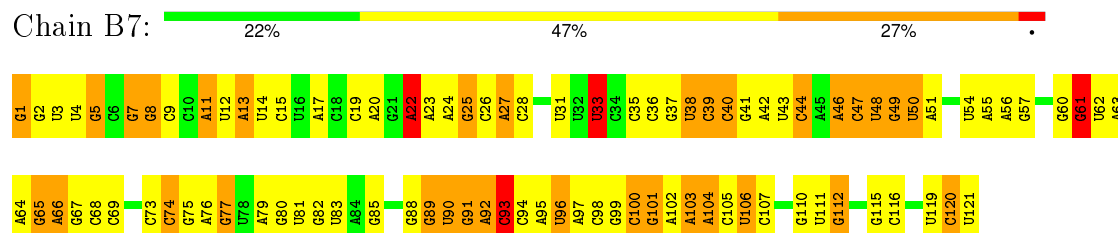

WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM

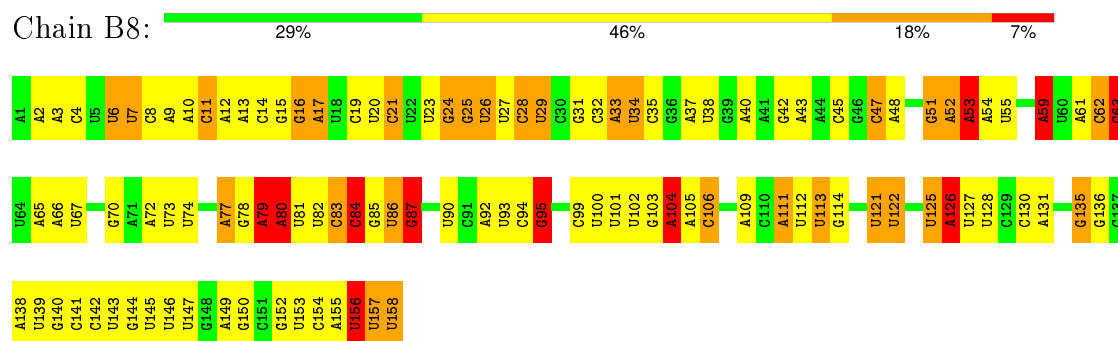
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U3282	U3214	U3152	A3086	G2953	U2891	A2694	U2757	A2695	U2633	A2562	U	A2441	G2381	U2319	U2319
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G3284	G3216	C3154	G3088	U2955	C2893	G2830	A2762	A2696	A2635	U2565	G	A2443	C2383	A2321	A2321
C3285	C3217	U3155	C3089	U2956	G2894	C2831	U2763	G2697	A2636	C2566	U	C2444	A2384	C2322	C2322
A3286	A3218	U3156	U3090	C2957	G2895	G2832	C2764	G2698	A2637	U2567	A	U2445	G2385	G2323	G2323
U3287	G3219	U3157	A3091	A2958	A2896	A2833	C2765	C2699	C2638	C2568	U	U2446	A2386	A2324	A2324
G3288	C3158	G3158	C3092	C2959	A2897	G2834	C2766	G2700	G2639	C2569	A	U2447	G2387	G2325	G2325
G3289	C3159	C3159	C3093	C2960	C2898	U2835	U2767	U2701	A2640	U2570	G	U2448	U2388	A2326	A2326
G3290	A3223	U3160	A3094	C2961	C2899	C2836	U2768	A2702	U2641	U2571	A	U2449	U2389	U2327	U2327
G3291	G3224	C3161	U3095	G3028	A2900	A2837	U2769	A2703	A2642	C2572	G	U2450	U2390	U2328	U2328
A3292	C3225	C3162	C3096	A3029	G2901	A2838	A2770	A2704	C2573	A2511	G	U2451	G2391	C2329	C2329
U3293	A3226	A3163	C3097	G2965	G2902	G2839	G2771	A2705	G2644	G2574	G	U2452	C2392	G2330	G2330
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A3308	G3245	G3178	G3112	A3046	U2916	C2852	C2792	U2718	G2657	A2596	G	U2465	C2405	A2345	A2345
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A3310	G3247	A3180	A3114	A3048	G2918	U2854	G2794	A2721	G2659	U2597	G	U2467	C2407	U2347	U2347
U3311	C3248	C3181	G3115	A3049	A2919	U2855	U2795	U2722	G2660	G2598	A	U2468	U2408	A2348	A2348
A3313	G3249	U3182	C3116	C2984	U2920	G2856	U2796	U2723	G2661	U2599	G	U2469	U2409	U2349	U2349
U3314	U3250	A3183	C3120	C2985	U2921	U2857	C2797	U2724	G2662	C2600	U	U2470	C2350	C2350	C2350
G3315	U3251	A3184	G3052	U2986	G2922	U2858	C2798	U2725	C2663	C2601	C	U2471	U2351	U2351	U2351
A3316	G3252	U3185	G3053	A2987	C2923	U2859	C2799	U2726	G2664	U2602	U	U2472	G2412	A2352	A2352
U3317	G3253	A3186	A3122	C2988	U2923	U2860	A2800	A2727	U2665	G2603	C	U2473	A2353	G2353	G2353
G3318	G3254	G3124	A3123	U2989	A2926	U2861	G2801	G2728	C2666	G2604	C	U2474	G2413	A2354	A2354
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A3320	G3256	G3189	C3126	U2992	C2928	U2866	A2802	G2730	U2668	G2606	U	U2476	U2415	A2356	A2356
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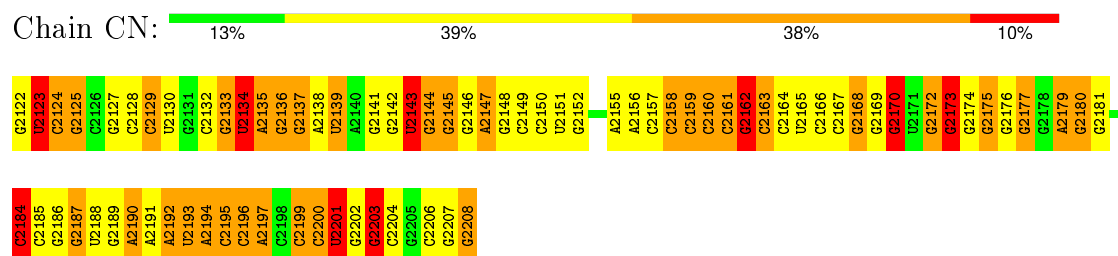
- Molecule 82: 5S RIBOSOMAL RNA



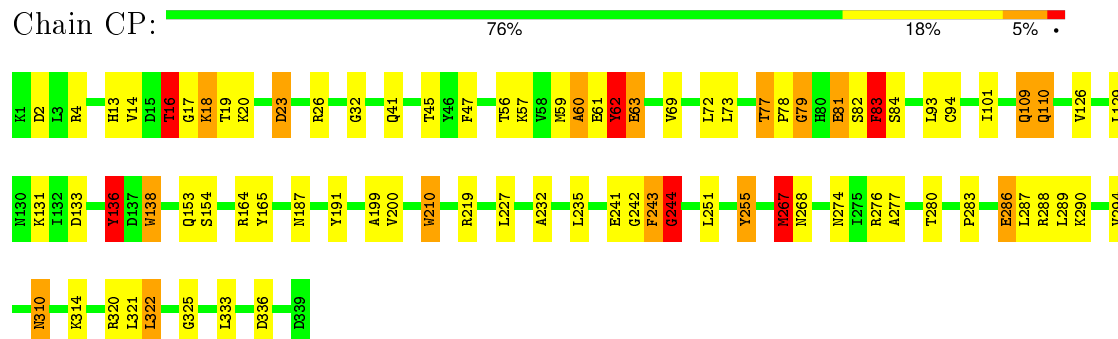
- Molecule 83: 5.8S RIBOSOMAL RNA



- Molecule 84: EUKARYOTIC RIBOSOMAL L1_RRNA

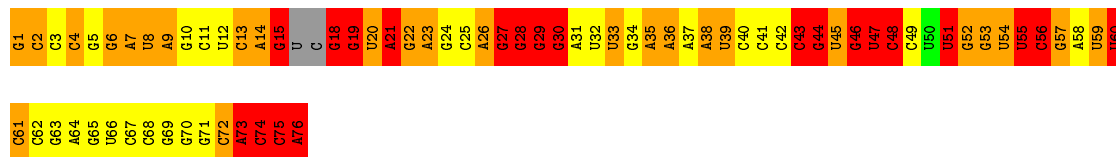


- Molecule 85: EUKARYOTIC TRANSLATION INITIATION FACTOR 5B



- Molecule 86: EUKARYOTIC RIBOSOMAL P_E TRNA

Chain CW:  34% 34% 28% .



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON (BACKTHINNED)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, OHX, MG, HSO

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A0	0.54	0/782	0.77	0/1047
10	AB	0.45	0/1735	0.81	0/2335
11	AC	0.60	0/1665	0.77	0/2263
12	AD	0.59	0/1759	0.74	0/2368
13	AE	0.57	0/2109	0.86	1/2839 (0.0%)
14	AF	0.49	0/1629	0.72	0/2202
15	AG	0.55	0/1823	0.75	0/2439
16	AH	0.52	0/1506	0.77	0/2028
17	AI	0.68	0/1514	0.89	3/2021 (0.1%)
18	AJ	0.59	0/1519	0.81	0/2035
19	AK	0.55	0/789	0.83	3/1067 (0.3%)
2	A1	0.53	0/620	0.81	1/838 (0.1%)
20	AL	0.70	0/1239	0.81	0/1673
21	AM	0.49	0/898	0.76	0/1220
22	AN	0.61	0/1215	0.83	3/1638 (0.2%)
23	AO	0.48	0/901	0.82	1/1217 (0.1%)
24	AP	0.60	0/998	0.86	3/1341 (0.2%)
25	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
26	AR	0.54	0/935	0.81	0/1254
27	AS	0.59	0/1211	0.80	0/1628
28	AT	0.57	0/1130	0.81	0/1517
29	AU	0.55	0/865	0.76	0/1169
3	A2	0.43	0/499	0.72	0/670
30	AV	0.52	0/693	0.75	0/935
31	AW	0.65	0/1038	0.86	3/1395 (0.2%)
32	AX	0.72	0/1139	0.91	2/1518 (0.1%)
33	AY	0.56	0/1087	0.77	1/1449 (0.1%)
34	AZ	0.50	0/571	0.85	1/768 (0.1%)
35	BA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
36	BB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
37	BC	0.87	0/2800	1.07	11/3790 (0.3%)
38	BD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
4	A3	0.70	0/452	0.94	1/600 (0.2%)
40	BF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
41	BG	0.64	0/1795	0.81	1/2429 (0.0%)
42	BH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
43	BI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
44	BJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
46	BL	0.82	0/1573	1.04	6/2113 (0.3%)
47	BM	0.96	0/1074	1.01	4/1446 (0.3%)
48	BN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
49	BO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
5	A4	0.50	0/483	0.71	0/643
50	BP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
51	BQ	0.89	1/1465 (0.1%)	1.12	9/1965 (0.5%)
52	BR	0.78	1/1538 (0.1%)	0.87	2/2050 (0.1%)
53	BS	1.02	0/1481	1.09	7/1990 (0.4%)
54	BT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
55	BU	0.56	0/794	0.77	0/1076
56	BV	0.98	0/1018	1.09	4/1369 (0.3%)
57	BW	0.80	0/1052	0.90	2/1398 (0.1%)
58	BX	0.72	0/974	0.86	0/1314
59	BY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
6	A5	0.53	0/404	0.99	1/542 (0.2%)
60	BZ	0.55	0/1118	0.83	2/1497 (0.1%)
61	Ba	0.95	2/1204 (0.2%)	1.14	9/1612 (0.6%)
62	Bb	0.91	0/473	1.14	1/629 (0.2%)
63	Bc	0.61	0/775	0.77	0/1040
64	Bd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
65	Be	1.03	0/1041	1.27	12/1394 (0.9%)
66	Bf	1.12	0/868	1.09	3/1168 (0.3%)
67	Bg	0.72	0/890	0.92	0/1189
68	Bh	0.67	0/974	0.80	0/1297
69	Bi	0.67	0/777	0.85	0/1033
7	A6	0.49	0/2490	0.70	0/3389
70	Bj	0.87	0/696	1.04	3/923 (0.3%)
71	Bk	0.50	0/614	0.70	0/822
72	Bl	0.90	0/443	1.02	1/588 (0.2%)
73	Bm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
74	Bn	0.90	0/234	1.15	1/300 (0.3%)
75	Bo	0.83	0/860	0.89	1/1136 (0.1%)
76	Bq	1.07	0/1092	1.31	4/1474 (0.3%)
79	By	0.98	0/1749	1.24	8/2355 (0.3%)
79	CL	0.80	2/1749 (0.1%)	1.02	4/2355 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
8	A7	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
80	B2	0.92	33/42128 (0.1%)	1.49	828/65642 (1.3%)
81	B5	1.49	661/75336 (0.9%)	1.92	3722/117449 (3.2%)
82	B7	1.38	12/2883 (0.4%)	1.80	119/4491 (2.6%)
83	B8	1.16	4/3746 (0.1%)	1.70	128/5832 (2.2%)
84	CN	0.76	7/2097 (0.3%)	1.20	23/3273 (0.7%)
85	CP	2.24	8/2623 (0.3%)	1.38	24/3532 (0.7%)
86	CW	1.86	27/1761 (1.5%)	2.72	212/2743 (7.7%)
9	AA	0.54	0/1617	0.80	0/2215
All	All	1.13	792/226118 (0.4%)	1.51	5267/331349 (1.6%)

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
10	AB	0	1
16	AH	0	1
2	A1	0	1
20	AL	0	1
23	AO	0	1
26	AR	0	2
34	AZ	0	3
35	BA	0	2
37	BC	0	1
38	BD	0	1
39	BE	0	1
40	BF	0	2
49	BO	0	2
53	BS	0	1
56	BV	0	1
59	BY	0	1
6	A5	0	2
60	BZ	0	1
61	Ba	0	3
62	Bb	0	1
76	Bq	0	7
77	Br	0	1
79	By	0	4
79	CL	0	3
8	A7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	B5	0	35
85	CP	0	8
86	CW	0	19
All	All	0	107

The worst 5 of 792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CP	63	GLU	N-CA	69.03	2.84	1.46
85	CP	210	TRP	CD2-CE3	34.76	1.92	1.40
85	CP	210	TRP	CD2-CE2	33.01	1.80	1.41
85	CP	210	TRP	CE2-CZ2	31.95	1.94	1.39
85	CP	210	TRP	CE3-CZ3	26.33	1.83	1.38

The worst 5 of 5267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B5	1152	G	N3-C4-C5	33.59	145.40	128.60
81	B5	1256	G	P-O3'-C3'	32.78	159.04	119.70
81	B5	1152	G	N3-C4-N9	-31.65	107.01	126.00
81	B5	1152	G	N3-C2-N2	-26.89	101.08	119.90
81	B5	1152	G	C2-N3-C4	-23.94	99.93	111.90

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	42	ASN	Peptide
6	A5	105	TYR	Peptide
6	A5	138	ARG	Peptide
8	A7	134	ASP	Sidechain
10	AB	131	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	769	0	814	117	0
2	A1	610	0	630	53	0
3	A2	497	0	535	32	0
4	A3	442	0	428	57	0
5	A4	475	0	525	21	0
6	A5	516	0	517	41	0
7	A6	2437	0	2386	84	0
8	A7	1105	0	959	200	0
9	AA	1577	0	1567	101	0
10	AB	1709	0	1784	197	0
11	AC	1635	0	1723	80	0
12	AD	1734	0	1817	121	0
13	AE	2068	0	2154	95	0
14	AF	1609	0	1675	114	0
15	AG	1799	0	1874	441	0
16	AH	1481	0	1572	83	0
17	AI	1489	0	1523	192	0
18	AJ	1494	0	1573	96	0
19	AK	772	0	727	45	0
20	AL	1213	0	1257	107	0
21	AM	890	0	887	48	0
22	AN	1192	0	1252	62	0
23	AO	891	0	880	295	0
24	AP	977	0	1002	71	0
25	AQ	1105	0	1166	139	0
26	AR	926	0	930	134	0
27	AS	1192	0	1220	112	0
28	AT	1112	0	1123	107	0
29	AU	855	0	917	117	0
30	AV	684	0	672	42	0
31	AW	1021	0	1060	70	0
32	AX	1121	0	1196	73	0
33	AY	1073	0	1132	113	0
34	AZ	563	0	602	52	0
35	BA	1912	0	1973	290	0
36	BB	3075	0	3142	147	0
37	BC	2748	0	2859	139	0
38	BD	2359	0	2311	266	0
39	BE	1248	0	1339	38	0
40	BF	1791	0	1869	56	0
41	BG	1763	0	1819	154	0
42	BH	1518	0	1587	82	0
43	BI	1722	0	1755	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BJ	1353	0	1380	116	0
45	BK	751	756	195	2	0
46	BL	1548	0	1613	90	0
47	BM	1059	0	1154	51	0
48	BN	1720	0	1779	136	0
49	BO	3119	0	3302	97	0
50	BP	1227	0	1236	41	0
51	BQ	1441	0	1543	68	0
52	BR	1521	0	1605	197	0
53	BS	1445	0	1487	63	0
54	BT	1276	0	1323	137	0
55	BU	778	0	791	23	0
56	BV	1003	0	1048	49	0
57	BW	1038	0	1071	43	0
58	BX	959	0	1023	37	0
59	BY	993	0	1081	155	0
60	BZ	1092	0	1154	111	0
61	Ba	1173	0	1215	0	0
62	Bb	462	0	491	0	0
63	Bc	767	0	816	0	0
64	Bd	883	0	918	0	0
65	Be	1020	0	1090	0	0
66	Bf	850	0	880	0	0
67	Bg	880	0	944	0	0
68	Bh	965	0	1067	0	0
69	Bi	770	0	846	0	0
70	Bj	681	0	683	0	0
71	Bk	608	0	671	0	0
72	Bl	436	0	475	0	0
73	Bm	417	0	455	0	0
74	Bn	233	0	271	0	0
75	Bo	847	0	916	0	0
76	Bq	1077	1110	1041	0	0
77	Br	236	237	65	0	0
78	Bs	231	232	67	0	0
79	By	1719	1773	1619	0	0
79	CL	1719	0	1649	135	0
80	B2	37835	0	19048	2999	0
81	B5	67308	664	33793	2340	0
82	B7	2579	0	1303	188	0
83	B8	3353	0	1695	115	0
84	CN	1875	0	926	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	CP	2655	2725	2710	242	0
86	CW	1576	803	797	72	0
87	A0	1	0	0	0	0
87	A1	1	0	0	0	0
87	A3	1	0	0	0	0
87	A5	1	0	0	0	0
87	Bj	1	0	0	0	0
87	Bm	1	0	0	0	0
88	A0	2	0	0	0	0
88	A3	3	0	0	0	0
88	A5	1	0	0	0	0
88	AB	1	0	0	0	0
88	AC	2	0	0	0	0
88	AE	1	0	0	0	0
88	AG	1	0	0	0	0
88	AI	1	0	0	0	0
88	AJ	1	0	0	0	0
88	AL	2	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0
88	AS	1	0	0	0	0
88	AU	1	0	0	0	0
88	B2	169	0	0	0	0
88	B5	3	0	0	0	0
89	A3	7	0	0	4	0
89	A6	7	0	0	2	0
89	AC	7	0	0	5	0
89	AI	14	0	0	2	0
89	AL	7	0	0	8	0
89	AN	7	0	0	2	0
89	AP	7	0	0	3	0
89	B2	1288	0	0	232	0
89	B5	21	0	0	4	0
89	BR	7	0	0	9	0
89	Bn	7	0	0	0	0
90	CP	32	0	7	63	0
All	All	214255	8300	157976	8607	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 35.

The worst 5 of 8607 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)
15:AG:175:ILE:HG12	80:B2:78:A:C4	1.29	1.65
85:CP:210:TRP:CH2	85:CP:210:TRP:CZ3	1.78	1.63
81:B5:2443:A:C6	84:CN:2208:G:H5'	1.32	1.61
85:CP:210:TRP:CZ3	85:CP:210:TRP:CE3	1.83	1.61
85:CP:210:TRP:CH2	85:CP:210:TRP:CZ2	1.82	1.59

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	3
2	A1	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	2	31
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	18
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	4	37
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	5	42
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	1
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	36
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	16
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	8
10	AB	212/255 (83%)	132 (62%)	42 (20%)	38 (18%)	0	3
11	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	2	29
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	2	26
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	19
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	1	16
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	3	32
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	18
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	25
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	11
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	2	28
21	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
22	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	2	30
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	9
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	8
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	19
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	1	12
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	1	14
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	17
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	3	32
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	9
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	7	49
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	8
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	1	14
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	5
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	6	46
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	8	50
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	2	28
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	9	52
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	7	47
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	11	55
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	1	16
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	9	52
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	2	28
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	20
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	2	28
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	26	71
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	6	46
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	15	60
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	5	43
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	12	57
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	30	74
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	15	60
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	5	44
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	13	58
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	2	27
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	24
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	4	37
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	1	14
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	5	42
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	17
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	5	44
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	2	29
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	3	32
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	6	45
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	4	40
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	5	42
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	23
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	7	49
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	2	30
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	9	52
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	53
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	3	35
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	10	54
76	Bq	139/312 (45%)	104 (75%)	14 (10%)	21 (15%)	0	5
79	By	219/229 (96%)	178 (81%)	24 (11%)	17 (8%)	1	20
79	CL	219/229 (96%)	165 (75%)	35 (16%)	19 (9%)	1	17
85	CP	331/339 (98%)	276 (83%)	32 (10%)	23 (7%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12051/13155 (92%)	10001 (83%)	1275 (11%)	775 (6%)	3	26

5 of 775 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	LYS
1	A0	45	VAL
1	A0	46	GLU
1	A0	62	TYR
1	A0	65	PRO

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	
1	A0	83/101 (82%)	65 (78%)	18 (22%)	1	10
2	A1	70/71 (99%)	62 (89%)	8 (11%)	7	36
3	A2	56/60 (93%)	38 (68%)	18 (32%)	0	3
4	A3	47/49 (96%)	38 (81%)	9 (19%)	2	14
5	A4	51/54 (94%)	43 (84%)	8 (16%)	3	23
6	A5	43/116 (37%)	32 (74%)	11 (26%)	0	6
7	A6	259/262 (99%)	221 (85%)	38 (15%)	4	26
8	A7	97/195 (50%)	74 (76%)	23 (24%)	1	8
9	AA	164/210 (78%)	122 (74%)	42 (26%)	0	6
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0	4
11	AC	176/205 (86%)	130 (74%)	46 (26%)	0	6
12	AD	182/195 (93%)	138 (76%)	44 (24%)	1	7
13	AE	221/222 (100%)	166 (75%)	55 (25%)	1	7
14	AF	173/191 (91%)	137 (79%)	36 (21%)	1	11
15	AG	188/201 (94%)	149 (79%)	39 (21%)	1	11
16	AH	165/170 (97%)	124 (75%)	41 (25%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AI	150/161 (93%)	118 (79%)	32 (21%)	1	11
18	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	6
19	AK	77/98 (79%)	58 (75%)	19 (25%)	1	7
20	AL	129/137 (94%)	105 (81%)	24 (19%)	2	15
21	AM	88/119 (74%)	55 (62%)	33 (38%)	0	1
22	AN	127/128 (99%)	91 (72%)	36 (28%)	0	4
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	4
24	AP	101/118 (86%)	82 (81%)	19 (19%)	2	15
25	AQ	117/119 (98%)	83 (71%)	34 (29%)	0	4
26	AR	94/124 (76%)	70 (74%)	24 (26%)	1	6
27	AS	128/129 (99%)	87 (68%)	41 (32%)	0	3
28	AT	115/116 (99%)	84 (73%)	31 (27%)	0	5
29	AU	100/114 (88%)	71 (71%)	29 (29%)	0	4
30	AV	74/74 (100%)	56 (76%)	18 (24%)	1	7
31	AW	110/111 (99%)	84 (76%)	26 (24%)	1	8
32	AX	119/120 (99%)	97 (82%)	22 (18%)	2	15
33	AY	112/113 (99%)	84 (75%)	28 (25%)	1	7
34	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	4
35	BA	192/195 (98%)	153 (80%)	39 (20%)	1	12
36	BB	321/322 (100%)	251 (78%)	70 (22%)	1	10
37	BC	288/288 (100%)	223 (77%)	65 (23%)	1	9
38	BD	243/244 (100%)	196 (81%)	47 (19%)	2	14
39	BE	135/152 (89%)	115 (85%)	20 (15%)	4	26
40	BF	187/204 (92%)	158 (84%)	29 (16%)	3	24
41	BG	177/207 (86%)	138 (78%)	39 (22%)	1	10
42	BH	171/171 (100%)	132 (77%)	39 (23%)	1	9
43	BI	179/186 (96%)	142 (79%)	37 (21%)	1	11
44	BJ	147/149 (99%)	114 (78%)	33 (22%)	1	10
46	BL	154/158 (98%)	124 (80%)	30 (20%)	2	14
47	BM	108/108 (100%)	84 (78%)	24 (22%)	1	10
48	BN	175/175 (100%)	143 (82%)	32 (18%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BO	323/178 (182%)	267 (83%)	56 (17%)	2	18
50	BP	125/145 (86%)	103 (82%)	22 (18%)	2	18
51	BQ	150/150 (100%)	123 (82%)	27 (18%)	2	17
52	BR	153/153 (100%)	121 (79%)	32 (21%)	1	11
53	BS	156/156 (100%)	123 (79%)	33 (21%)	1	11
54	BT	136/136 (100%)	109 (80%)	27 (20%)	1	13
55	BU	85/106 (80%)	62 (73%)	23 (27%)	0	5
56	BV	104/104 (100%)	96 (92%)	8 (8%)	16	55
57	BW	100/129 (78%)	85 (85%)	15 (15%)	3	25
58	BX	104/117 (89%)	81 (78%)	23 (22%)	1	10
59	BY	109/109 (100%)	85 (78%)	24 (22%)	1	10
60	BZ	115/115 (100%)	89 (77%)	26 (23%)	1	9
61	Ba	118/118 (100%)	95 (80%)	23 (20%)	2	14
62	Bb	46/46 (100%)	35 (76%)	11 (24%)	1	7
63	Bc	84/87 (97%)	68 (81%)	16 (19%)	2	14
64	Bd	94/96 (98%)	73 (78%)	21 (22%)	1	10
65	Be	109/110 (99%)	89 (82%)	20 (18%)	2	16
66	Bf	90/90 (100%)	79 (88%)	11 (12%)	6	33
67	Bg	95/102 (93%)	71 (75%)	24 (25%)	1	7
68	Bh	103/104 (99%)	77 (75%)	26 (25%)	1	7
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	53 (76%)	17 (24%)	1	7
71	Bk	67/68 (98%)	53 (79%)	14 (21%)	1	11
72	Bl	45/45 (100%)	34 (76%)	11 (24%)	1	7
73	Bm	47/116 (40%)	34 (72%)	13 (28%)	0	4
74	Bn	23/23 (100%)	16 (70%)	7 (30%)	0	3
75	Bo	90/90 (100%)	74 (82%)	16 (18%)	2	17
76	Bq	105/254 (41%)	94 (90%)	11 (10%)	8	39
79	By	177/181 (98%)	171 (97%)	6 (3%)	44	77
79	CL	177/181 (98%)	153 (86%)	24 (14%)	5	29
85	CP	290/290 (100%)	275 (95%)	15 (5%)	29	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10154/10976 (92%)	8030 (79%)	2124 (21%)	4 11

5 of 2124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	AY	96	LEU
38	BD	155	THR
69	Bi	9	ILE
35	BA	15	ILE
36	BB	284	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
35	BA	209	HIS
41	BG	59	GLN
79	CL	101	GLN
35	BA	215	ASN
37	BC	221	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
80	B2	1764/1800 (98%)	545 (30%)	86 (4%)
81	B5	3140/3396 (92%)	741 (23%)	131 (4%)
82	B7	120/121 (99%)	18 (15%)	0
83	B8	157/158 (99%)	32 (20%)	3 (1%)
84	CN	86/87 (98%)	41 (47%)	8 (9%)
86	CW	73/76 (96%)	26 (35%)	7 (9%)
All	All	5340/5638 (94%)	1403 (26%)	235 (4%)

5 of 1403 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
80	B2	2	A
80	B2	4	C
80	B2	8	U
80	B2	16	G
80	B2	20	G

5 of 235 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
81	B5	715	A
81	B5	1236	G
83	B8	111	A
81	B5	735	A
81	B5	993	G

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

6 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	$\# Z > 2$
85	HSO	CP	105	85	6,10,10	2.40	2 (33%)	4,12,12	1.78	1 (25%)
85	HSO	CP	13	85	6,10,10	2.21	1 (16%)	4,12,12	2.21	2 (50%)
85	HSO	CP	229	85	6,10,10	2.05	1 (16%)	4,12,12	2.43	2 (50%)
85	HSO	CP	295	85	6,10,10	2.16	1 (16%)	4,12,12	1.75	1 (25%)
85	HSO	CP	296	85	6,10,10	2.40	2 (33%)	4,12,12	2.05	2 (50%)
85	HSO	CP	80	85	6,10,10	2.49	2 (33%)	4,12,12	1.96	2 (50%)

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
85	HSO	CP	105	85	-	0/5/6/6	0/1/1/1
85	HSO	CP	13	85	-	0/5/6/6	0/1/1/1
85	HSO	CP	229	85	-	0/5/6/6	0/1/1/1
85	HSO	CP	295	85	-	0/5/6/6	0/1/1/1
85	HSO	CP	296	85	-	0/5/6/6	0/1/1/1
85	HSO	CP	80	85	-	0/5/6/6	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CP	296	HSO	O-C	-4.53	1.22	1.42
85	CP	295	HSO	O-C	-4.51	1.22	1.42
85	CP	13	HSO	O-C	-4.47	1.23	1.42
85	CP	80	HSO	O-C	-4.47	1.23	1.42
85	CP	105	HSO	O-C	-4.46	1.23	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CP	229	HSO	CG-CB-CA	-2.87	107.48	114.06
85	CP	296	HSO	CG-CB-CA	-2.08	109.28	114.06
85	CP	80	HSO	CG-CB-CA	2.29	119.30	114.06
85	CP	13	HSO	CG-CB-CA	2.40	119.55	114.06
85	CP	80	HSO	O-C-CA	2.81	119.21	111.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	CP	13	HSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 395 ligands modelled in this entry, 197 are monoatomic - leaving 198 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
89	OHX	A3	102	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	A6	401	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AC	301	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AI	301	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AI	302	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AL	201	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AN	201	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	AP	201	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1906	88	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1909	89	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1918	89	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1935	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1978	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2031	89	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2050	88	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2064	88,89	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2071	80	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B5	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B5	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	B5	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	BR	201	-	0,6,6	0.00	-	0,15,15	0.00	-
89	OHX	Bn	101	-	0,6,6	0.00	-	0,15,15	0.00	-
90	GCP	CP	401	-	29,34,34	6.14	8 (27%)	32,54,54	2.86	10 (31%)

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
89	OHX	A3	102	-	-	0/0/0/0	0/0/0/0
89	OHX	A6	401	-	-	0/0/0/0	0/0/0/0
89	OHX	AC	301	-	-	0/0/0/0	0/0/0/0
89	OHX	AI	301	-	-	0/0/0/0	0/0/0/0
89	OHX	AI	302	-	-	0/0/0/0	0/0/0/0
89	OHX	AL	201	-	-	0/0/0/0	0/0/0/0
89	OHX	AN	201	-	-	0/0/0/0	0/0/0/0
89	OHX	AP	201	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1901	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	OHX	B2	1902	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1903	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1904	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1905	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1906	88	-	0/0/0/0	0/0/0/0
89	OHX	B2	1907	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1908	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1909	89	-	0/0/0/0	0/0/0/0
89	OHX	B2	1910	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1911	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1912	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1913	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1914	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1915	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1916	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1917	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1918	89	-	0/0/0/0	0/0/0/0
89	OHX	B2	1919	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1920	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1921	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1922	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1923	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1924	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1925	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1926	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1927	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1928	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1929	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1930	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1931	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1932	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1933	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1934	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1935	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1936	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1937	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1938	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1939	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1940	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1941	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1942	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1943	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	OHX	B2	1944	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1945	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1946	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1947	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1948	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1949	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1950	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1951	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1952	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1953	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1954	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1955	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1956	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1957	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1958	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1959	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1960	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1961	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1962	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1963	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1964	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1965	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1966	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1967	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1968	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1969	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1970	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1971	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1972	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1973	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1974	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1975	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1976	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1977	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1978	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1979	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1980	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1981	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1982	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1983	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1984	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1985	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	OHX	B2	1986	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1987	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1988	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1989	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1990	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1991	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1992	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1993	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1994	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1995	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1996	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1997	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1998	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	1999	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2000	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2001	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2002	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2003	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2004	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2005	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2006	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2007	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2008	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2009	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2010	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2011	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2012	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2013	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2014	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2015	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2016	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2017	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2018	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2019	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2020	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2021	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2022	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2023	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2024	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2025	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2026	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2027	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	OHX	B2	2028	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2029	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2030	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2031	89	-	0/0/0/0	0/0/0/0
89	OHX	B2	2032	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2033	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2034	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2035	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2036	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2037	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2038	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2039	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2040	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2041	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2042	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2043	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2044	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2045	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2046	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2047	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2048	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2049	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2050	88	-	0/0/0/0	0/0/0/0
89	OHX	B2	2051	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2052	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2053	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2054	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2055	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2056	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2057	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2058	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2059	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2060	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2061	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2062	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2063	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2064	88,89	-	0/0/0/0	0/0/0/0
89	OHX	B2	2065	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2066	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2067	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2068	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2069	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	OHX	B2	2070	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2071	80	-	0/0/0/0	0/0/0/0
89	OHX	B2	2072	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2073	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2074	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2075	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2076	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2077	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2078	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2079	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2080	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2081	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2082	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2083	-	-	0/0/0/0	0/0/0/0
89	OHX	B2	2084	-	-	0/0/0/0	0/0/0/0
89	OHX	B5	3401	-	-	0/0/0/0	0/0/0/0
89	OHX	B5	3402	-	-	0/0/0/0	0/0/0/0
89	OHX	B5	3403	-	-	0/0/0/0	0/0/0/0
89	OHX	BR	201	-	-	0/0/0/0	0/0/0/0
89	OHX	Bn	101	-	-	0/0/0/0	0/0/0/0
90	GCP	CP	401	-	-	0/15/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	CP	401	GCP	PB-C3B	-22.47	1.56	1.80
90	CP	401	GCP	PG-C3B	-21.79	1.57	1.80
90	CP	401	GCP	C2'-C1'	-6.11	1.43	1.53
90	CP	401	GCP	PB-O3A	-2.27	1.55	1.58
90	CP	401	GCP	C8-N7	-2.16	1.30	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	CP	401	GCP	C5-C6-N1	-7.44	113.79	123.52
90	CP	401	GCP	O3G-PG-C3B	-7.42	88.55	106.13
90	CP	401	GCP	C1'-N9-C4	-4.48	121.81	126.81
90	CP	401	GCP	N3-C2-N1	-3.74	122.46	127.56
90	CP	401	GCP	C6-C5-C4	-2.54	117.96	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

126 monomers are involved in 322 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	A3	102	OHX	4	0
89	A6	401	OHX	2	0
89	AC	301	OHX	5	0
89	AI	302	OHX	2	0
89	AL	201	OHX	8	0
89	AN	201	OHX	2	0
89	AP	201	OHX	3	0
89	B2	1901	OHX	1	0
89	B2	1906	OHX	3	0
89	B2	1907	OHX	6	0
89	B2	1909	OHX	2	0
89	B2	1910	OHX	2	0
89	B2	1914	OHX	3	0
89	B2	1915	OHX	6	0
89	B2	1916	OHX	1	0
89	B2	1917	OHX	2	0
89	B2	1918	OHX	8	0
89	B2	1919	OHX	1	0
89	B2	1921	OHX	6	0
89	B2	1922	OHX	7	0
89	B2	1923	OHX	1	0
89	B2	1924	OHX	1	0
89	B2	1925	OHX	1	0
89	B2	1926	OHX	1	0
89	B2	1928	OHX	1	0
89	B2	1929	OHX	1	0
89	B2	1930	OHX	1	0
89	B2	1933	OHX	1	0
89	B2	1937	OHX	1	0
89	B2	1938	OHX	1	0
89	B2	1940	OHX	5	0
89	B2	1942	OHX	1	0
89	B2	1943	OHX	2	0
89	B2	1945	OHX	1	0
89	B2	1946	OHX	1	0
89	B2	1948	OHX	1	0
89	B2	1949	OHX	1	0
89	B2	1950	OHX	2	0
89	B2	1952	OHX	2	0
89	B2	1953	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B2	1954	OHX	6	0
89	B2	1955	OHX	1	0
89	B2	1957	OHX	1	0
89	B2	1960	OHX	1	0
89	B2	1961	OHX	4	0
89	B2	1962	OHX	1	0
89	B2	1963	OHX	4	0
89	B2	1964	OHX	6	0
89	B2	1965	OHX	2	0
89	B2	1968	OHX	4	0
89	B2	1969	OHX	7	0
89	B2	1970	OHX	1	0
89	B2	1972	OHX	2	0
89	B2	1973	OHX	1	0
89	B2	1974	OHX	7	0
89	B2	1975	OHX	3	0
89	B2	1977	OHX	7	0
89	B2	1978	OHX	1	0
89	B2	1979	OHX	1	0
89	B2	1982	OHX	5	0
89	B2	1983	OHX	1	0
89	B2	1986	OHX	3	0
89	B2	1987	OHX	1	0
89	B2	1988	OHX	8	0
89	B2	1989	OHX	1	0
89	B2	1990	OHX	1	0
89	B2	1991	OHX	3	0
89	B2	1996	OHX	6	0
89	B2	2001	OHX	3	0
89	B2	2004	OHX	1	0
89	B2	2006	OHX	1	0
89	B2	2008	OHX	1	0
89	B2	2009	OHX	2	0
89	B2	2011	OHX	2	0
89	B2	2012	OHX	1	0
89	B2	2013	OHX	11	0
89	B2	2014	OHX	1	0
89	B2	2015	OHX	1	0
89	B2	2016	OHX	7	0
89	B2	2022	OHX	3	0
89	B2	2024	OHX	1	0
89	B2	2025	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B2	2026	OHX	2	0
89	B2	2027	OHX	7	0
89	B2	2030	OHX	1	0
89	B2	2031	OHX	1	0
89	B2	2034	OHX	1	0
89	B2	2035	OHX	2	0
89	B2	2038	OHX	1	0
89	B2	2039	OHX	1	0
89	B2	2040	OHX	1	0
89	B2	2042	OHX	1	0
89	B2	2043	OHX	1	0
89	B2	2044	OHX	1	0
89	B2	2045	OHX	1	0
89	B2	2046	OHX	5	0
89	B2	2047	OHX	1	0
89	B2	2048	OHX	1	0
89	B2	2049	OHX	3	0
89	B2	2050	OHX	7	0
89	B2	2053	OHX	1	0
89	B2	2058	OHX	1	0
89	B2	2059	OHX	1	0
89	B2	2060	OHX	1	0
89	B2	2061	OHX	1	0
89	B2	2063	OHX	1	0
89	B2	2064	OHX	6	0
89	B2	2065	OHX	2	0
89	B2	2068	OHX	6	0
89	B2	2069	OHX	2	0
89	B2	2070	OHX	1	0
89	B2	2071	OHX	17	0
89	B2	2073	OHX	6	0
89	B2	2075	OHX	1	0
89	B2	2076	OHX	1	0
89	B2	2077	OHX	2	0
89	B2	2078	OHX	1	0
89	B2	2079	OHX	5	0
89	B2	2080	OHX	3	0
89	B2	2082	OHX	1	0
89	B2	2083	OHX	11	0
89	B2	2084	OHX	1	0
89	B5	3401	OHX	1	0
89	B5	3402	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	BR	201	OHX	9	0
90	CP	401	GCP	63	0

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
45	BK	2
81	B5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	52:UNK	C	54:UNK	N	9.71
1	BK	23:UNK	C	28:UNK	N	8.84
1	B5	1285:G	O3'	1286:A	P	6.77