



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 2, 2019 – 10:10 PM EST

PDB ID : 4V8Z
EMDB ID: : EMD-2422
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 : 6.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

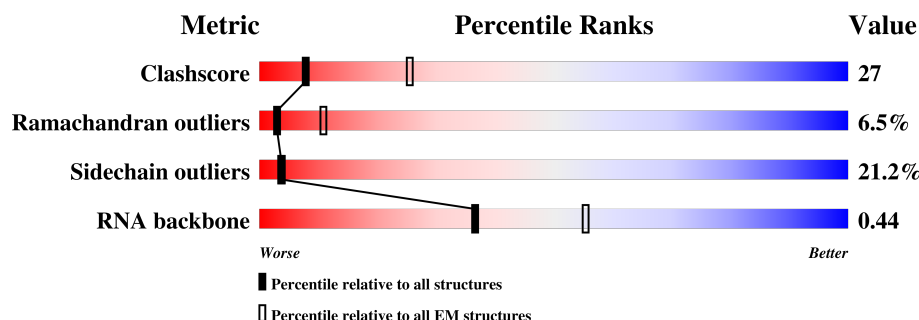
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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.



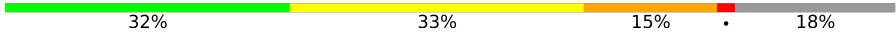


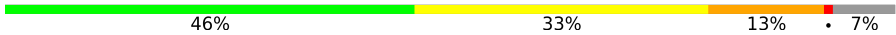
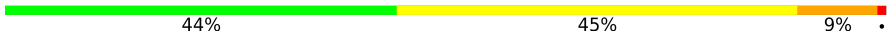
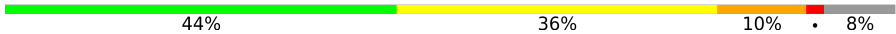
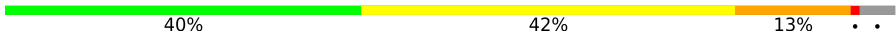
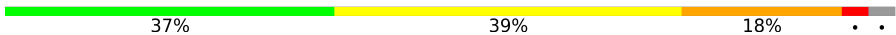
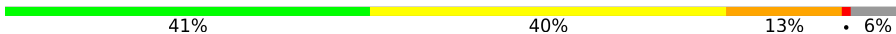
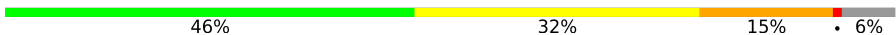
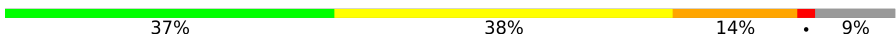
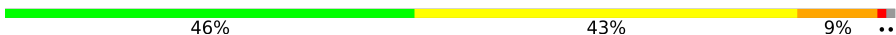
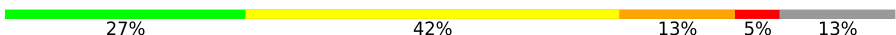







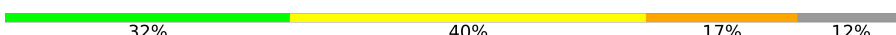




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	









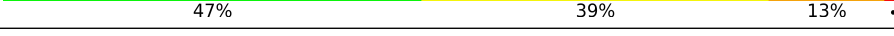

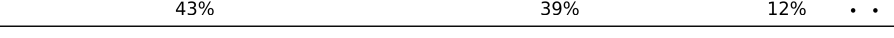
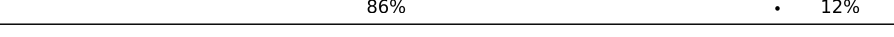

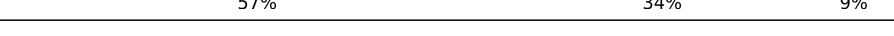


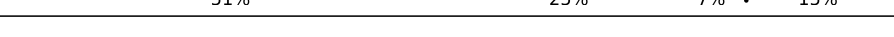

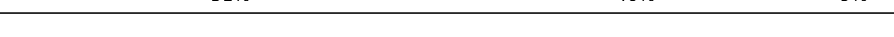






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Mol	Chain	Length	Quality of chain
9	AA	252	
10	AB	255	
11	AC	254	
12	AD	240	
13	AE	261	
14	AF	225	
15	AG	236	
16	AH	190	
17	AI	200	
18	AJ	197	
19	AK	105	
20	AL	156	
21	AM	143	
22	AN	151	
23	AO	137	
24	AP	142	
25	AQ	143	
26	AR	136	
27	AS	146	
28	AT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


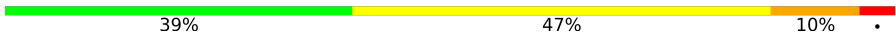









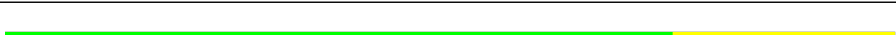

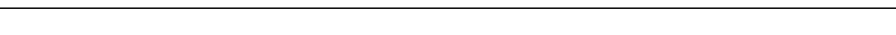
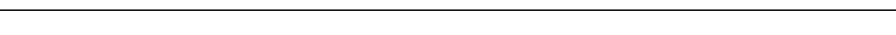
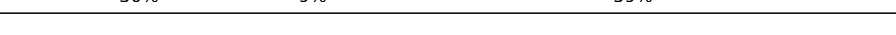

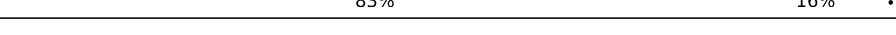

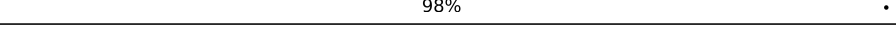
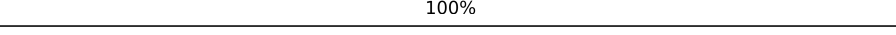
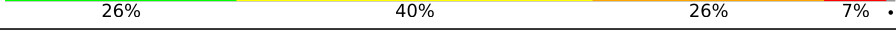


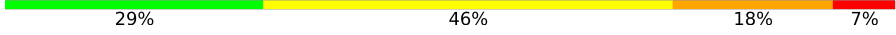
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Mol	Chain	Length	Quality of chain
34	AZ	108	
35	BA	253	
36	BB	386	
37	BC	361	
38	BD	296	
39	BE	175	
40	BF	243	
41	BG	255	
42	BH	191	
43	BI	220	
44	BJ	173	
45	BK	174	
46	BL	198	
47	BM	137	
48	BN	203	
49	BO	218	
50	BP	183	
51	BQ	185	
52	BR	188	
53	BS	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	 51% 39% 8% .
60	BZ	135	 39% 47% 10% .
61	Ba	148	 76% 22% ..
62	Bb	58	 72% 24% .
63	Bc	104	 79% 16% . .
64	Bd	112	 73% 21% . .
65	Be	129	 76% 20% . . .
66	Bf	106	 86% 12% .
67	Bg	120	 71% 22% . 7%
68	Bh	119	 76% 22% .
69	Bi	99	 68% 28% .
70	Bj	87	 75% 25%
71	Bk	77	 77% 23%
72	Bl	50	 76% 22% .
73	Bm	128	 30% 9% . 59%
74	Bn	25	 72% 20% 8%
75	Bo	105	 83% 16% .
76	Bq	312	 34% 11% . 54%
77	Br	47	 98% .
78	Bs	46	 100%
79	B2	1800	 26% 40% 26% 7% .
80	B5	3396	 21% 41% 24% 7% 7%
81	B7	121	 21% 48% 27% .
82	B8	158	 29% 46% 18% 7%
83	CV	586	 63% 26% 5% . .

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Mol	Chain	Length	Quality of chain
84	CW	76	
85	CX	3	

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
88	OHX	A3	102	-	-	X	-
88	OHX	AC	301	-	-	X	-
88	OHX	AL	201	-	-	X	-
88	OHX	B2	1907	-	-	X	-
88	OHX	B2	1915	-	-	X	-
88	OHX	B2	1918	-	-	X	-
88	OHX	B2	1921	-	-	X	-
88	OHX	B2	1922	-	-	X	-
88	OHX	B2	1939	-	-	X	-
88	OHX	B2	1953	-	-	X	-
88	OHX	B2	1960	-	-	X	-
88	OHX	B2	1962	-	-	X	-
88	OHX	B2	1963	-	-	X	-
88	OHX	B2	1967	-	-	X	-
88	OHX	B2	1968	-	-	X	-
88	OHX	B2	1973	-	-	X	-
88	OHX	B2	1976	-	-	X	-
88	OHX	B2	1981	-	-	X	-
88	OHX	B2	1987	-	-	X	-
88	OHX	B2	1995	-	-	X	-
88	OHX	B2	2011	-	-	X	-
88	OHX	B2	2014	-	-	X	-
88	OHX	B2	2025	-	-	X	-
88	OHX	B2	2044	-	-	X	-
88	OHX	B2	2048	-	-	X	-
88	OHX	B2	2062	-	-	X	-
88	OHX	B2	2066	-	-	X	-
88	OHX	B2	2069	-	-	X	-
88	OHX	B2	2071	-	-	X	-
88	OHX	B2	2077	-	-	X	-
88	OHX	B2	2081	-	-	X	-
88	OHX	B7	203	-	-	X	-
88	OHX	B7	219	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	BR	201	-	-	X	-
88	OHX	CV	601	-	-	X	-
89	GCP	CV	602	-	-	X	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 219371 atoms, of which 8407 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	153	Total	C	H	N	O	0	3
			1509	450	756	153	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	145	Total	C	H	N	O	S	0	2
			2185	683	1110	194	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 RNA chain called 18S RIBOSOMAL RNA.

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

- Molecule 80 is a RNA chain called 25S RIBOSOMAL RNA.

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

- Molecule 81 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 82 is a RNA chain called 5.8S RIBOSOMAL RNA.

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

- Molecule 83 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 5B, PROBABLE TRANSLATION INITIATION FACTOR IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
83	CV	570	Total	C	H	N	O	S	0	2
			9036	2819	4585	766	847	19		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CV	340	ASP	-	linker	UNP P39730
CV	341	LEU	-	linker	UNP P39730
CV	342	THR	-	linker	UNP P39730
CV	343	GLY	-	linker	UNP P39730
CV	344	LEU	-	linker	UNP P39730
CV	345	LEU	-	linker	UNP P39730
CV	346	ASP	-	linker	UNP P39730
CV	347	SER	-	linker	UNP P39730
CV	348	VAL	-	linker	UNP P39730
CV	349	ASP	-	linker	UNP P39730
CV	350	THR	-	linker	UNP P39730

- Molecule 84 is a RNA chain called EUKARYOTIC RIBOSOMAL PI TRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	CW	76	Total	C	H	N	O	P	0	0
			2403	721	789	285	533	75		

- Molecule 85 is a RNA chain called 5'-R(*AP*UP*GP)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	CX	3	Total	C	H	N	O	P	0	0
			96	29	34	12	19	2		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	A0	1	Total	Zn	0
			1	1	

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

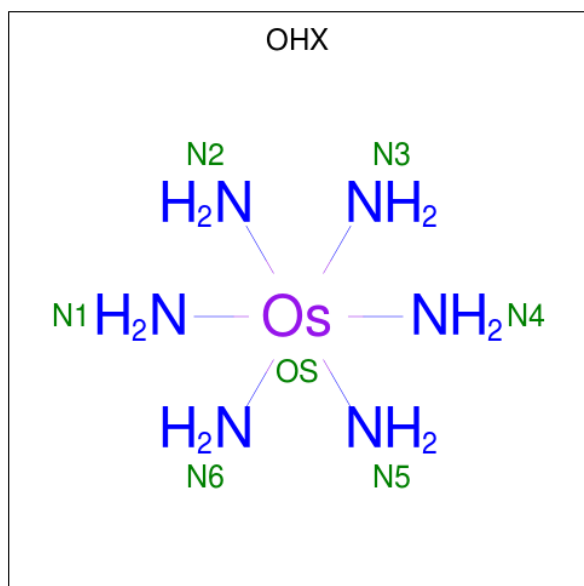
Mol	Chain	Residues	Atoms		AltConf
87	A0	2	Total 2	Mg 2	0
87	AG	1	Total 1	Mg 1	0
87	AJ	1	Total 1	Mg 1	0
87	B7	27	Total 27	Mg 27	0
87	BF	1	Total 1	Mg 1	0
87	AE	1	Total 1	Mg 1	0
87	AB	1	Total 1	Mg 1	0
87	AI	1	Total 1	Mg 1	0
87	AC	2	Total 2	Mg 2	0
87	BS	3	Total 3	Mg 3	0
87	AS	1	Total 1	Mg 1	0
87	B2	168	Total 168	Mg 168	0
87	BD	4	Total 4	Mg 4	0
87	AU	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
87	AN	1	Total	Mg	0
			1	1	
87	A5	1	Total	Mg	0
			1	1	
87	B5	3	Total	Mg	0
			3	3	
87	CW	1	Total	Mg	0
			1	1	
87	AL	2	Total	Mg	0
			2	2	
87	A3	3	Total	Mg	0
			3	3	
87	AP	1	Total	Mg	0
			1	1	

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			AltConf
88	A3	1	Total	N	Os	0
			7	6	1	
88	A6	1	Total	N	Os	0
			7	6	1	
88	AC	1	Total	N	Os	0
			7	6	1	
88	AI	1	Total	N	Os	0
			14	12	2	

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Mol	Chain	Residues	Atoms			AltConf
88	AI	1	Total 14	N 12	Os 2	0
88	AL	1	Total 7	N 6	Os 1	0
88	AN	1	Total 7	N 6	Os 1	0
88	AP	1	Total 7	N 6	Os 1	0
88	BR	1	Total 7	N 6	Os 1	0
88	Bn	1	Total 7	N 6	Os 1	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0

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Mol	Chain	Residues	Atoms			AltConf
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	

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Mol	Chain	Residues	Atoms			AltConf
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	

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[illegible]

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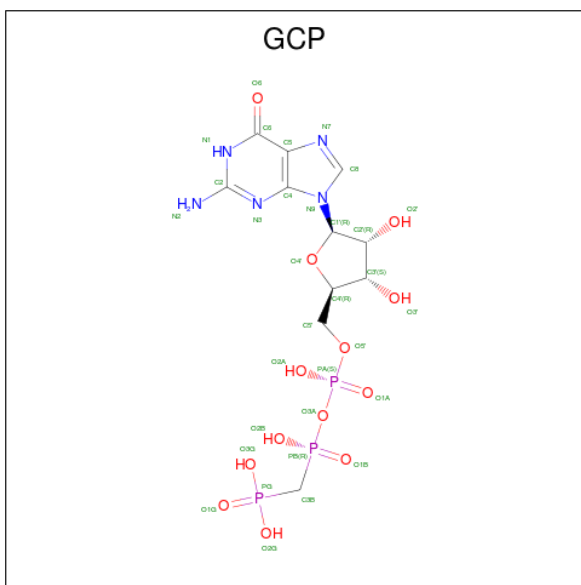
Mol	Chain	Residues	Atoms			AltConf
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B5	1	Total	N	Os	0
			21	18	3	

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Mol	Chain	Residues	Atoms			AltConf
88	B5	1	Total	N	Os	0
			21	18	3	
88	B5	1	Total	N	Os	0
			21	18	3	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	CV	1	Total	N	Os	0
			7	6	1	
88	CX	1	Total	N	Os	0
			7	6	1	

- Molecule 89 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

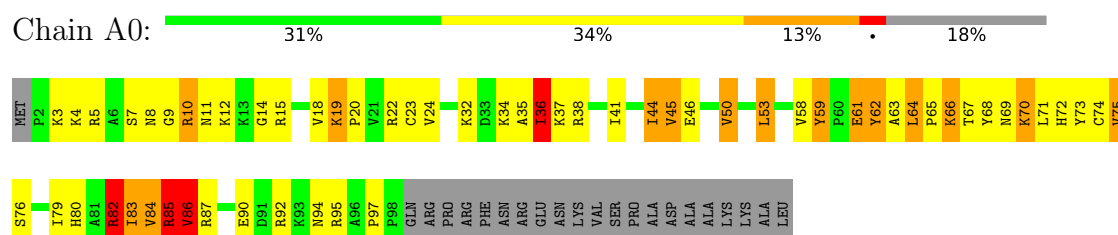


Mol	Chain	Residues	Atoms					AltConf
89	CV	1	Total	C	N	O	P	0
			32	11	5	13	3	

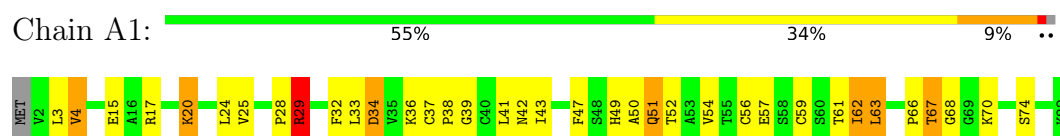
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

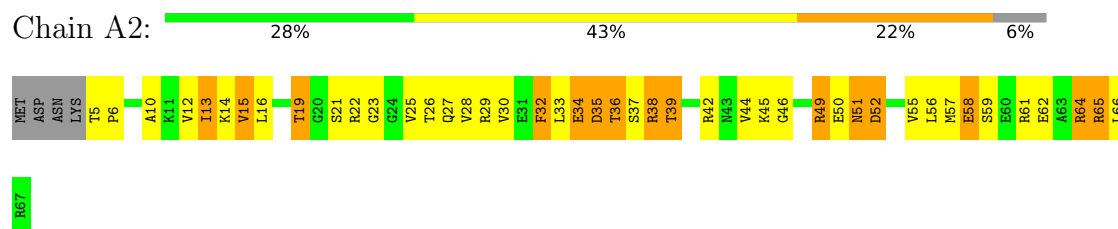
• Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



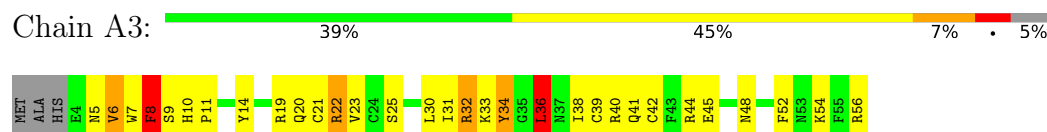
• Molecule 2: 40S RIBOSOMAL PROTEIN S27-A



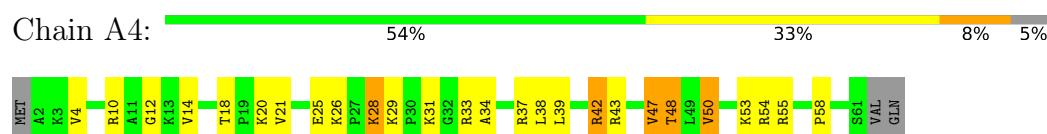
• Molecule 3: 40S RIBOSOMAL PROTEIN S28-A



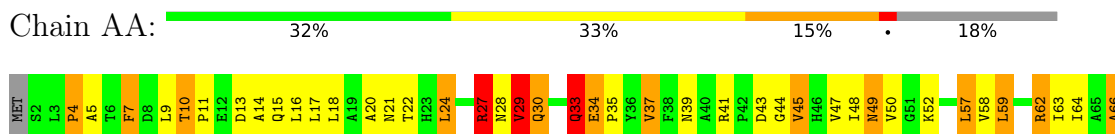
• Molecule 4: 40S RIBOSOMAL PROTEIN S29-A

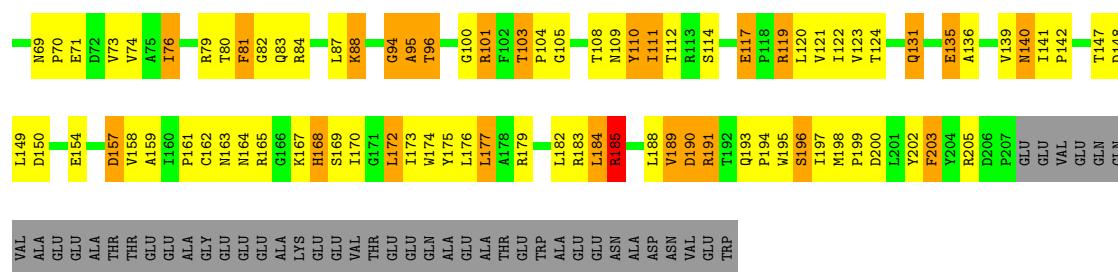


• Molecule 5: 40S RIBOSOMAL PROTEIN S30-A



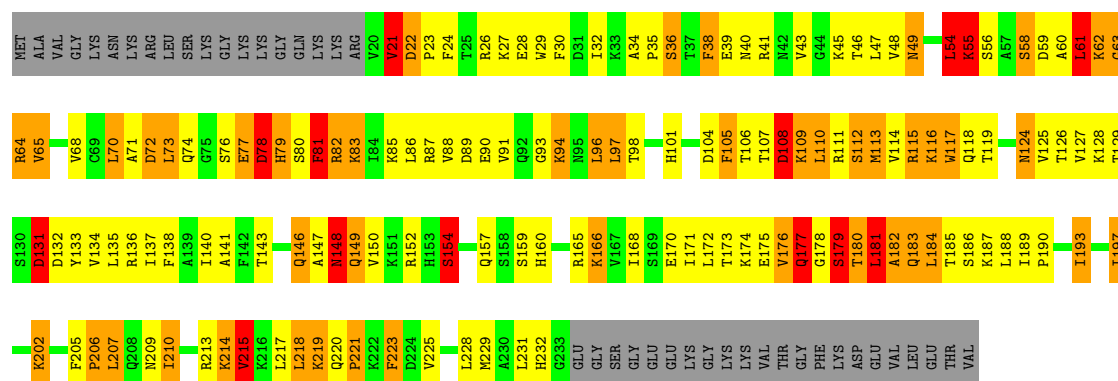
• Molecule 6: UBIQUITIN-40S RIBOSOMAL PROTEIN S31





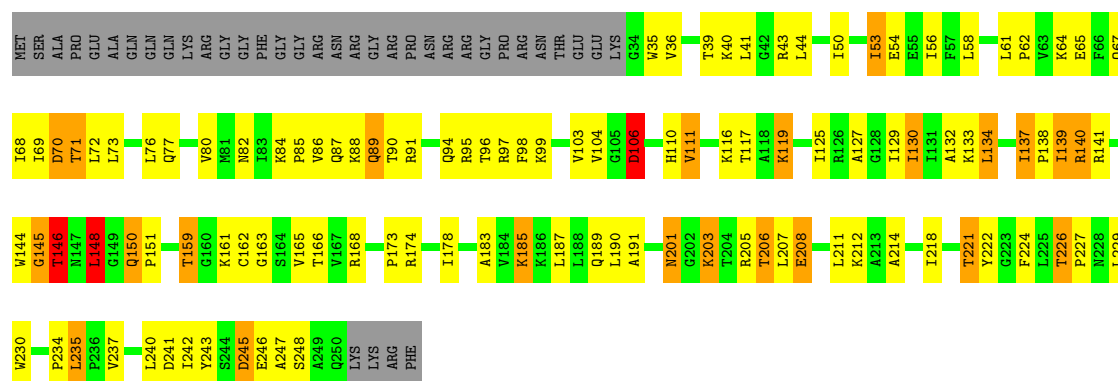
• Molecule 10: 40S RIBOSOMAL PROTEIN S1-A

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



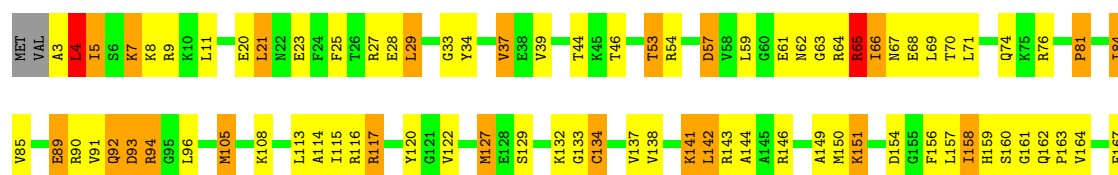
• Molecule 11: 40S RIBOSOMAL PROTEIN S2

Chain AC: 42% 33% 9% 15%



• Molecule 12: 40S RIBOSOMAL PROTEIN S3

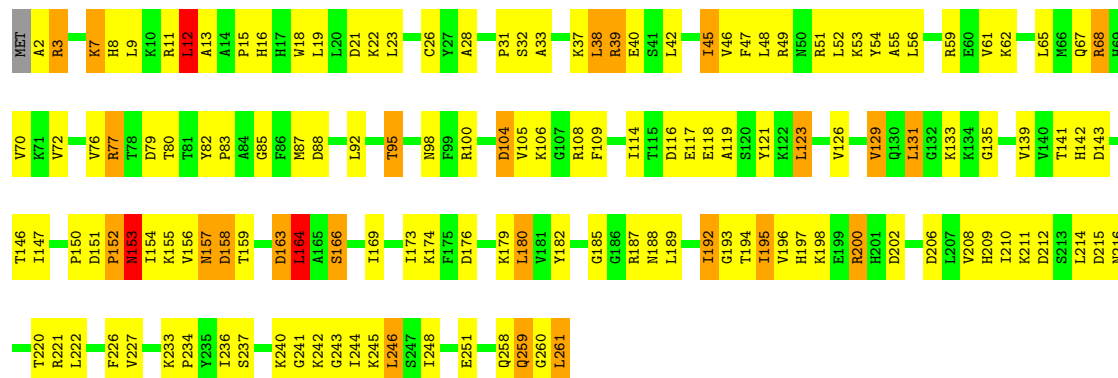
Chain AD: 46% 33% 13% 7%





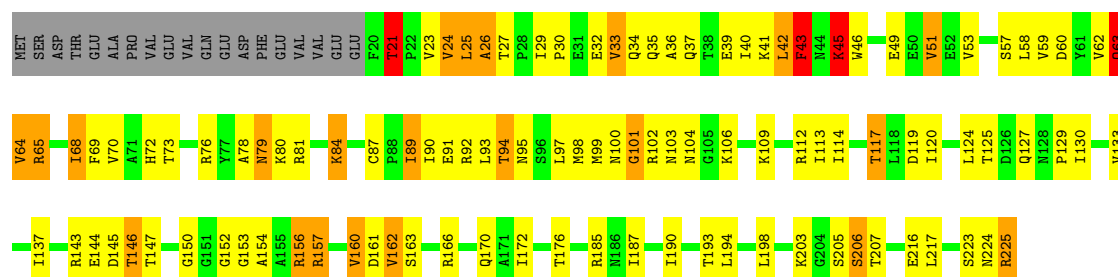
• Molecule 13: 40S RIBOSOMAL PROTEIN S4-A

Chain AE: 44% 45% 9%



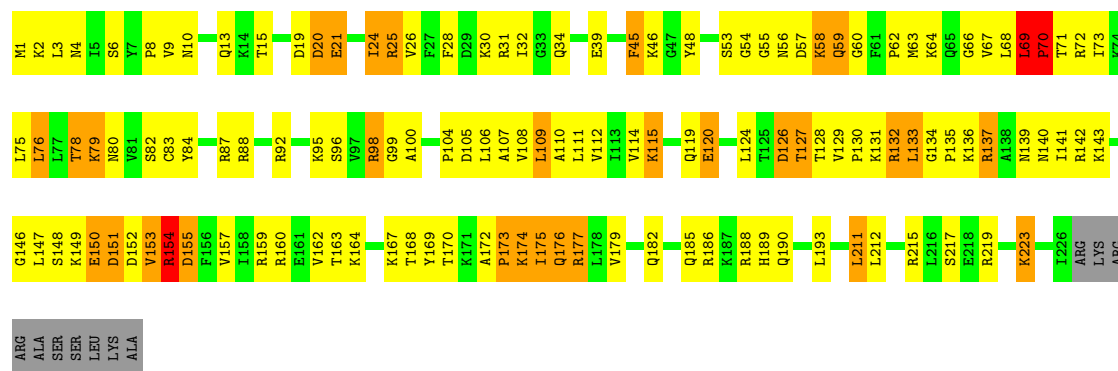
• Molecule 14: 40S RIBOSOMAL PROTEIN S5

Chain AF: 44% 36% 10% 8%



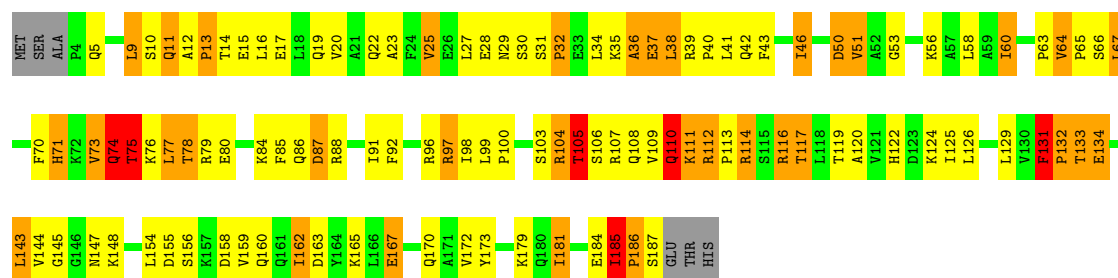
• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A

Chain AG: 40% 42% 13%



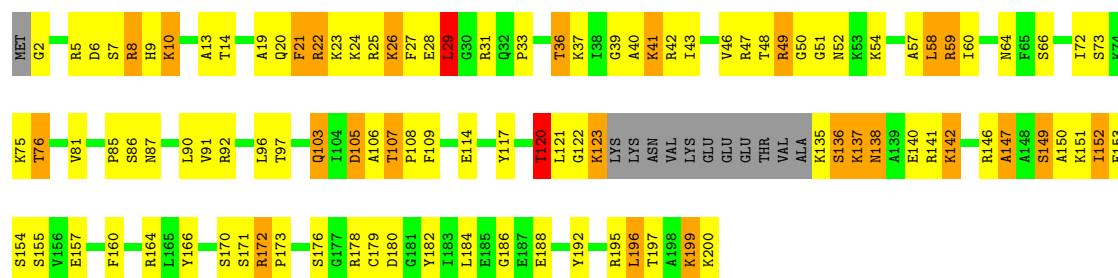
• Molecule 16: 40S RIBOSOMAL PROTEIN S7-A

Chain AH: 37% 39% 18%



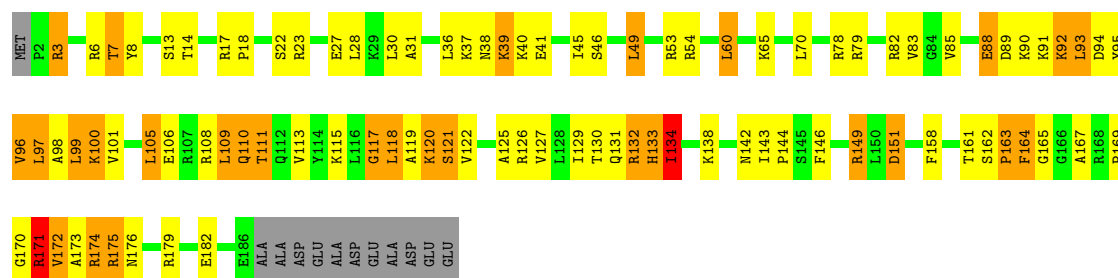
• Molecule 17: 40S RIBOSOMAL PROTEIN S8-A

Chain AI: 41% 40% 13% 6%



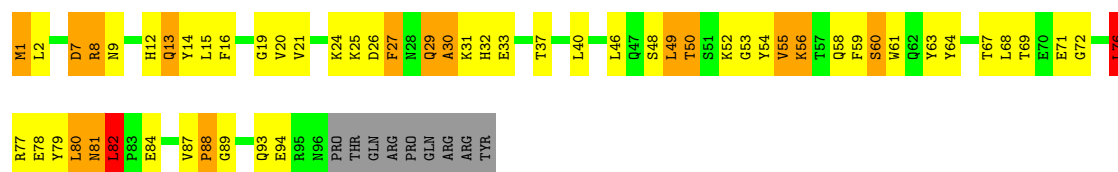
• Molecule 18: 40S RIBOSOMAL PROTEIN S9-A

Chain AJ: 46% 32% 15% 6%



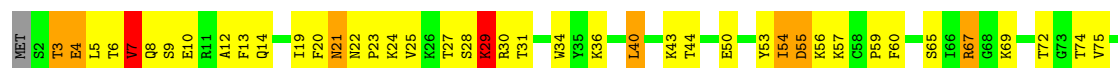
• Molecule 19: 40S RIBOSOMAL PROTEIN S10-A

Chain AK: 37% 38% 14% 9%



• Molecule 20: 40S RIBOSOMAL PROTEIN S11-A

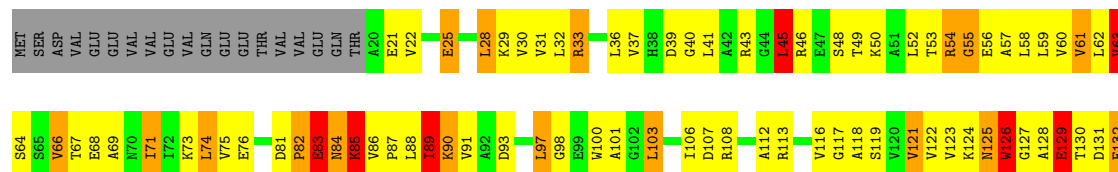
Chain AL: 46% 43% 9% ..





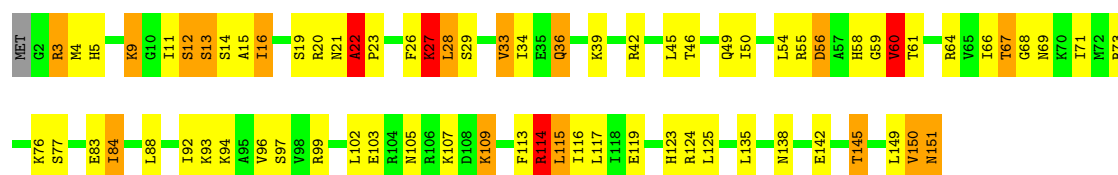
• Molecule 21: 40S RIBOSOMAL PROTEIN S12

Chain AM: 27% 42% 13% 5% 13%



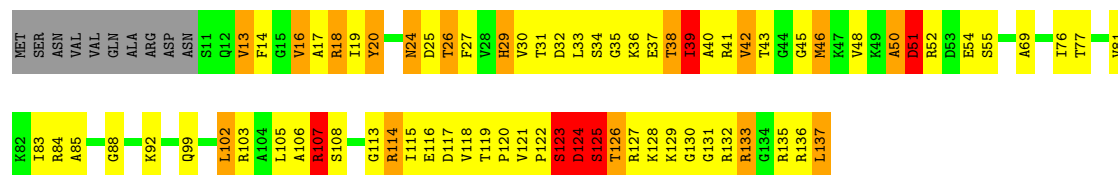
• Molecule 22: 40S RIBOSOMAL PROTEIN S13

Chain AN: 50% 36% 11% ..



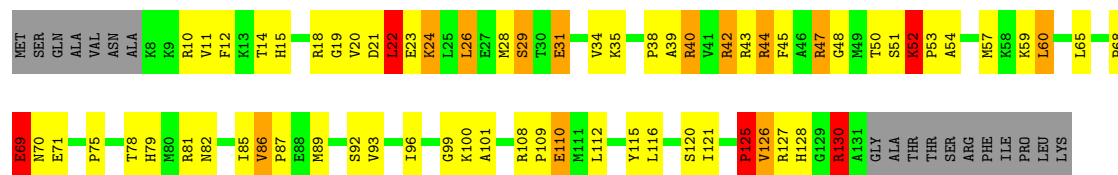
• Molecule 23: 40S RIBOSOMAL PROTEIN S14-A

Chain AO: 39% 38% 12% 7%



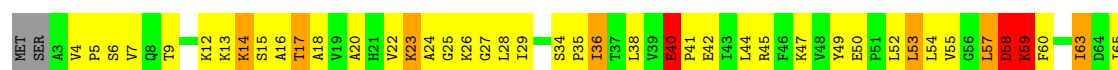
• Molecule 24: 40S RIBOSOMAL PROTEIN S15

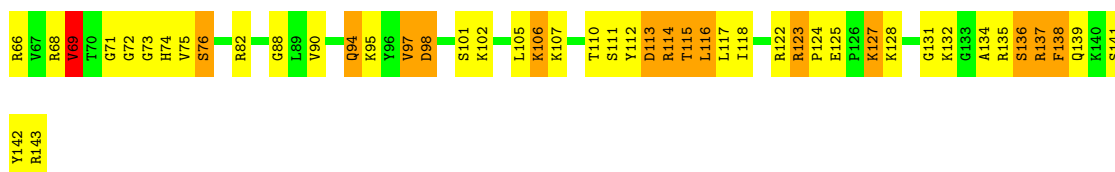
Chain AP: 39% 36% 8% 13%



• Molecule 25: 40S RIBOSOMAL PROTEIN S16-A

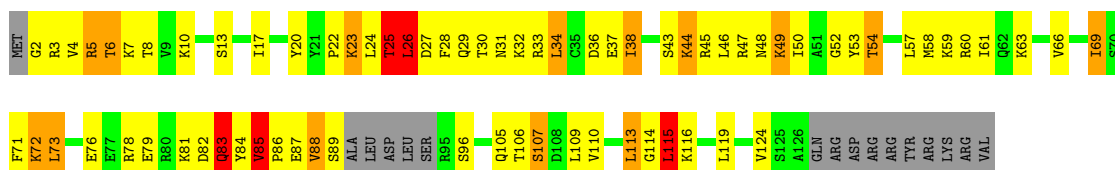
Chain AQ: 36% 45% 15%





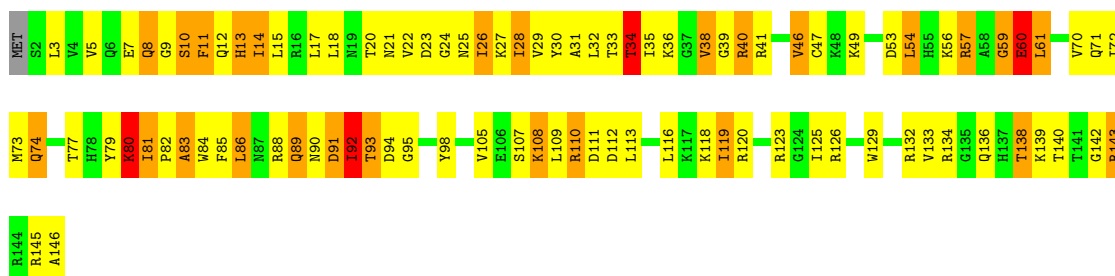
• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A

Chain AR: 35% 40% 10% 12%



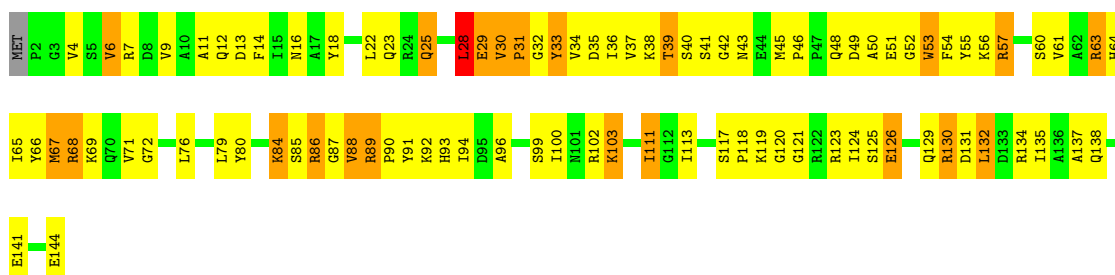
• Molecule 27: 40S RIBOSOMAL PROTEIN S18-A

Chain AS: 35% 44% 18%



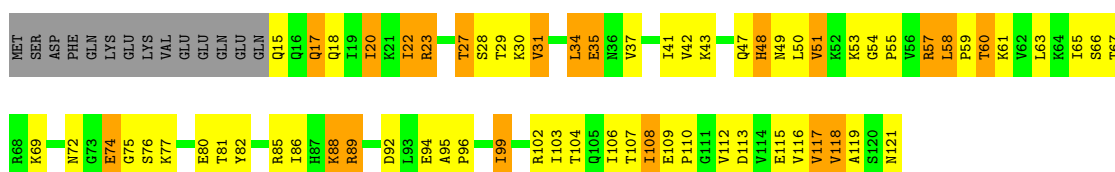
• Molecule 28: 40S RIBOSOMAL PROTEIN S19-A

Chain AT: 35% 49% 15%

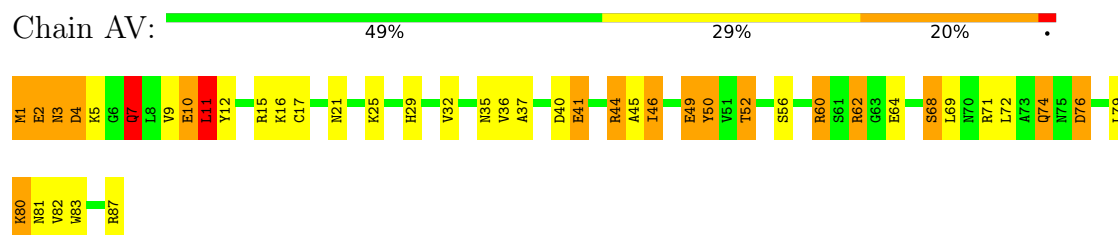


• Molecule 29: 40S RIBOSOMAL PROTEIN S20

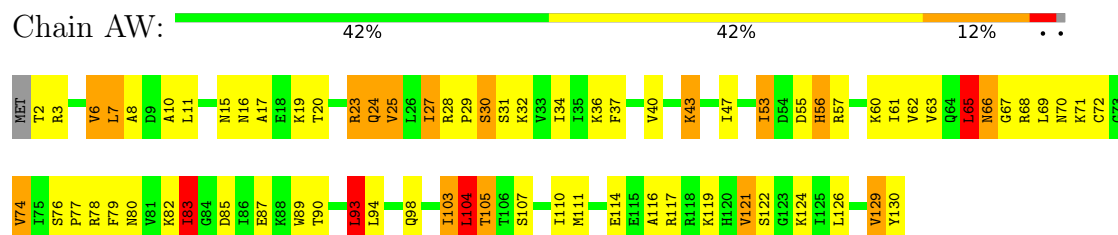
Chain AU: 32% 40% 17% 12%



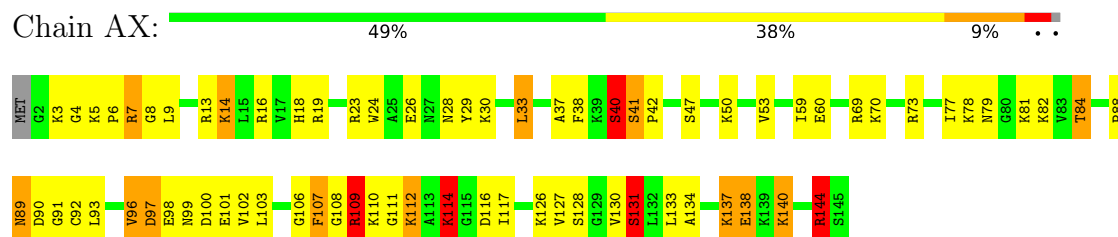
- Molecule 30: 40S RIBOSOMAL PROTEIN S21-A



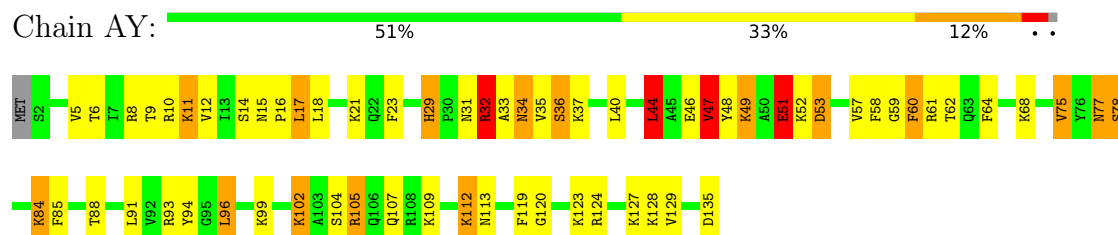
- Molecule 31: 40S RIBOSOMAL PROTEIN S22-A



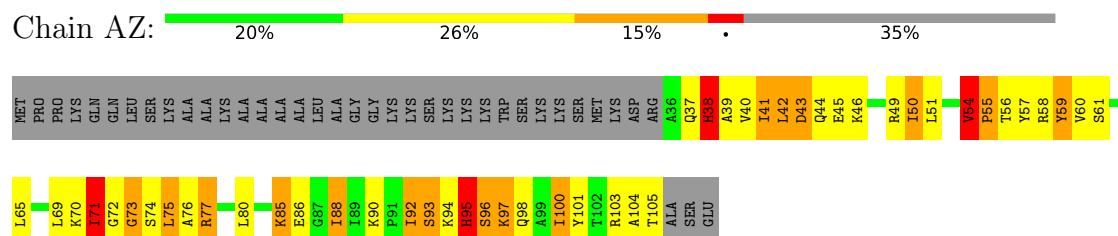
- Molecule 32: 40S RIBOSOMAL PROTEIN S23-A



- Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

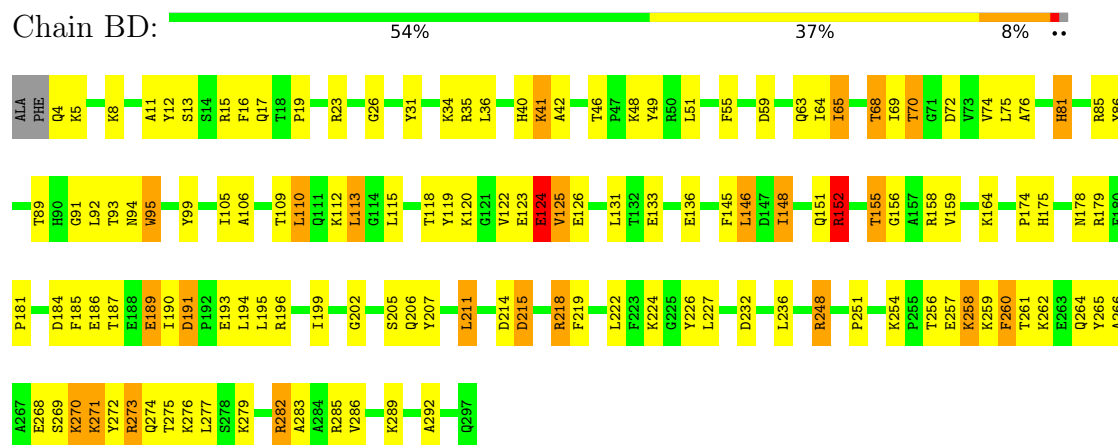


- Molecule 34: 40S RIBOSOMAL PROTEIN S25-A

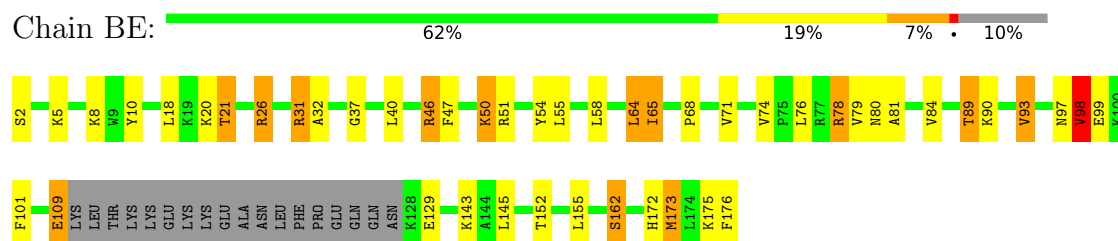


- Molecule 35: 60S RIBOSOMAL PROTEIN L2-B

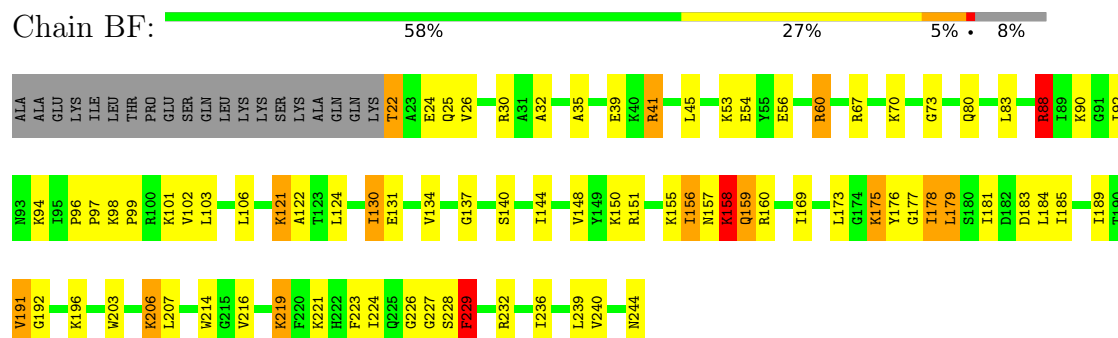




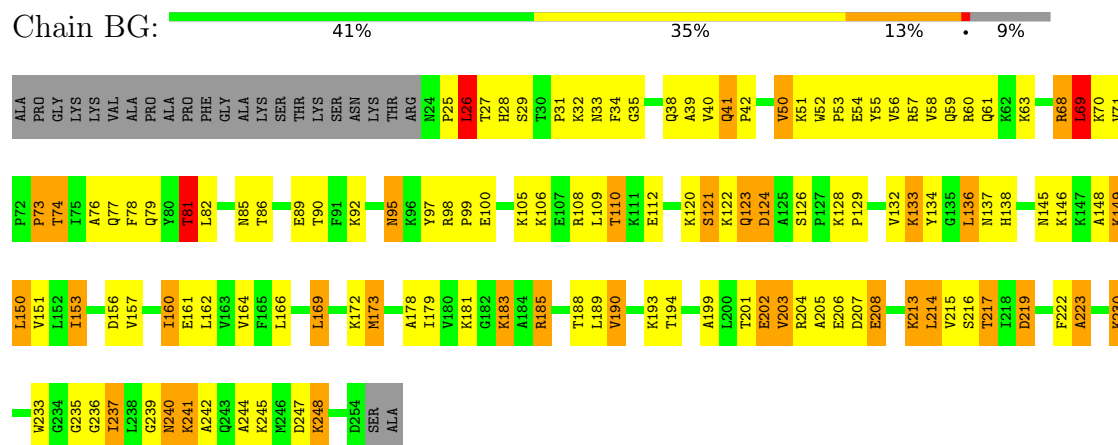
• Molecule 39: 60S RIBOSOMAL PROTEIN L6-A



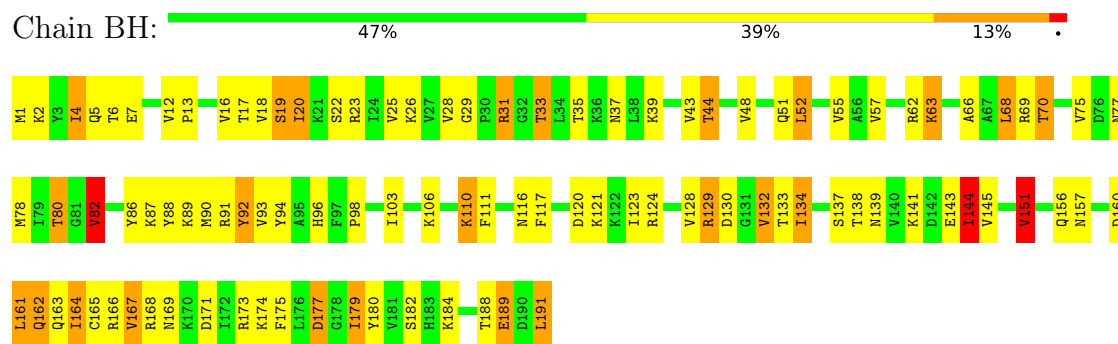
• Molecule 40: 60S RIBOSOMAL PROTEIN L7-A



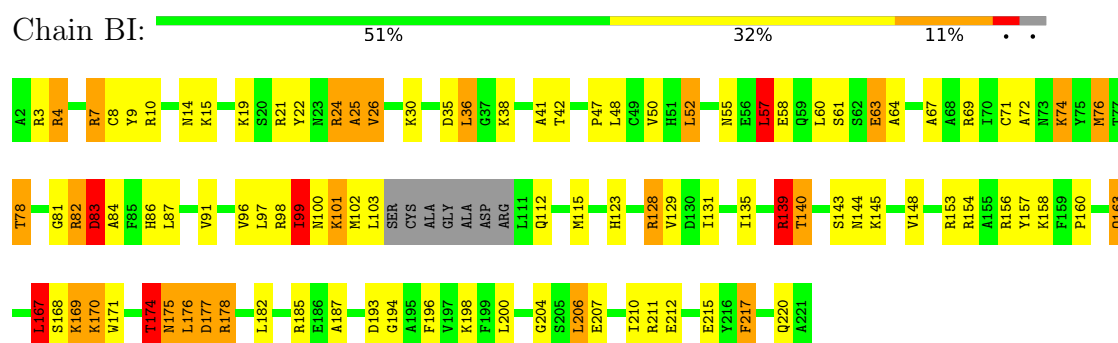
• Molecule 41: 60S RIBOSOMAL PROTEIN L8-A



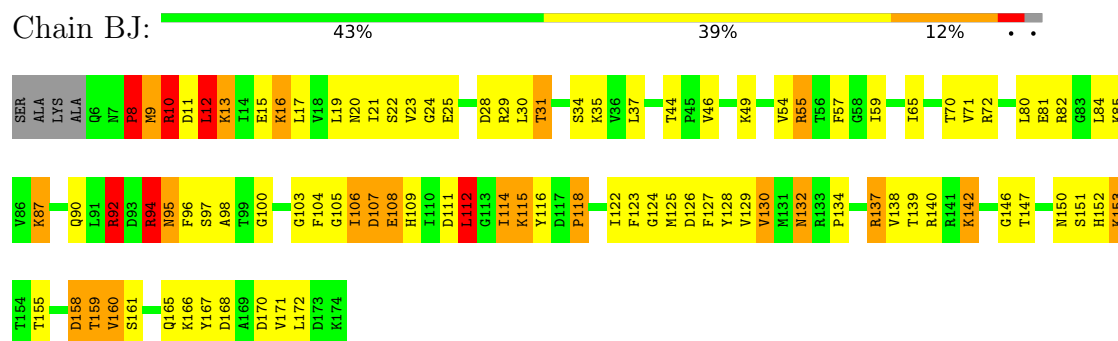
- Molecule 42: 60S RIBOSOMAL PROTEIN L9-A



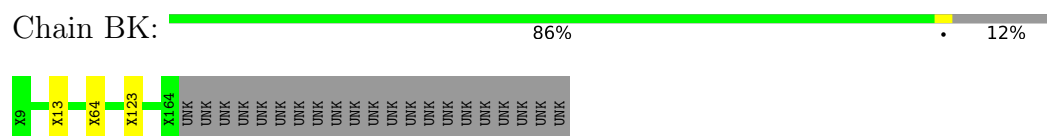
- Molecule 43: 60S RIBOSOMAL PROTEIN L10



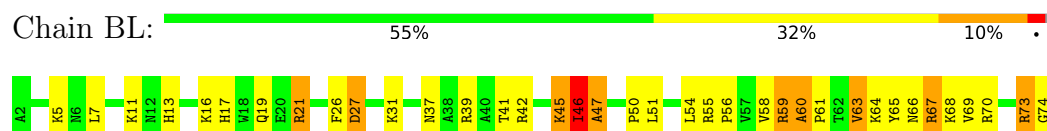
- Molecule 44: 60S RIBOSOMAL PROTEIN L11-A

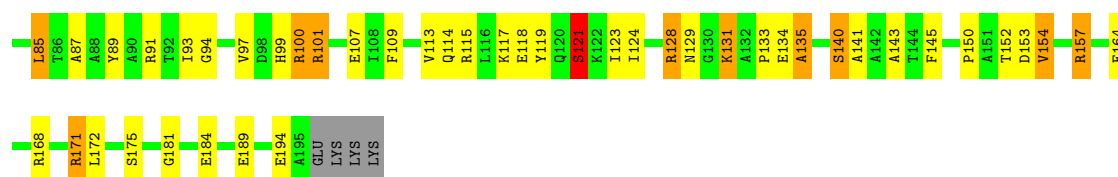


- Molecule 45: 60S RIBOSOMAL PROTEIN L11-A



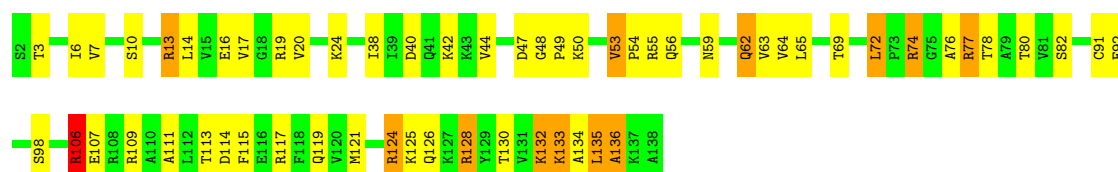
- Molecule 46: 60S RIBOSOMAL PROTEIN L13-A





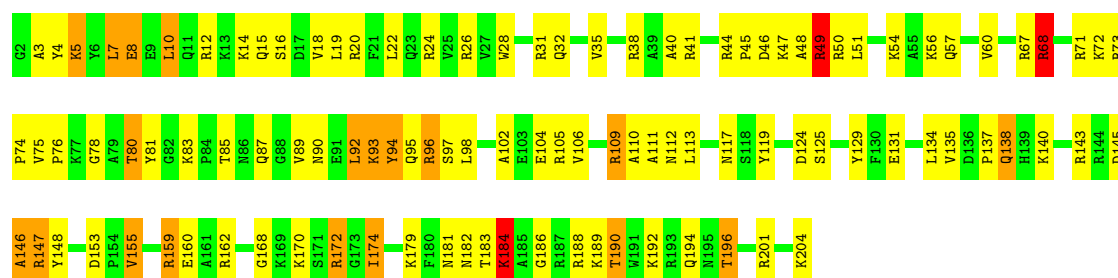
• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

Chain BM: 57% 34% 9% .



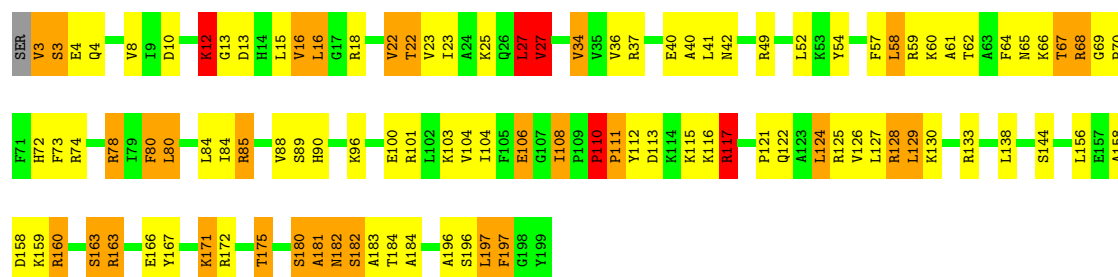
• Molecule 48: 60S RIBOSOMAL PROTEIN L15-A

Chain BN: 48% 41% 9% .



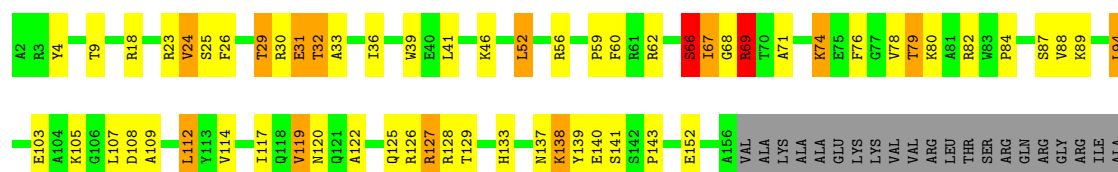
• Molecule 49: 60S RIBOSOMAL PROTEIN L16-A

Chain BO: 51% 32% 14% .



• Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

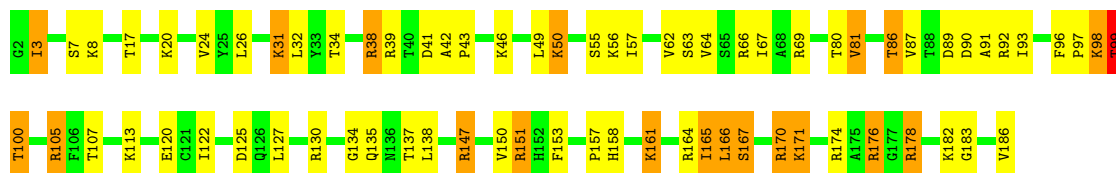
Chain BP: 51% 25% 7% . 15%



ALA
GLN
LYS
ARG
ILE
ALA
ALA

• Molecule 51: 60S RIBOSOMAL PROTEIN L18-A

Chain BQ:  61% 28% 10%



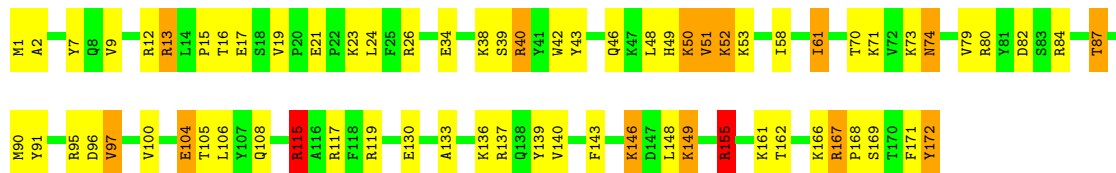
• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B

Chain BR:  51% 40% 9%



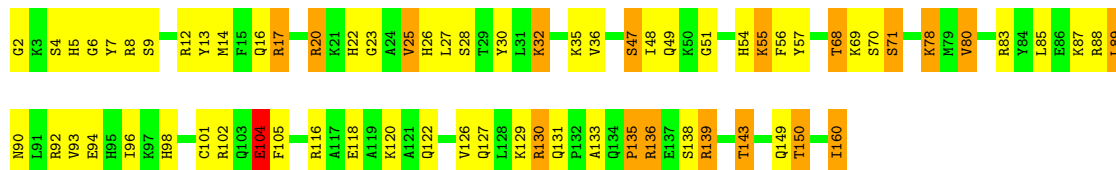
• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B

Chain BS:  59% 31% 8%



• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A

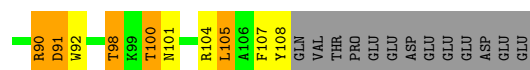
Chain BT:  56% 32% 11%



• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A

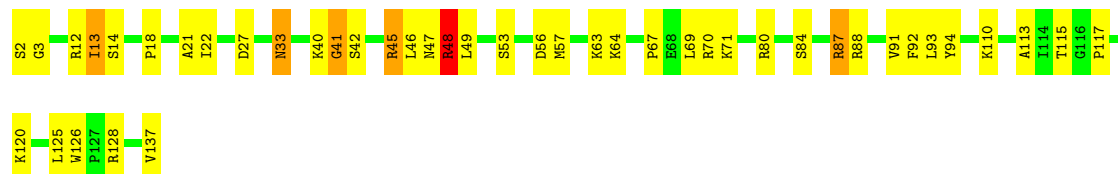
Chain BU:  44% 26% 12% 18%





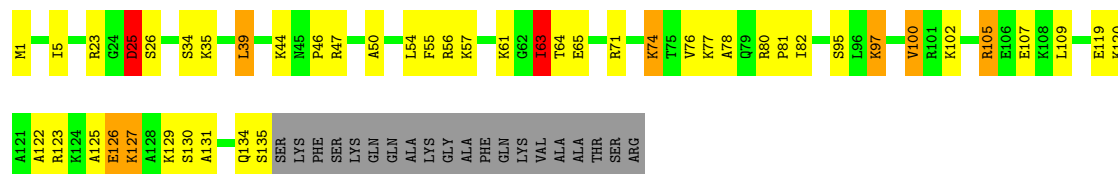
• Molecule 56: 60S RIBOSOMAL PROTEIN L23-A

Chain BV: 68% 28% . .



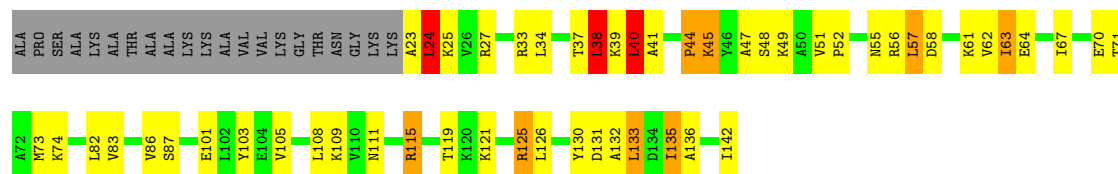
• Molecule 57: 60S RIBOSOMAL PROTEIN L24-A

Chain BW: 57% 25% 5% . 13%



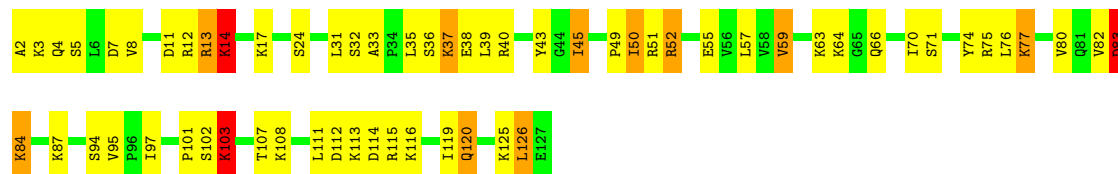
• Molecule 58: 60S RIBOSOMAL PROTEIN L25

Chain BX: 48% 30% 6% . 15%



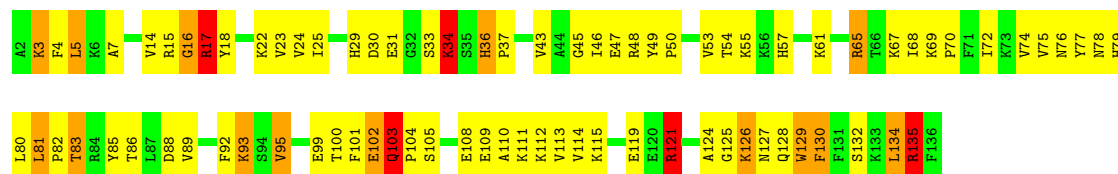
• Molecule 59: 60S RIBOSOMAL PROTEIN L26-A

Chain BY: 51% 39% 8% .

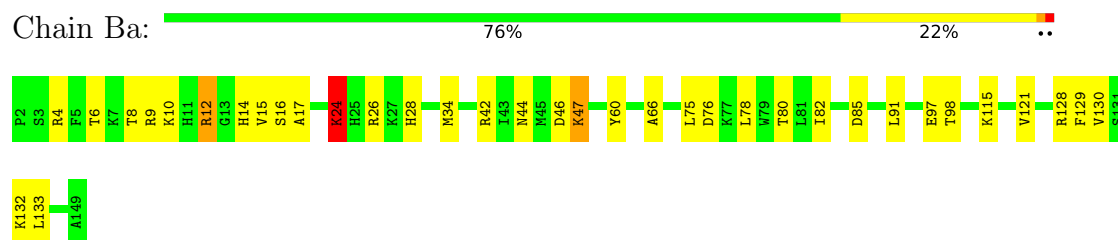


• Molecule 60: 60S RIBOSOMAL PROTEIN L27-A

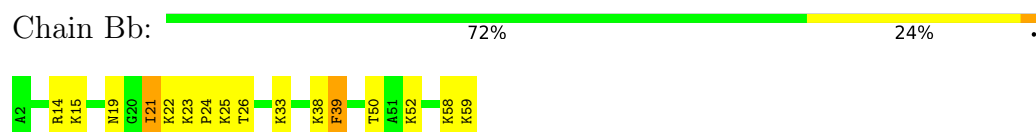
Chain BZ: 39% 47% 10% .



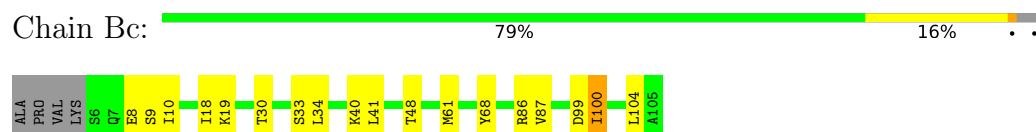
- Molecule 61: 60S RIBOSOMAL PROTEIN L28



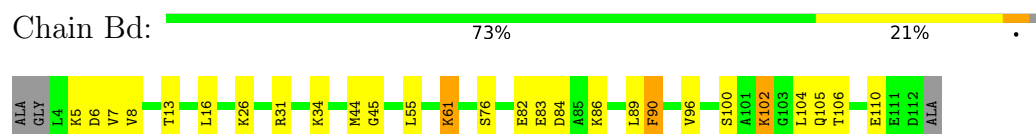
- Molecule 62: 60S RIBOSOMAL PROTEIN L29



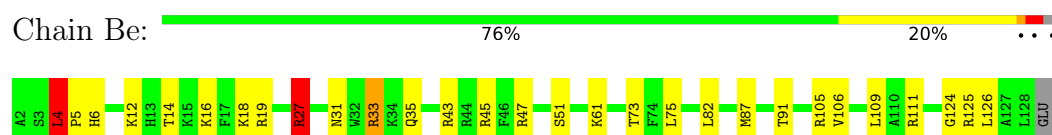
- Molecule 63: 60S RIBOSOMAL PROTEIN L30



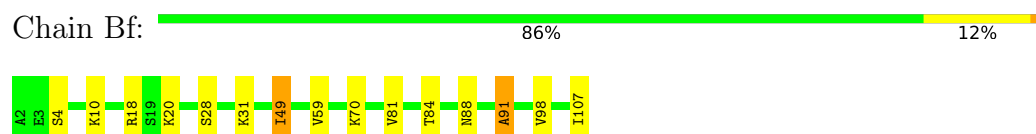
- Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



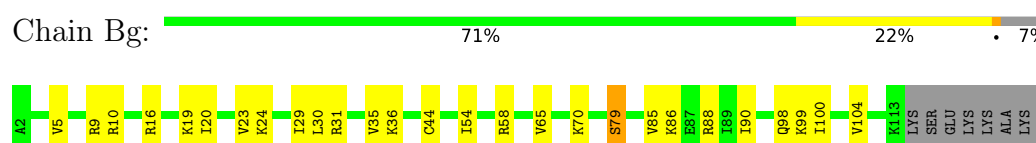
- Molecule 65: 60S RIBOSOMAL PROTEIN L32



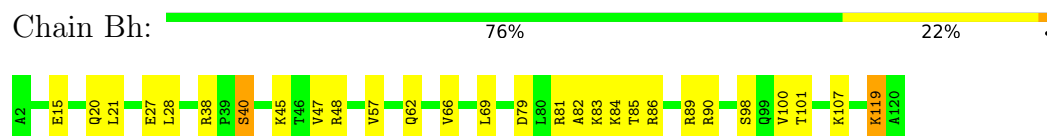
- Molecule 66: 60S RIBOSOMAL PROTEIN L33-A



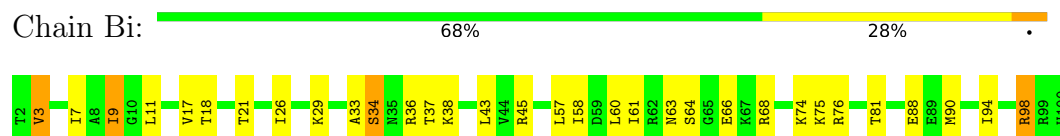
- Molecule 67: 60S RIBOSOMAL PROTEIN L34-A



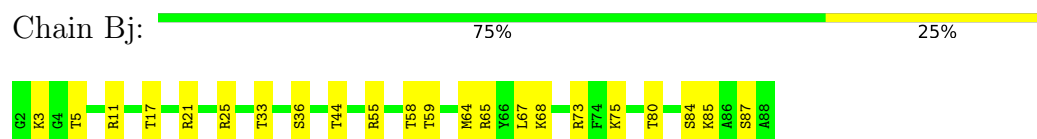
- Molecule 68: 60S RIBOSOMAL PROTEIN L35-B



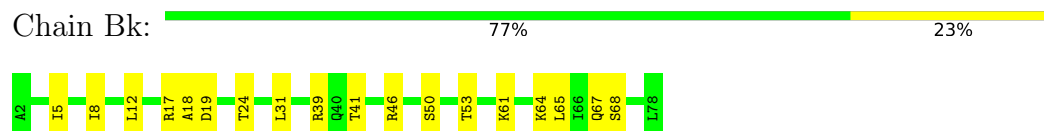
- Molecule 69: 60S RIBOSOMAL PROTEIN L36-A



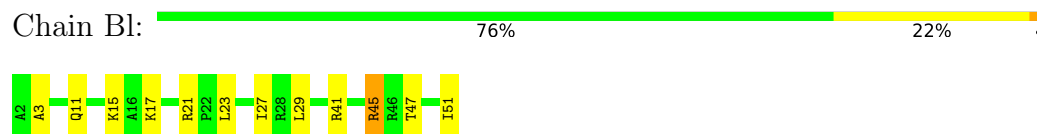
- Molecule 70: 60S RIBOSOMAL PROTEIN L37-A



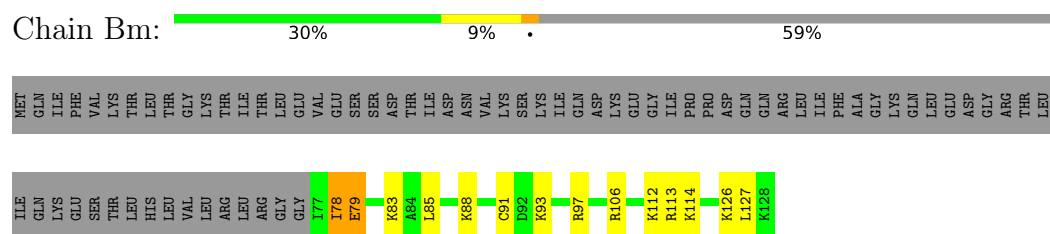
- Molecule 71: 60S RIBOSOMAL PROTEIN L38



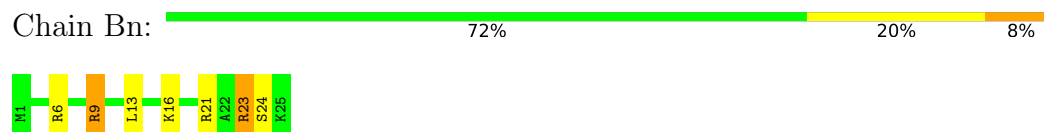
- Molecule 72: 60S RIBOSOMAL PROTEIN L39



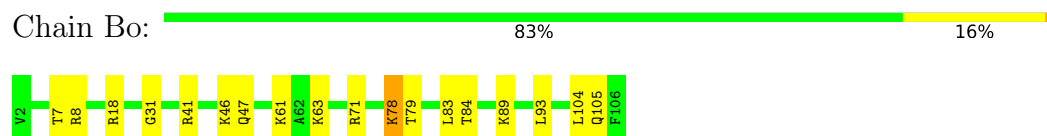
- Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



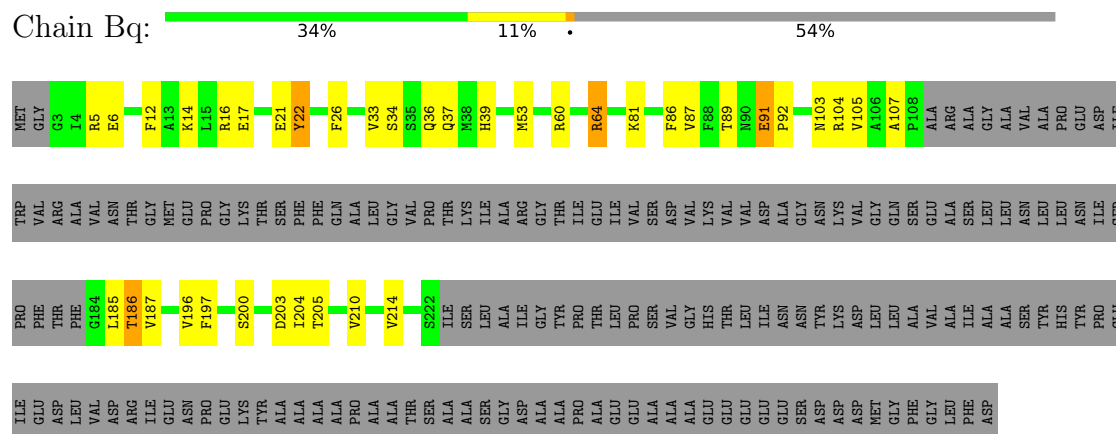
- Molecule 74: 60S RIBOSOMAL PROTEIN L41-B



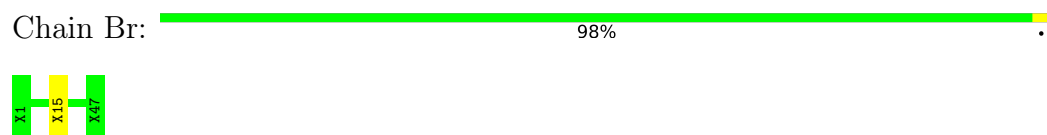
- Molecule 75: 60S RIBOSOMAL PROTEIN L42-A



• Molecule 76: 60S ACIDIC RIBOSOMAL PROTEIN P0



• Molecule 77: 60S ACIDIC RIBOSOMAL PROTEIN P1

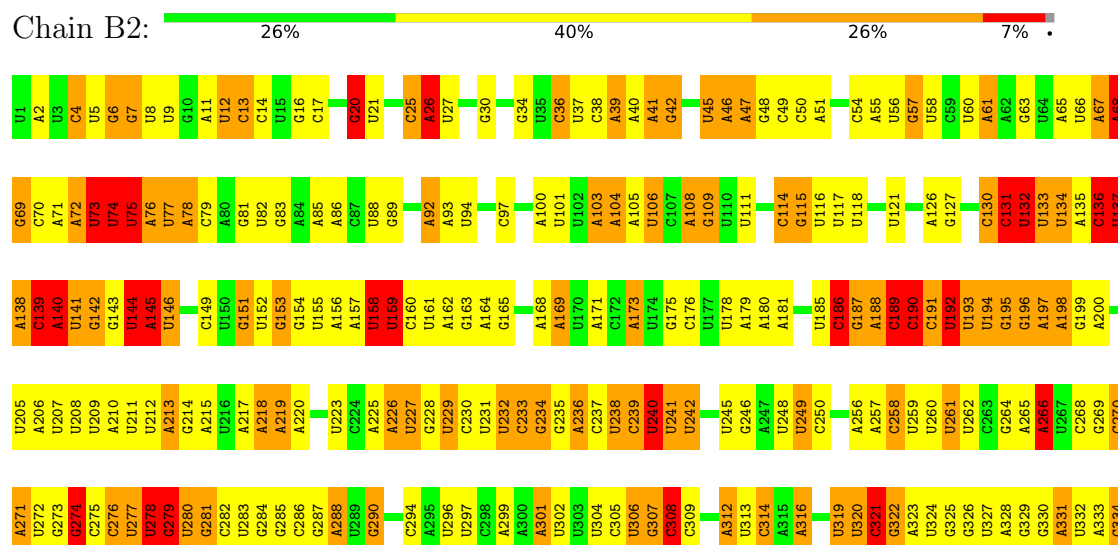


• Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2



There are no outlier residues recorded for this chain.

• Molecule 79: 18S RIBOSOMAL RNA



G1352	U1286	U1214	G1149	G1074	A1005	U935	G867	A803	G738	G676	U609	A541	A477	G409	U335
U1353	A1287	C1215	G1150	C1075	C1006	G836	G868	A804	G739	G677	G610	A542	A478	A410	G336
C1355	A1152	C1216	A1151	U1079	G1007	C937	A869	U805	A740	A678	U612	C543	C480	C411	C337
U1356	U1290	A1217	G1153	U1081	U1009	G842	G871	G810	U743	U680	G614	A545	C484	U414	C339
A1357	G1291	G1218	G1154	C1082	G1011	C943	U873	A811	U744	G682	A615	U647	A485	C415	A341
G1358	C1292	A1219	G1155	G1083	U1012	A944	C874	A812	U745	C683	G616	G548	G487	A416	C342
C1359	C1156	C1220	A1157	G1084	A1013	U945	G875	U813	U746	A684	U619	G553	G488	G418	C343
A1360	A1221	U1225	G1158	G1085	G1014	U946	G876	A814	U747	A685	A620	C554	C489	G419	A344
U1361	U1226	C1159	C1159	A1087	U1015	U947	G877	G815	U748	C686	A621	A555	C490	A420	U345
U1362	A1227	C1160	A1160	U1087	U1016	G948	G878	A816	U749	G687	A622	A556	C491	A421	U348
U1363	C1161	C1162	C1162	A1091	U1017	C949	U882	A817	U750	G688	A623	G557	A492	G422	U349
C1365	G1228	G1228	C1163	A1092	U1018	C950	C883	C818	U751	U692	G624	U558	U493	G423	U350
U1366	G1229	A1163	A1163	A1093	A1019	A951	A884	G819	A753	C692	C625	U559	U494	C424	C351
G1367	G1164	G1230	G1164	G1094	A1020	U958	G885	U820	A754	U693	G626	C560	U495	G425	A352
G1368	U1231	G1165	G1165	U1095	C1021	U959	U886	U821	A755	U694	U626	U560	G496	A426	U358
U1369	U1232	G1166	G1166	U1096	U1024	U960	A887	U822	A756	U695	G627	G561	G497	A427	U359
U1370	G1233	G1233	G1167	C1096	A1025	U961	U888	G823	A757	C697	U628	G562	G498	C427	G355
A1371	U1234	C1234	U1168	U1097	A1026	U962	U889	G824	U758	C698	U629	U563	G499	A428	G356
U1372	C1235	C1235	G1169	U1098	U1027	U963	A892	C827	U759	U698	A630	C565	U499	G429	G357
U1373	G1236	G1236	G1170	U1099	A1027	U964	U893	U828	A760	U699	U633	C566	C500	G430	U360
C1374	A1237	A1237	A1171	G1100	C1028	U965	U894	U829	G763	C700	G634	C567	U501	C431	A359
U1375	G1238	A1238	G1172	G1101	U1029	A966	G895	A829	U764	U701	A635	A567	U502	G432	A360
U1376	C1173	C1173	C1173	G1102	A1030	A967	U896	U830	G765	G702	G635	G568	G503	C433	C361
U1377	C1174	G1241	C1174	U1103	U1031	U968	C897	U831	G766	C703	A636	C569	U504	G434	G372
U1378	G1178	G1242	G1178	U1104	G1032	A970	A898	U832	U767	C704	C637	A570	C505	C435	G373
C1379	G1243	A1243	G1179	C1105	C1033	A971	G899	U833	U768	U705	U638	C572	U507	A437	G374
A1381	U1244	G1244	C1180	U1106	C1034	G972	A900	U836	A769	A706	U640	C573	U508	A438	G377
A1382	G1178	G1245	C1181	G1111	G1037	G973	G901	U837	A770	C708	U641	C575	U509	U439	A378
A1383	U1181	G1246	U1181	G1112	U1038	A974	G902	G838	A771	C709	G647	C576	G510	U440	U379
C1384	U1182	U1247	U1182	A1113	U1039	C975	A905	U839	G772	U710	G648	C577	G511	C443	U380
G1385	C1248	C1248	A1183	G1114	G1040	G976	A906	U840	C773	U711	U649	U578	A512	C444	C381
G1386	U1249	U1249	U1184	U1115	G1041	A977	U909	U841	A774	G712	U650	A579	U513	C445	C382
A1387	G1185	G1250	U1185	U1116	G1042	A978	U910	C842	G775	A713	G651	A580	G514	A445	C383
C1388	U1251	U1251	U1186	G1119	A1043	A979	C910	U843	G776	G714	G652	U581	A515	A446	G384
C1327	C1252	C1252	U1187	U1120	U1044	G980	U911	A844	C777	U715	C653	U582	G516	U447	A385
G1328	U1253	U1253	G1188	C1121	U1049	U981	U912	G845	G778	C716	C654	C583	U517	C448	G386
A1329	U1254	G1255	A1189	G1127	G1050	U982	U913	G846	U779	C717	G655	C584	A518	C449	G387
G1330	G1256	C1256	C1190	U1128	G1051	U983	G914	A847	A780	U718	U656	A585	C519	U450	G388
A1331	A1257	A1257	U1191	C1128	U1052	G984	A915	C848	U781	U719	G657	G586	A520	A451	C389
C1332	U1258	U1258	U1192	G1129	G1053	G987	U916	C849	U782	G720	C658	C590	U521	U452	G390
G1333	U1259	U1259	A1193	U1130	U1062	G988	U917	A850	G783	U721	C	A591	U522	U453	A391
U1334	U1260	U1260	C1195	A1131	U1067	A988	U918	U851	C784	G722	G	A592	G523	U454	G392
U1335	U1261	U1261	A1196	U1132	U1068	U989	U919	C852	U785	G723	A	U593	U524	G458	C393
C1336	G1267	G1267	C1197	A1133	U1059	C990	U920	G853	C786	C724	U	U594	A525	G459	C394
A1400	G1268	G1268	G1198	C1134	U1060	G991	U921	U854	G787	U725	U	A595	A526	A460	U395
A1401	U1269	U1269	G1199	U1135	A1061	A992	U922	A855	A788	C726	U	G596	A527	G461	G396
G1402	G1270	G1270	G1200	A1137	A1062	A993	G925	A856	A789	U727	U	C597	U528	A397	A397
C1403	U1340	U1340	A1138	U1138	U1063	G994	G926	U857	U790	U728	U	U598	A529	G467	G398
C1404	A1341	C1274	A1139	A1139	G1064	A995	A926	G858	C784	G729	U	G599	U530	A468	C400
G1405	A1275	A1275	A1140	U1140	A1065	U996	C927	A859	A793	G730	C	U600	U532	C469	A400
U1408	U1276	U1276	U1141	A1142	C1066	G997	U928	U860	U794	C731	U	G601	U533	A470	A401
A1346	G1277	G1277	U1143	A1143	C1067	U1000	U929	U861	U795	G732	U	A604	U534	A471	C402
A1410	U1278	U1278	C1207	U1144	C1070	A1081	A930	A862	U796	A733	G	G605	A535	U472	C403
A1411	C1279	C1279	U1145	U1145	U1071	A1082	C931	A863	U797	A734	U	A606	A536	A473	G404
A1348	A1208	A1208	G1146	G1146	U1072	G1002	U932	U864	U801	C735	U	G607	A537	A474	A407
G1349	C1209	C1209	U1147	U1147	G1073	A1003	U933	A865	G802	C736	A	A608	G538	A475	C408
U1413	G1210	G1210	A1148	C1148	G1073	U1004	C934	G866			U			U476	



G1565	U1494	G1429	G1365	U1305	A1294	U1181	U1121	A1048	G984	U922	G860	G795	A720	G652	G658
A1566	U1495	U1430	A1366	G1306	A1245	A1182	U1122	C1049	U985	C923	C861	U796	G721	A653	A589
U1567	C1496	G1431	G1367	G1307	G1246	C1183	U1123	U1050	U986	G924	U862	U797	G722	C654	G590
G1497	C1497	A1432	U1368	A1308	U1247	A1184	U1124	U1051	U987	A925	C863	G798		G591	G591
U1569	A1498	A1433	A1369	U1309	G1248		U1125	A1054		A926	G864	G799	G725	A656	A592
U1570	C1499	G1434	G1370	G1310	G1249	C1187	U1126	A1055	U990	C927	U865	G800	G726	A657	C593
A1571	G1500		G1371	G1311	G1250	U1188	G1127	U1056	G981	C928	A866	A801	G727	G658	U584
U1572	U1501	C1437	C1372	G1312	A1251	U1189	U1128	A1057	A992	A929	G867	C802	G728	G659	G595
G1573	C1502	U1438	A1373	G1313	A1252	C1189	U1129	U1060	G993	U930	C968	C803	G729	A660	C599
C1574	A1503	G1439	G1374	C1314	U1253	U1191	A1130	U1061	G994	C931	U871	C804	U731	G661	G600
A1575	U1504	G1440	G1375	U1315	C1254	C1192	G1131	A1062	U995	U932	G873	G805	U730	U662	G601
G1576	A1505	A1441	C1376	C1316	C1255	A1193	C1132	A1063	A996	A933	U872	A806	C732	C663	
G1577	U1506	U1442	G1377	A1317	G1256	G1194	A1133	G1063	A997	G934	C873	A807	G733	U664	
C1578	G1507	G1443	U1378	A1318	C1257	A1195	G1134	A1064	A998	U935	U874	A808	C734	A665	
C1579	U1508	U1444	G1379	G1319	U1258	C1196	A1135	A1065	G999	A936	G875	G809	C735	A666	
A1580	A1509	U1445	G1380	C1320	A1259	A1197	A1136	A1066	C1000	A937	A876	A810	A736	C667	
C1581	G1510	A1446	A1381	U1321	A1260	C1198	U1137	A1067	G1001	C938	C877	U811	G737	G668	A608
C1582	U1511	G1447	G1382	G1322	G1261	C1199	U1138	U1071	A1002	U939	G878	G812		U669	G609
A1583	U1512	U1448	G1383	G1323	G1262	A1200	G1139	G1072	A1003	G940	U879	G813	U741	C670	G610
	G1513	A1449	U1384	U1324	A1263	C1201	G1140	U1073	U1004	G941	G880	U814	G742	U671	A611
G1586	G1514	C1451	U1385	U1325	G1264	C1202	C1141	U1077	U1007	C947	G887	A820	C749	A677	G617
A1587	U1515		A1386	A1326	U1265	A1203	G1142	U1078	U1008	C948	A888	U821	G750	G678	C618
A1588	C1516		G1387	C1327	G1266	A1204	A1143	A1079	U1009	C949	U889	G822	U759	U679	A619
A1589	G1517	A1454	U1388	U1328	U1267	A1205	U1144	A1080	G1010	C945	A882	C818	C752	G675	G620
G1590	U1518	U1455	G1389	U1329	G1268	G1206	G1145	A1081	U1011	U946	A884	U819	C753	U681	A621
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A1593	A1524	U1458	G1392	A1332	A1271	G1209	A1148	G1084	U1014	C949	U889	G822	C756	U679	A619
A1594	G1525	A1459	C1393	C1333	C1272	U1210	G1149	A1085	G1015	G950	A883	C824	C757	G681	G620
U1595	U1526	A1460	U1334	U1334	A1273	U1211	A1150	A1086	U1016	C951	A884	U825	C758	U682	A622
C1596	G1527	A1461	C1335	C1335	A1274	A1212	U1151	C1086	G1017	U954	C893	A828	C759	U687	
C1597	G1528	U1462	U1336	U1336	C1275	G1213	G1152	C1087	G1018	U955	C894	U829	C759	G688	G624
	U1529	U1463	A1337	A1337	U1276	U1214	A1153	U1093	G1019	U956	A895	U829	C759	G688	G625
A1534		A1464	A1401	C1338	C1277	U1215	A1154	U1094	G1020	C957	A896	U830	C759	U689	U626
G1538	G1538	A1466	C1403	G1340	C1278	C1156	G1157	U1095	G1021	C958	U897	G831	C760	A690	U627
		A1467	G1404	U1341	G1280	G1157	G1157	U1096	U1022	C959	U898	G832	C760	A691	A628
A1605	U1605	U1468	U1405	C1342	G1281	A1158	A1158	G1097	C1023	U960	U899	G833	C765	A692	U629
U1606	G1541	C1469	A1406	A1343	C1282	A1159		A1098	G1024	C961	G900	U834	C766	A693	U630
U1607	G1542	U1470	U1407	G1344	C1283	A	C1160	A1099	A1025	A962	C901	G835	U767	C694	U631
C1608	G1543	U1471	G1345	G1345	C1284	C	G1161	U1100	A1026	G963	G902	U838	U767	C695	G632
C1609	U1544	U1472	G1408	G1346	C1285	A1225	U1162	G1101	A1027	G964	U903	G838	C769	C633	C633
G1610	A1545	G1473	U1410	U1347	A1286	G1226	A1163	A1102	U1028	A965	A904	C839	C769	C634	C634
	U1546		C1411	U1348	A1287	C1227	G1164	A1103	G1029	U966	U905	C840	U768	C635	C635
C1614	G1547	G1476	G1412	G1349	U1288	C1228	A1165	G1104		A967	A906	A841	U777	C701	C636
C1615	C1548	A1477	G1413	A1350	G1289	G1229	G1166		C1032	G968	G907	G842	U778	C702	C636
U1616			G1414	C1351		G1230	U1167	C1107	U1033	C969	G908	A843	U778	G703	C637
			U1415	A1352	C1292	A1231	U1168	U1108	U1034	A970	G909	G844	A780	U704	C638
U1620	U1553	A1481	C1416	U1353	U1293	C1232	A1169	U1109	G1035	G971	G910	G845	A781	A705	G639
A1621	U1554	A1482	G1417	G1354	A1294	G1233	A1170	U1110	A1036	A972	G911	A846	U782	U706	U640
U1622	U1555	G1483	A1418	A1355	G1295	G1234	G1171	U1111	C1037	A973	G912	A847	U783	U707	C641
G1623	U1556	U1484	U1356	U1356	C1296	U1235	G1172	A1112		G974	A913	A848	A783	G708	U642
	A1557	G1485	C1357	C1357	C1297	G1236	U1173	G1113	A1040	C975	A914	A849	A786	A709	U643
C1628	U1558	G1486	G1421	C1358	C1298	G1237	U1174	U1114	U1041	U976	A915	C851	A786	A710	G644
U1629	A1559	G1487	U1359	C1359	U1299	C1238	G1175	G1115	U1042	U976	G916	U852	A787	G712	A646
U1630	G1560		C1360	C1360	C1300	C1239	C1176	G1116	C1043	C979	A917	U852	C788	A647	
C1631	G1561	A1490	U1361	U1361	A1301	A1240	G1177	G1117	U1044	A980	G916	G856	C788	C648	
A1632	C1562	A1491	C1362	A1362	A1302	U1241	G1178	G1118	C1045	U981	U919	G857	C792	A716	A649
C1633	U1563	G1492	A1363	A1363	A1303	G1242	G1179	C1119	U1046	C982	A920	A858	C793	G650	
G1634	U1564	G1493	C1364	C1364	A1304	G1243	A1180	A1120	A1047	A983	A921	G859	U794	G651	






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5143	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.09	0/1090	1.31	4/1474 (0.3%)
79	B2	0.92	33/42128 (0.1%)	1.49	828/65642 (1.3%)
8	A7	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
80	B5	1.49	661/75336 (0.9%)	1.92	3722/117449 (3.2%)
81	B7	1.38	12/2883 (0.4%)	1.80	119/4491 (2.6%)
82	B8	1.16	4/3746 (0.1%)	1.70	128/5832 (2.2%)
83	CV	1.87	8/4407 (0.2%)	1.47	47/5931 (0.8%)
84	CW	2.08	51/1801 (2.8%)	3.23	250/2803 (8.9%)
85	CX	2.12	4/69 (5.8%)	3.20	11/106 (10.4%)
9	AA	0.54	0/1617	0.80	0/2215
All	All	1.14	811/222414 (0.4%)	1.53	5304/325931 (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
8	A7	0	1
80	B5	0	35
83	CV	0	18
84	CW	0	32
85	CX	0	2
All	All	0	125

The worst 5 of 811 bond length outliers are listed below:

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

The worst 5 of 5304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	36	U	P-O3'-C3'	-59.91	47.81	119.70
80	B5	1152	G	N3-C4-C5	33.59	145.40	128.60
80	B5	1256	G	P-O3'-C3'	32.78	159.04	119.70
80	B5	1152	G	N3-C4-N9	-31.65	107.01	126.00
80	B5	1152	G	N3-C2-N2	-26.89	101.08	119.90

There are no chirality outliers.

5 of 125 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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A7	1105	0	933	449	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	76	0
25	AQ	1105	0	1164	144	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	1195	88	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	1754	130	0
44	BJ	1353	0	1380	125	0
45	BK	753	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	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	918	0	0
76	Bq	1075	1110	1021	0	0
77	Br	236	237	65	0	0
78	Bs	231	232	67	0	0
79	B2	37835	0	19045	3138	0
80	B5	67308	664	33785	2411	0
81	B7	2579	0	1303	190	0
82	B8	3353	0	1695	115	0
83	CV	4451	4585	4534	558	0
84	CW	1614	789	802	457	0
85	CX	62	34	34	35	0
86	A0	1	0	0	0	0
86	A1	1	0	0	0	0
86	A3	1	0	0	0	0
86	A5	1	0	0	0	0
86	Bj	1	0	0	0	0
86	Bm	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	A0	2	0	0	0	0
87	A3	3	0	0	0	0
87	A5	1	0	0	0	0
87	AB	1	0	0	0	0
87	AC	2	0	0	0	0
87	AE	1	0	0	0	0
87	AG	1	0	0	0	0
87	AI	1	0	0	0	0
87	AJ	1	0	0	0	0
87	AL	2	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AS	1	0	0	0	0
87	AU	1	0	0	0	0
87	B2	168	0	0	0	0
87	B5	3	0	0	0	0
87	B7	27	0	0	0	0
87	BD	4	0	0	0	0
87	BF	1	0	0	0	0
87	BS	3	0	0	0	0
87	CW	1	0	0	0	0
88	A3	7	0	0	4	0
88	A6	7	0	0	2	0
88	AC	7	0	0	5	0
88	AI	14	0	0	2	0
88	AL	7	0	0	8	0
88	AN	7	0	0	2	0
88	AP	7	0	0	3	0
88	B2	1274	0	0	231	0
88	B5	21	0	0	4	0
88	B7	91	0	0	9	0
88	BR	7	0	0	9	0
88	Bn	7	0	0	0	0
88	CV	7	0	0	10	0
88	CX	7	0	0	2	0
89	CV	32	0	7	63	0
All	All	210964	8407	155586	9058	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 27.

The worst 5 of 9058 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)
80:B5:2621:G:C8	84:CW:75:C:C5	1.76	1.69
8:A7:85:SER:HB2	84:CW:30:G:C8	1.24	1.66
15:AG:175:ILE:HG12	79:B2:78:A:C4	1.29	1.65
83:CV:210:TRP:CZ3	83:CV:210:TRP:CH2	1.78	1.63
83:CV:210:TRP:CE3	83:CV:210:TRP:CZ3	1.83	1.61

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	25
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	15
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	29
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	4	33
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	2
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	29
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	14
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	6
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	24
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	1	21
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	16
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	1	13
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	2	26
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	15
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	20
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	9
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	2	22
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	24
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	7
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	6
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	16
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	10
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	1	12
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	15
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	26
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	7
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	6	40
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	6
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	1	12
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	4
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	5	37
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	7	41
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	2	23
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	8	43
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	6	38
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	9	47
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	1	14
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	8	43
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	2	23
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	17
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	2	23
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	24	67
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	5	37
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	13	54
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	4	33
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	11	50
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	27	70
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	13	54
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	4	34
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	11	51
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	2	22
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	19
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3	29
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	1	12
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	4	33
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	14
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	4	34
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	2	24
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	2	26
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	5	36
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	4	32
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	4	33
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	18
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	40
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	2	24
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	8	43
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	8	45
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	3	28
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	9	45
76	Bq	141/312 (45%)	105 (74%)	14 (10%)	22 (16%)	0	4
83	CV	555/586 (95%)	450 (81%)	61 (11%)	44 (8%)	1	16
All	All	11839/12944 (92%)	9833 (83%)	1245 (10%)	761 (6%)	3	21

5 of 761 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	7
2	A1	70/71 (99%)	62 (89%)	8 (11%)	6	26
3	A2	56/60 (93%)	38 (68%)	18 (32%)	0	2
4	A3	47/49 (96%)	38 (81%)	9 (19%)	1	10
5	A4	51/54 (94%)	43 (84%)	8 (16%)	3	17
6	A5	43/116 (37%)	32 (74%)	11 (26%)	0	4
7	A6	259/262 (99%)	221 (85%)	38 (15%)	3	19
8	A7	97/195 (50%)	74 (76%)	23 (24%)	1	5
9	AA	164/210 (78%)	122 (74%)	42 (26%)	0	4
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0	3
11	AC	176/205 (86%)	130 (74%)	46 (26%)	0	4
12	AD	182/195 (93%)	138 (76%)	44 (24%)	1	5
13	AE	221/222 (100%)	166 (75%)	55 (25%)	0	5
14	AF	173/191 (91%)	137 (79%)	36 (21%)	1	8
15	AG	188/201 (94%)	149 (79%)	39 (21%)	1	8
16	AH	165/170 (97%)	124 (75%)	41 (25%)	0	5
17	AI	150/161 (93%)	118 (79%)	32 (21%)	1	7
18	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	4
19	AK	77/98 (79%)	58 (75%)	19 (25%)	0	5
20	AL	129/137 (94%)	105 (81%)	24 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AM	88/119 (74%)	55 (62%)	33 (38%)	0	1
22	AN	127/128 (99%)	91 (72%)	36 (28%)	0	3
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	3
24	AP	101/118 (86%)	82 (81%)	19 (19%)	1	11
25	AQ	117/119 (98%)	83 (71%)	34 (29%)	0	3
26	AR	94/124 (76%)	70 (74%)	24 (26%)	0	4
27	AS	128/129 (99%)	87 (68%)	41 (32%)	0	2
28	AT	115/116 (99%)	84 (73%)	31 (27%)	0	4
29	AU	100/114 (88%)	71 (71%)	29 (29%)	0	3
30	AV	74/74 (100%)	56 (76%)	18 (24%)	1	5
31	AW	110/111 (99%)	84 (76%)	26 (24%)	1	5
32	AX	119/120 (99%)	97 (82%)	22 (18%)	2	11
33	AY	112/113 (99%)	84 (75%)	28 (25%)	0	4
34	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	3
35	BA	192/195 (98%)	153 (80%)	39 (20%)	1	8
36	BB	320/322 (99%)	250 (78%)	70 (22%)	1	7
37	BC	288/288 (100%)	223 (77%)	65 (23%)	1	6
38	BD	243/244 (100%)	196 (81%)	47 (19%)	1	10
39	BE	135/152 (89%)	115 (85%)	20 (15%)	3	19
40	BF	187/204 (92%)	158 (84%)	29 (16%)	3	17
41	BG	177/207 (86%)	138 (78%)	39 (22%)	1	7
42	BH	171/171 (100%)	132 (77%)	39 (23%)	1	6
43	BI	179/186 (96%)	142 (79%)	37 (21%)	1	8
44	BJ	147/149 (99%)	114 (78%)	33 (22%)	1	7
46	BL	154/158 (98%)	124 (80%)	30 (20%)	1	10
47	BM	108/108 (100%)	84 (78%)	24 (22%)	1	7
48	BN	175/175 (100%)	143 (82%)	32 (18%)	2	12
49	BO	323/178 (182%)	267 (83%)	56 (17%)	2	14
50	BP	125/145 (86%)	103 (82%)	22 (18%)	2	13
51	BQ	150/150 (100%)	123 (82%)	27 (18%)	2	12
52	BR	153/153 (100%)	121 (79%)	32 (21%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BS	156/156 (100%)	123 (79%)	33 (21%)	1	7
54	BT	136/136 (100%)	109 (80%)	27 (20%)	1	9
55	BU	85/106 (80%)	62 (73%)	23 (27%)	0	4
56	BV	104/104 (100%)	96 (92%)	8 (8%)	14	44
57	BW	100/129 (78%)	85 (85%)	15 (15%)	3	18
58	BX	104/117 (89%)	81 (78%)	23 (22%)	1	7
59	BY	109/109 (100%)	85 (78%)	24 (22%)	1	7
60	BZ	115/115 (100%)	89 (77%)	26 (23%)	1	6
61	Ba	118/118 (100%)	95 (80%)	23 (20%)	1	10
62	Bb	46/46 (100%)	35 (76%)	11 (24%)	1	5
63	Bc	84/87 (97%)	68 (81%)	16 (19%)	1	10
64	Bd	94/96 (98%)	73 (78%)	21 (22%)	1	7
65	Be	109/110 (99%)	89 (82%)	20 (18%)	2	12
66	Bf	90/90 (100%)	79 (88%)	11 (12%)	5	24
67	Bg	95/102 (93%)	71 (75%)	24 (25%)	0	4
68	Bh	103/104 (99%)	77 (75%)	26 (25%)	0	4
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	53 (76%)	17 (24%)	1	5
71	Bk	67/68 (98%)	53 (79%)	14 (21%)	1	8
72	Bl	45/45 (100%)	34 (76%)	11 (24%)	1	5
73	Bm	47/116 (40%)	34 (72%)	13 (28%)	0	3
74	Bn	23/23 (100%)	16 (70%)	7 (30%)	0	2
75	Bo	90/90 (100%)	74 (82%)	16 (18%)	2	13
76	Bq	101/254 (40%)	91 (90%)	10 (10%)	8	31
83	CV	481/497 (97%)	450 (94%)	31 (6%)	19	50
All	All	9986/10821 (92%)	7877 (79%)	2109 (21%)	4	7

5 of 2109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	AY	61	ARG
38	BD	118	THR
68	Bh	79	ASP

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Mol	Chain	Res	Type
34	AZ	85	LYS
36	BB	232	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
32	AX	48	HIS
38	BD	40	HIS
83	CV	65	GLN
35	BA	50	HIS
35	BA	215	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
79	B2	1764/1800 (98%)	545 (30%)	86 (4%)
80	B5	3140/3396 (92%)	741 (23%)	131 (4%)
81	B7	120/121 (99%)	18 (15%)	0
82	B8	157/158 (99%)	32 (20%)	3 (1%)
84	CW	74/76 (97%)	23 (31%)	5 (6%)
85	CX	2/3 (66%)	0	0
All	All	5257/5554 (94%)	1359 (25%)	225 (4%)

5 of 1359 RNA backbone outliers are listed below:

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

5 of 225 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
80	B5	588	G
80	B5	1094	U
80	B5	3228	C
80	B5	647	A
80	B5	896	A

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

9 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
83	HSO	CV	105	83	6,10,10	2.34	2 (33%)	4,12,12	1.87	2 (50%)
83	HSO	CV	13	83	6,10,10	2.17	1 (16%)	4,12,12	1.52	1 (25%)
83	HSO	CV	229	83	6,10,10	2.02	1 (16%)	4,12,12	1.75	1 (25%)
83	HSO	CV	295	83	6,10,10	2.11	1 (16%)	4,12,12	1.50	1 (25%)
83	HSO	CV	296	83	6,10,10	2.33	2 (33%)	4,12,12	2.27	2 (50%)
83	HSO	CV	541	83	6,10,10	2.71	2 (33%)	4,12,12	1.67	2 (50%)
83	HSO	CV	554	83	6,10,10	2.48	2 (33%)	4,12,12	1.52	1 (25%)
83	HSO	CV	556	83	6,10,10	2.38	2 (33%)	4,12,12	2.06	2 (50%)
83	HSO	CV	80	83	6,10,10	2.39	2 (33%)	4,12,12	1.38	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	HSO	CV	105	83	-	3/6/6/6	0/1/1/1
83	HSO	CV	13	83	-	5/6/6/6	0/1/1/1
83	HSO	CV	229	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	295	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	296	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	541	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	554	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	556	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	80	83	-	4/6/6/6	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CV	296	HSO	O-C	-4.66	1.22	1.42
83	CV	556	HSO	O-C	-4.66	1.22	1.42
83	CV	541	HSO	O-C	-4.65	1.22	1.42
83	CV	295	HSO	O-C	-4.64	1.22	1.42
83	CV	13	HSO	O-C	-4.61	1.23	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CV	296	HSO	CB-CA-C	-3.68	105.49	112.25
83	CV	556	HSO	CB-CA-C	-2.82	107.07	112.25
83	CV	556	HSO	O-C-CA	2.80	121.97	111.55
83	CV	229	HSO	O-C-CA	2.78	121.91	111.55
83	CV	105	HSO	CB-CA-C	-2.62	107.44	112.25

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	CV	105	HSO	O-C-CA-N
83	CV	105	HSO	O-C-CA-CB
83	CV	105	HSO	CA-CB-CG-ND1
83	CV	80	HSO	N-CA-CB-CG
83	CV	80	HSO	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	CV	13	HSO	1	0
83	CV	541	HSO	1	0
83	CV	554	HSO	1	0
83	CV	556	HSO	1	0
83	CV	80	HSO	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 443 ligands modelled in this entry, 232 are monoatomic - leaving 211 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
88	OHX	A3	102	-	0,6,6	0.00	-	-		
88	OHX	A6	401	-	0,6,6	0.00	-	-		
88	OHX	AC	301	-	0,6,6	0.00	-	-		
88	OHX	AI	301	-	0,6,6	0.00	-	-		
88	OHX	AI	302	-	0,6,6	0.00	-	-		
88	OHX	AL	201	-	0,6,6	0.00	-	-		
88	OHX	AN	201	-	0,6,6	0.00	-	-		
88	OHX	AP	201	-	0,6,6	0.00	-	-		
88	OHX	B2	1901	-	0,6,6	0.00	-	-		
88	OHX	B2	1902	-	0,6,6	0.00	-	-		
88	OHX	B2	1903	-	0,6,6	0.00	-	-		
88	OHX	B2	1904	-	0,6,6	0.00	-	-		
88	OHX	B2	1905	-	0,6,6	0.00	-	-		
88	OHX	B2	1906	87	0,6,6	0.00	-	-		
88	OHX	B2	1907	-	0,6,6	0.00	-	-		
88	OHX	B2	1908	-	0,6,6	0.00	-	-		
88	OHX	B2	1909	88	0,6,6	0.00	-	-		
88	OHX	B2	1910	-	0,6,6	0.00	-	-		
88	OHX	B2	1911	-	0,6,6	0.00	-	-		
88	OHX	B2	1912	-	0,6,6	0.00	-	-		
88	OHX	B2	1913	-	0,6,6	0.00	-	-		
88	OHX	B2	1914	-	0,6,6	0.00	-	-		
88	OHX	B2	1915	-	0,6,6	0.00	-	-		
88	OHX	B2	1916	-	0,6,6	0.00	-	-		
88	OHX	B2	1917	-	0,6,6	0.00	-	-		
88	OHX	B2	1918	88	0,6,6	0.00	-	-		
88	OHX	B2	1919	-	0,6,6	0.00	-	-		
88	OHX	B2	1920	-	0,6,6	0.00	-	-		
88	OHX	B2	1921	-	0,6,6	0.00	-	-		
88	OHX	B2	1922	-	0,6,6	0.00	-	-		
88	OHX	B2	1923	-	0,6,6	0.00	-	-		
88	OHX	B2	1924	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	B2	1925	-	0,6,6	0.00	-	-		
88	OHX	B2	1926	-	0,6,6	0.00	-	-		
88	OHX	B2	1927	-	0,6,6	0.00	-	-		
88	OHX	B2	1928	-	0,6,6	0.00	-	-		
88	OHX	B2	1929	-	0,6,6	0.00	-	-		
88	OHX	B2	1930	-	0,6,6	0.00	-	-		
88	OHX	B2	1931	-	0,6,6	0.00	-	-		
88	OHX	B2	1932	-	0,6,6	0.00	-	-		
88	OHX	B2	1933	-	0,6,6	0.00	-	-		
88	OHX	B2	1934	-	0,6,6	0.00	-	-		
88	OHX	B2	1935	-	0,6,6	0.00	-	-		
88	OHX	B2	1936	-	0,6,6	0.00	-	-		
88	OHX	B2	1937	-	0,6,6	0.00	-	-		
88	OHX	B2	1938	-	0,6,6	0.00	-	-		
88	OHX	B2	1939	-	0,6,6	0.00	-	-		
88	OHX	B2	1940	-	0,6,6	0.00	-	-		
88	OHX	B2	1941	-	0,6,6	0.00	-	-		
88	OHX	B2	1942	-	0,6,6	0.00	-	-		
88	OHX	B2	1943	-	0,6,6	0.00	-	-		
88	OHX	B2	1944	-	0,6,6	0.00	-	-		
88	OHX	B2	1945	-	0,6,6	0.00	-	-		
88	OHX	B2	1946	-	0,6,6	0.00	-	-		
88	OHX	B2	1947	-	0,6,6	0.00	-	-		
88	OHX	B2	1948	-	0,6,6	0.00	-	-		
88	OHX	B2	1949	-	0,6,6	0.00	-	-		
88	OHX	B2	1950	-	0,6,6	0.00	-	-		
88	OHX	B2	1951	-	0,6,6	0.00	-	-		
88	OHX	B2	1952	-	0,6,6	0.00	-	-		
88	OHX	B2	1953	-	0,6,6	0.00	-	-		
88	OHX	B2	1954	-	0,6,6	0.00	-	-		
88	OHX	B2	1955	-	0,6,6	0.00	-	-		
88	OHX	B2	1956	-	0,6,6	0.00	-	-		
88	OHX	B2	1957	-	0,6,6	0.00	-	-		
88	OHX	B2	1958	-	0,6,6	0.00	-	-		
88	OHX	B2	1959	-	0,6,6	0.00	-	-		
88	OHX	B2	1960	-	0,6,6	0.00	-	-		
88	OHX	B2	1961	-	0,6,6	0.00	-	-		
88	OHX	B2	1962	-	0,6,6	0.00	-	-		
88	OHX	B2	1963	-	0,6,6	0.00	-	-		
88	OHX	B2	1964	-	0,6,6	0.00	-	-		
88	OHX	B2	1965	-	0,6,6	0.00	-	-		
88	OHX	B2	1966	-	0,6,6	0.00	-	-		
88	OHX	B2	1967	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	B2	1968	-	0,6,6	0.00	-	-		
88	OHX	B2	1969	-	0,6,6	0.00	-	-		
88	OHX	B2	1970	-	0,6,6	0.00	-	-		
88	OHX	B2	1971	-	0,6,6	0.00	-	-		
88	OHX	B2	1972	-	0,6,6	0.00	-	-		
88	OHX	B2	1973	-	0,6,6	0.00	-	-		
88	OHX	B2	1974	-	0,6,6	0.00	-	-		
88	OHX	B2	1975	-	0,6,6	0.00	-	-		
88	OHX	B2	1976	-	0,6,6	0.00	-	-		
88	OHX	B2	1977	-	0,6,6	0.00	-	-		
88	OHX	B2	1978	-	0,6,6	0.00	-	-		
88	OHX	B2	1979	-	0,6,6	0.00	-	-		
88	OHX	B2	1980	-	0,6,6	0.00	-	-		
88	OHX	B2	1981	-	0,6,6	0.00	-	-		
88	OHX	B2	1982	-	0,6,6	0.00	-	-		
88	OHX	B2	1983	-	0,6,6	0.00	-	-		
88	OHX	B2	1984	-	0,6,6	0.00	-	-		
88	OHX	B2	1985	-	0,6,6	0.00	-	-		
88	OHX	B2	1986	-	0,6,6	0.00	-	-		
88	OHX	B2	1987	-	0,6,6	0.00	-	-		
88	OHX	B2	1988	-	0,6,6	0.00	-	-		
88	OHX	B2	1989	-	0,6,6	0.00	-	-		
88	OHX	B2	1990	-	0,6,6	0.00	-	-		
88	OHX	B2	1991	-	0,6,6	0.00	-	-		
88	OHX	B2	1992	-	0,6,6	0.00	-	-		
88	OHX	B2	1993	-	0,6,6	0.00	-	-		
88	OHX	B2	1994	-	0,6,6	0.00	-	-		
88	OHX	B2	1995	-	0,6,6	0.00	-	-		
88	OHX	B2	1996	-	0,6,6	0.00	-	-		
88	OHX	B2	1997	-	0,6,6	0.00	-	-		
88	OHX	B2	1998	-	0,6,6	0.00	-	-		
88	OHX	B2	1999	-	0,6,6	0.00	-	-		
88	OHX	B2	2000	-	0,6,6	0.00	-	-		
88	OHX	B2	2001	-	0,6,6	0.00	-	-		
88	OHX	B2	2002	-	0,6,6	0.00	-	-		
88	OHX	B2	2003	-	0,6,6	0.00	-	-		
88	OHX	B2	2004	-	0,6,6	0.00	-	-		
88	OHX	B2	2005	-	0,6,6	0.00	-	-		
88	OHX	B2	2006	-	0,6,6	0.00	-	-		
88	OHX	B2	2007	-	0,6,6	0.00	-	-		
88	OHX	B2	2008	-	0,6,6	0.00	-	-		
88	OHX	B2	2009	-	0,6,6	0.00	-	-		
88	OHX	B2	2010	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	B2	2011	-	0,6,6	0.00	-	-		
88	OHX	B2	2012	-	0,6,6	0.00	-	-		
88	OHX	B2	2013	-	0,6,6	0.00	-	-		
88	OHX	B2	2014	-	0,6,6	0.00	-	-		
88	OHX	B2	2015	-	0,6,6	0.00	-	-		
88	OHX	B2	2016	-	0,6,6	0.00	-	-		
88	OHX	B2	2017	-	0,6,6	0.00	-	-		
88	OHX	B2	2018	-	0,6,6	0.00	-	-		
88	OHX	B2	2019	-	0,6,6	0.00	-	-		
88	OHX	B2	2020	-	0,6,6	0.00	-	-		
88	OHX	B2	2021	-	0,6,6	0.00	-	-		
88	OHX	B2	2022	-	0,6,6	0.00	-	-		
88	OHX	B2	2023	-	0,6,6	0.00	-	-		
88	OHX	B2	2024	-	0,6,6	0.00	-	-		
88	OHX	B2	2025	-	0,6,6	0.00	-	-		
88	OHX	B2	2026	-	0,6,6	0.00	-	-		
88	OHX	B2	2027	-	0,6,6	0.00	-	-		
88	OHX	B2	2028	-	0,6,6	0.00	-	-		
88	OHX	B2	2029	88	0,6,6	0.00	-	-		
88	OHX	B2	2030	-	0,6,6	0.00	-	-		
88	OHX	B2	2031	-	0,6,6	0.00	-	-		
88	OHX	B2	2032	-	0,6,6	0.00	-	-		
88	OHX	B2	2033	-	0,6,6	0.00	-	-		
88	OHX	B2	2034	-	0,6,6	0.00	-	-		
88	OHX	B2	2035	-	0,6,6	0.00	-	-		
88	OHX	B2	2036	-	0,6,6	0.00	-	-		
88	OHX	B2	2037	-	0,6,6	0.00	-	-		
88	OHX	B2	2038	-	0,6,6	0.00	-	-		
88	OHX	B2	2039	-	0,6,6	0.00	-	-		
88	OHX	B2	2040	-	0,6,6	0.00	-	-		
88	OHX	B2	2041	-	0,6,6	0.00	-	-		
88	OHX	B2	2042	-	0,6,6	0.00	-	-		
88	OHX	B2	2043	-	0,6,6	0.00	-	-		
88	OHX	B2	2044	-	0,6,6	0.00	-	-		
88	OHX	B2	2045	-	0,6,6	0.00	-	-		
88	OHX	B2	2046	-	0,6,6	0.00	-	-		
88	OHX	B2	2047	-	0,6,6	0.00	-	-		
88	OHX	B2	2048	87	0,6,6	0.00	-	-		
88	OHX	B2	2049	-	0,6,6	0.00	-	-		
88	OHX	B2	2050	-	0,6,6	0.00	-	-		
88	OHX	B2	2051	-	0,6,6	0.00	-	-		
88	OHX	B2	2052	-	0,6,6	0.00	-	-		
88	OHX	B2	2053	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	B2	2054	-	0,6,6	0.00	-	-		
88	OHX	B2	2055	-	0,6,6	0.00	-	-		
88	OHX	B2	2056	-	0,6,6	0.00	-	-		
88	OHX	B2	2057	-	0,6,6	0.00	-	-		
88	OHX	B2	2058	-	0,6,6	0.00	-	-		
88	OHX	B2	2059	-	0,6,6	0.00	-	-		
88	OHX	B2	2060	-	0,6,6	0.00	-	-		
88	OHX	B2	2061	-	0,6,6	0.00	-	-		
88	OHX	B2	2062	88,87	0,6,6	0.00	-	-		
88	OHX	B2	2063	-	0,6,6	0.00	-	-		
88	OHX	B2	2064	-	0,6,6	0.00	-	-		
88	OHX	B2	2065	-	0,6,6	0.00	-	-		
88	OHX	B2	2066	-	0,6,6	0.00	-	-		
88	OHX	B2	2067	-	0,6,6	0.00	-	-		
88	OHX	B2	2068	-	0,6,6	0.00	-	-		
88	OHX	B2	2069	79	0,6,6	0.00	-	-		
88	OHX	B2	2070	-	0,6,6	0.00	-	-		
88	OHX	B2	2071	-	0,6,6	0.00	-	-		
88	OHX	B2	2072	-	0,6,6	0.00	-	-		
88	OHX	B2	2073	-	0,6,6	0.00	-	-		
88	OHX	B2	2074	-	0,6,6	0.00	-	-		
88	OHX	B2	2075	-	0,6,6	0.00	-	-		
88	OHX	B2	2076	-	0,6,6	0.00	-	-		
88	OHX	B2	2077	-	0,6,6	0.00	-	-		
88	OHX	B2	2078	-	0,6,6	0.00	-	-		
88	OHX	B2	2079	-	0,6,6	0.00	-	-		
88	OHX	B2	2080	-	0,6,6	0.00	-	-		
88	OHX	B2	2081	-	0,6,6	0.00	-	-		
88	OHX	B2	2082	-	0,6,6	0.00	-	-		
88	OHX	B5	3401	-	0,6,6	0.00	-	-		
88	OHX	B5	3402	-	0,6,6	0.00	-	-		
88	OHX	B5	3403	-	0,6,6	0.00	-	-		
88	OHX	B7	201	-	0,6,6	0.00	-	-		
88	OHX	B7	202	-	0,6,6	0.00	-	-		
88	OHX	B7	203	-	0,6,6	0.00	-	-		
88	OHX	B7	204	-	0,6,6	0.00	-	-		
88	OHX	B7	205	-	0,6,6	0.00	-	-		
88	OHX	B7	206	-	0,6,6	0.00	-	-		
88	OHX	B7	210	-	0,6,6	0.00	-	-		
88	OHX	B7	212	-	0,6,6	0.00	-	-		
88	OHX	B7	214	-	0,6,6	0.00	-	-		
88	OHX	B7	215	-	0,6,6	0.00	-	-		
88	OHX	B7	219	87	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	B7	220	-	0,6,6	0.00	-	-		
88	OHX	B7	221	-	0,6,6	0.00	-	-		
88	OHX	BR	201	-	0,6,6	0.00	-	-		
88	OHX	Bn	101	-	0,6,6	0.00	-	-		
88	OHX	CV	601	-	0,6,6	0.00	-	-		
89	GCP	CV	602	-	26,34,34	2.77	7 (26%)	31,54,54	2.39	7 (22%)
88	OHX	CX	101	-	0,6,6	0.00	-	-		

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	GCP	CV	602	-	-	2/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	CV	602	GCP	C4-N9	-9.57	1.35	1.47
89	CV	602	GCP	C6-N1	5.56	1.42	1.33
89	CV	602	GCP	C5-C6	-5.10	1.44	1.52
89	CV	602	GCP	C2'-C1'	-2.98	1.43	1.53
89	CV	602	GCP	C8-N9	-2.63	1.36	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	CV	602	GCP	O3G-PG-C3B	-7.36	88.55	106.40
89	CV	602	GCP	C4-C5-N7	6.46	111.02	102.46
89	CV	602	GCP	C5-C6-N1	-3.76	113.79	118.27
89	CV	602	GCP	O6-C6-C5	3.50	127.03	119.82
89	CV	602	GCP	O1B-PB-C3B	2.92	116.72	109.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

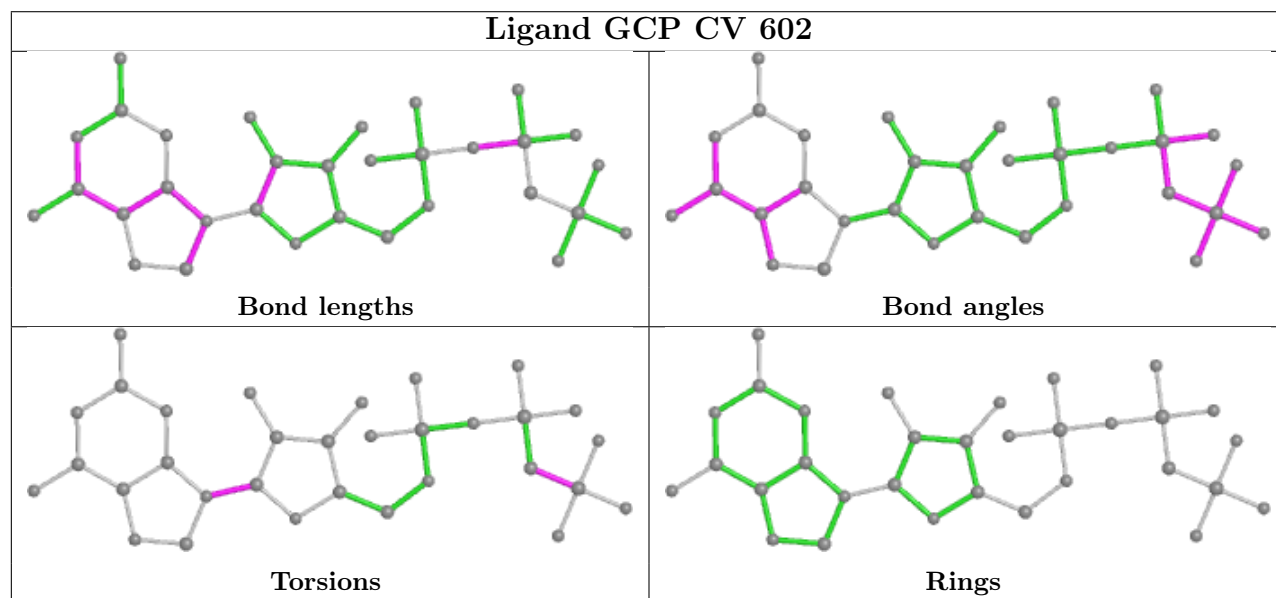
Mol	Chain	Res	Type	Atoms
89	CV	602	GCP	C2'-C1'-N9-C4
89	CV	602	GCP	PB-C3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	CV	602	GCP	63	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	B5	1
84	CW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	1285:G	O3'	1286:A	P	6.77
1	CW	33:U	O3'	34:C	P	4.25