



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:19 PM UTC

PDB ID : 4V5L / pdb_00004v5l
Title : The structure of EF-Tu and aminoacyl-tRNA bound to the 70S ribosome with a GTP analog
Authors : Voorhees, R.M.; Schmeing, T.M.; Ramakrishnan, V.
Deposited on : 2010-09-02
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

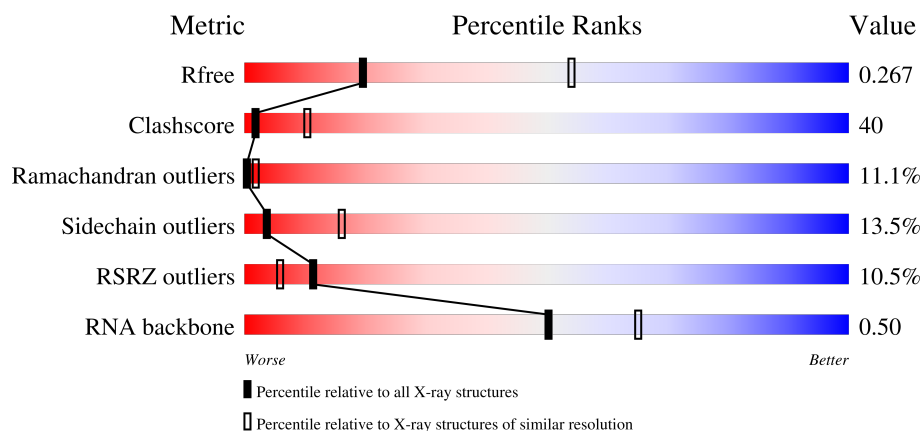
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	5% 33% 52% 10% ..
2	AB	256	6% 19% 49% 21% 9%
3	AC	239	% 23% 51% 12% 14%
4	AD	209	4% 35% 47% 16% .

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
22	AW	76	
23	AX	14	
24	AY	77	
25	AZ	405	
26	B0	85	
27	B1	98	
28	B2	72	

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Mol	Chain	Length	Quality of chain
29	B3	60	
30	B4	71	
31	B5	60	
32	B6	54	
33	B7	49	
34	B8	65	
35	B9	37	
36	BA	2915	
37	BB	122	
38	BC	229	
39	BD	276	
40	BE	206	
41	BF	210	
42	BG	182	
43	BH	180	
44	BJ	130	
45	BK	140	
46	BN	140	
47	BO	122	
48	BP	150	
49	BQ	141	
50	BR	118	
51	BS	112	
52	BT	146	
53	BU	118	

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Mol	Chain	Length	Quality of chain
54	BV	101	
55	BW	113	
56	BX	96	
57	BY	110	
58	BZ	206	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	expression tag	UNP P17293
AL	2	VAL	-	expression tag	UNP P17293
AL	3	ALA	-	expression tag	UNP P17293
AL	4	LEU	-	expression tag	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	14	Total	C	N	O	P	0	0	0
			298	135	56	94	13			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0
			1644	742	289	535	76	2		

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	405	Total	C	N	O	S	0	0	0
			3142	1983	550	597	12			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	27	ARG	LEU	conflict	UNP Q5SLP7

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O	S	0	0	0
			770	486	154	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

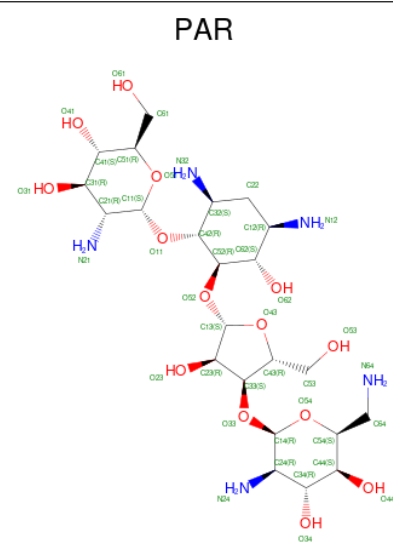
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 59 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).

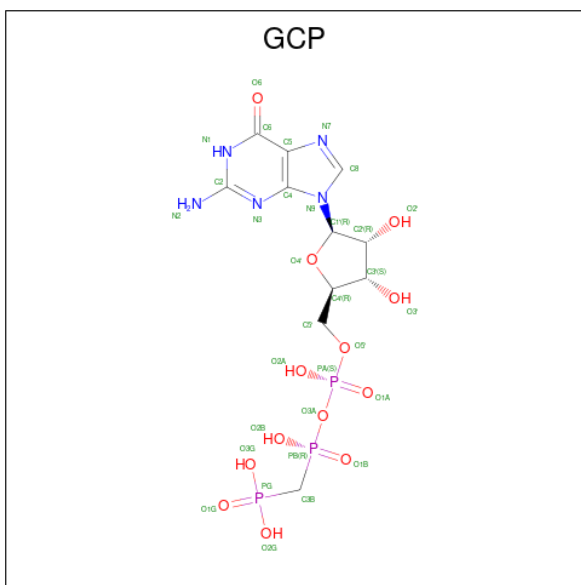


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total 42	C 23	N 5	O 14	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	1	Total 1	Zn 1	0	0
60	AN	1	Total 1	Zn 1	0	0
60	B4	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).



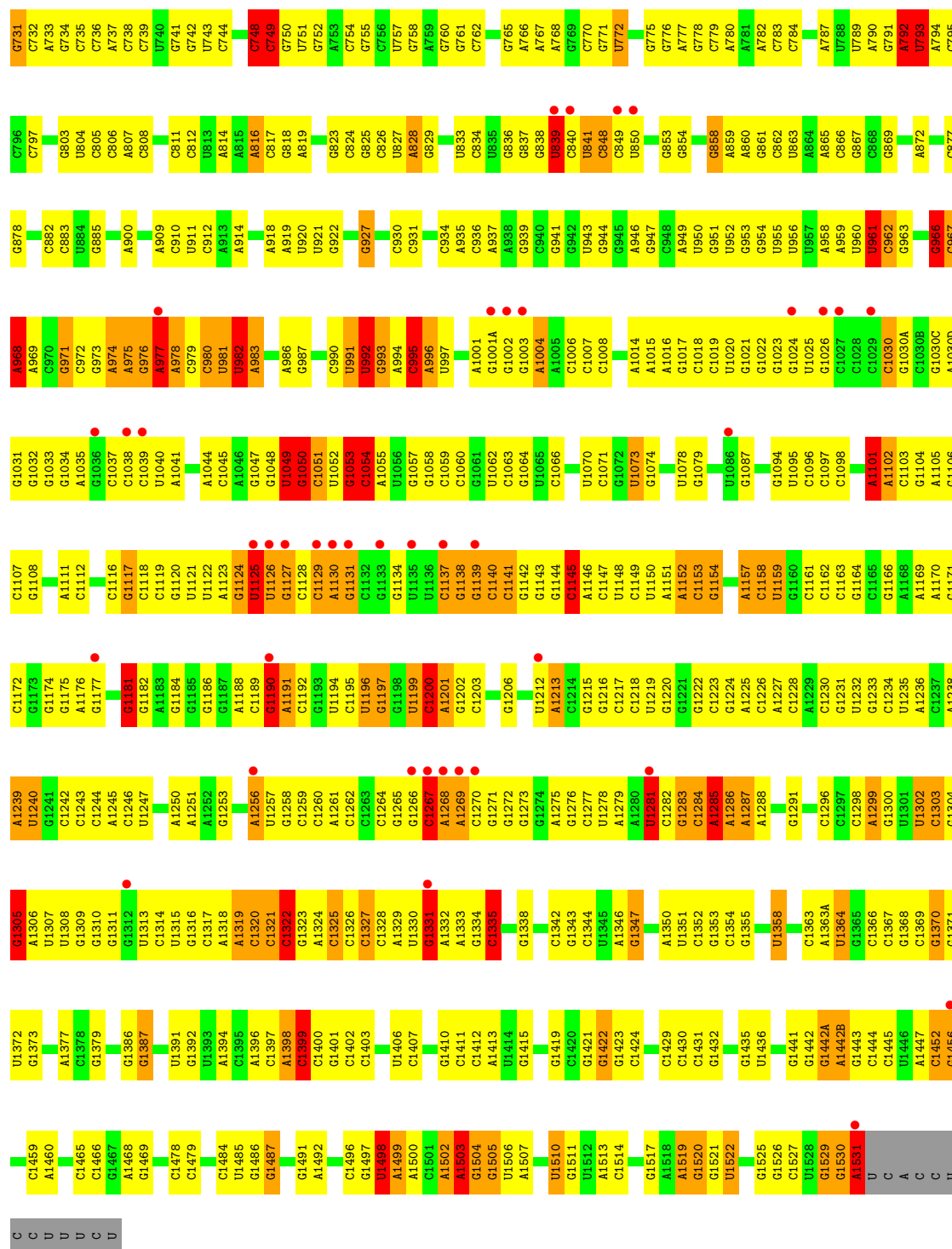
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
61	AZ	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

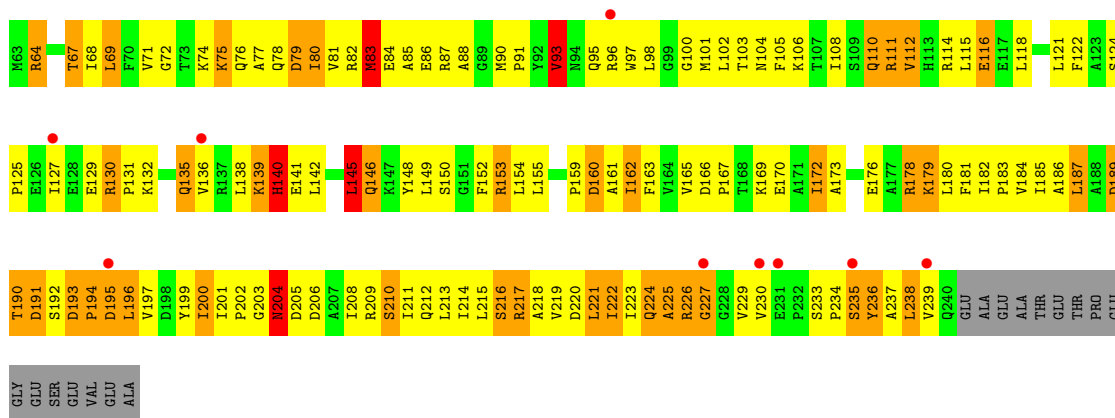
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AZ	1	Total Mg 1 1	0	0

- Molecule 63 is water.

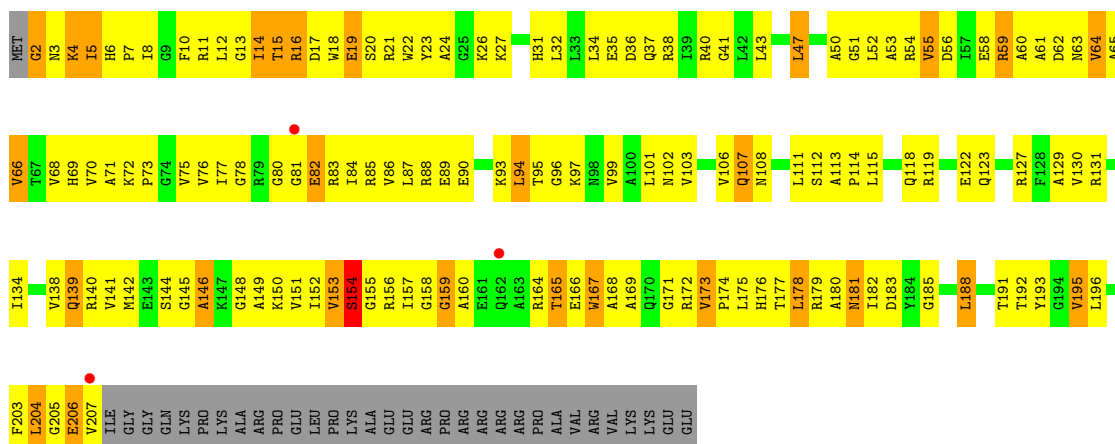
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AZ	1	Total O 1 1	0	0



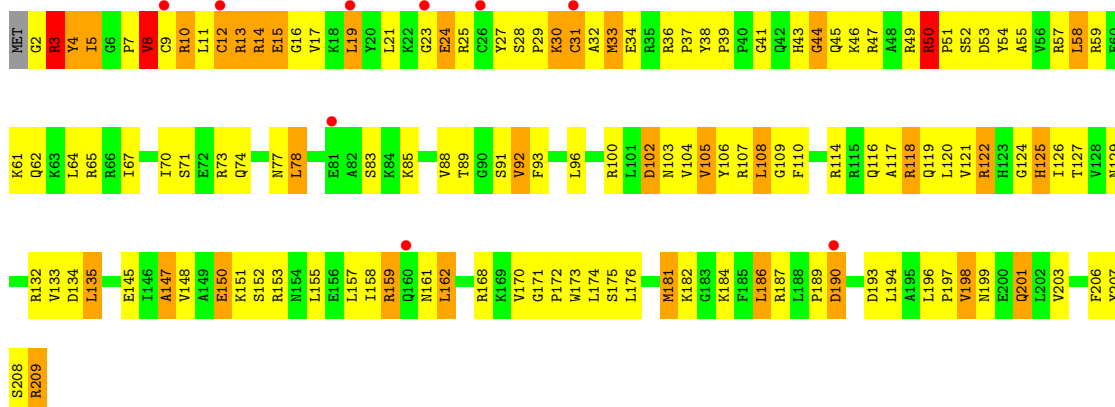
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

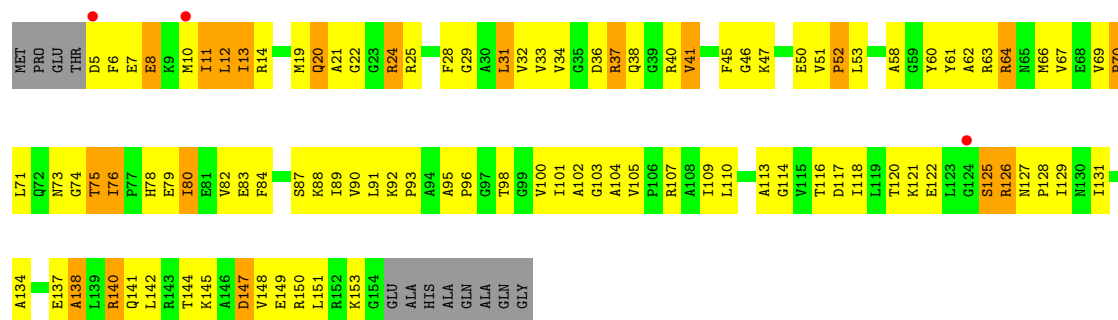


• Molecule 4: 30S RIBOSOMAL PROTEIN S4



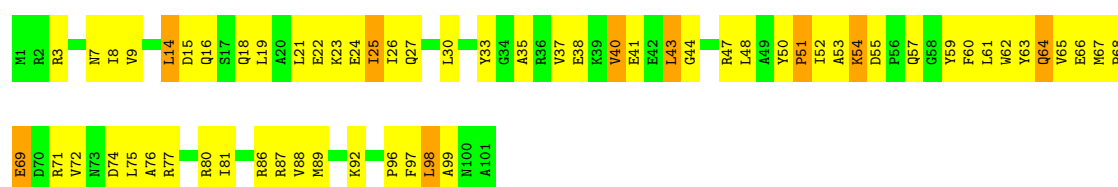
• Molecule 5: 30S RIBOSOMAL PROTEIN S5





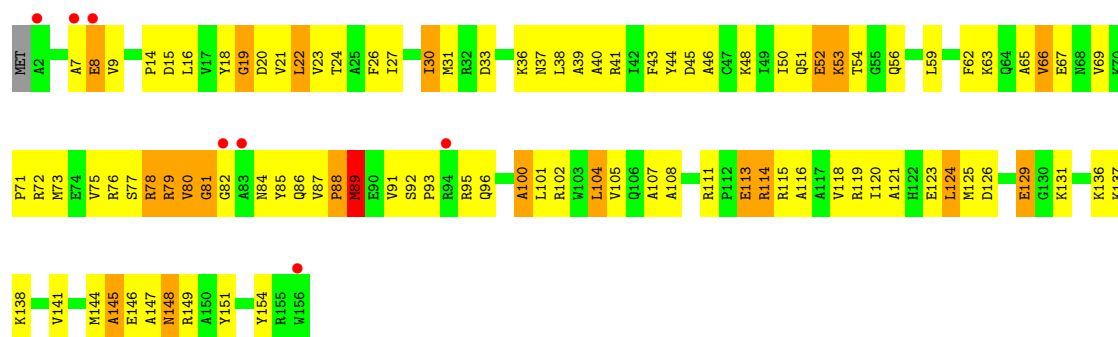
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 39% 52% 9%



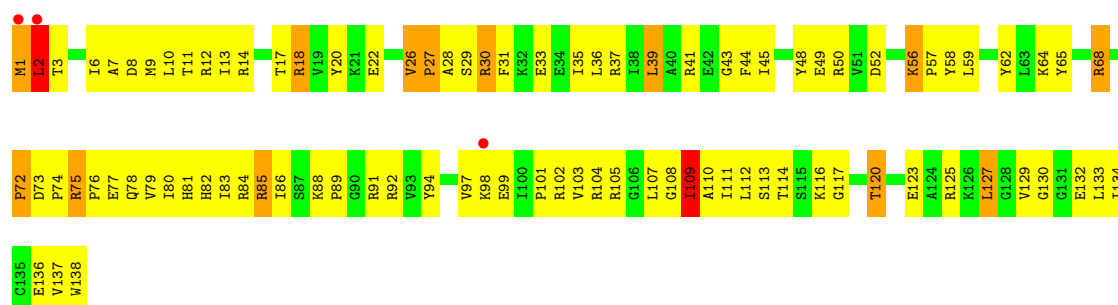
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG: 4% 37% 49% 13% ..

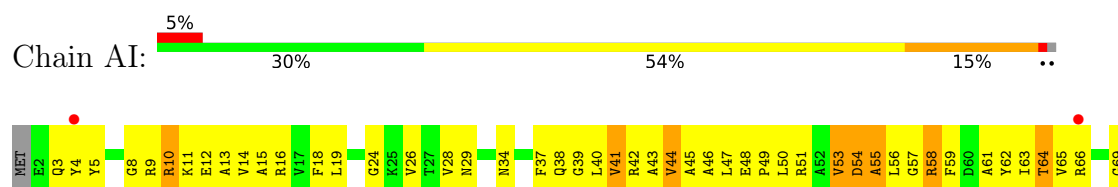


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

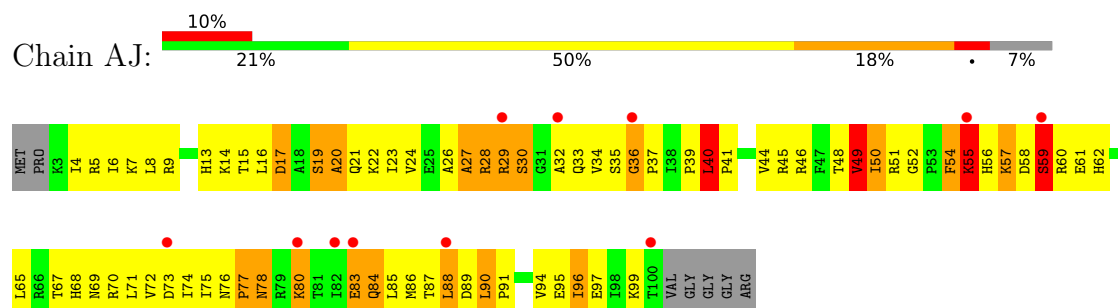
Chain AH: 2% 33% 57% 9% .



• Molecule 9: 30S RIBOSOMAL PROTEIN S9



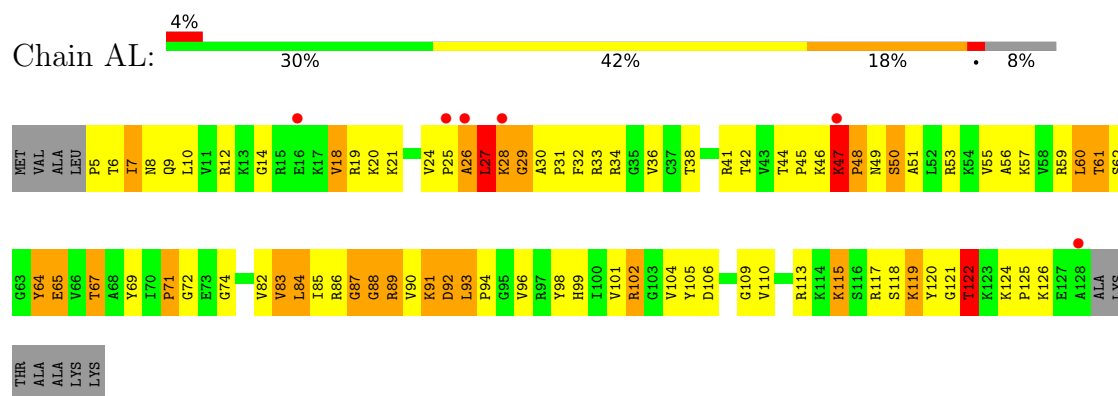
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



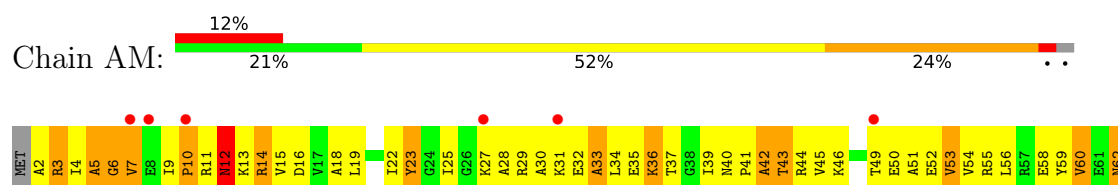
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

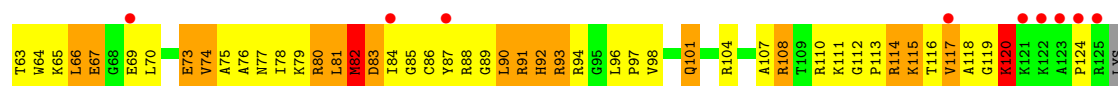


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

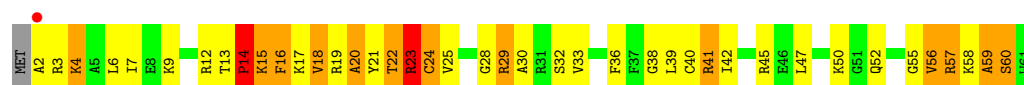


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

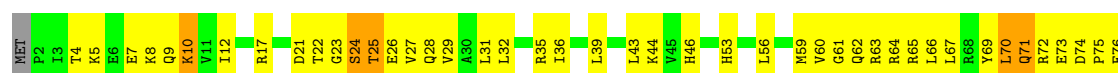




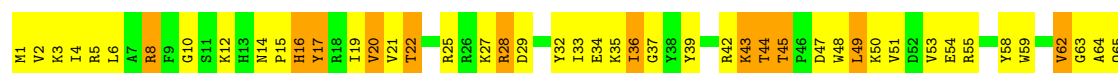
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



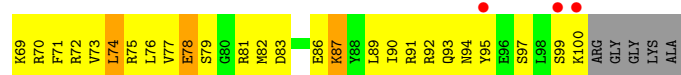
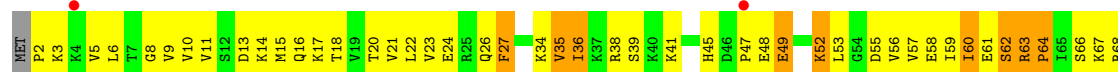
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



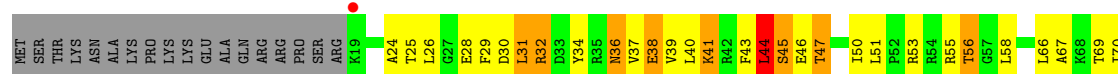
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

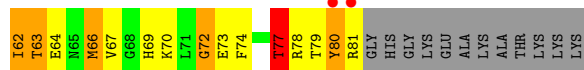
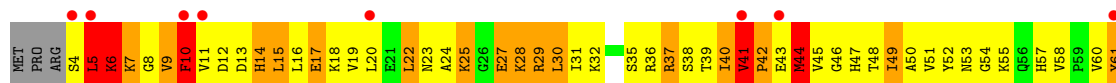


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

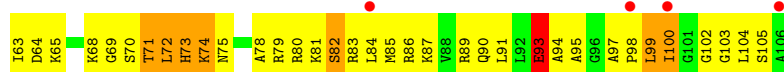
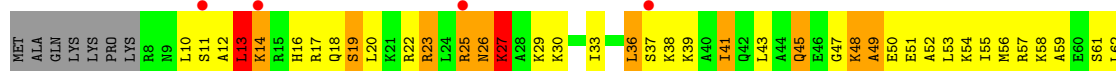




• Molecule 19: 30S RIBOSOMAL PROTEIN S19



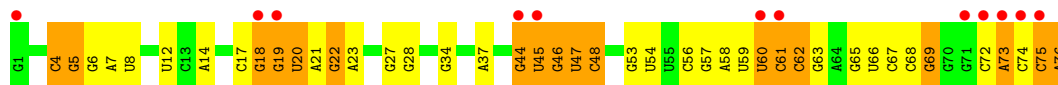
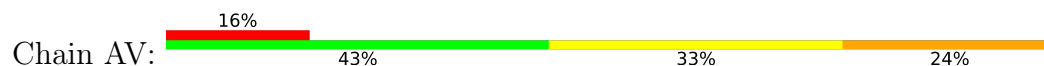
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



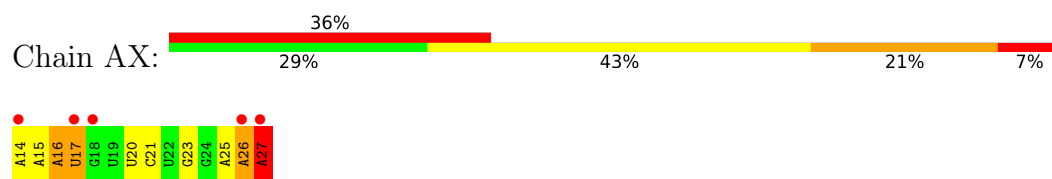
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



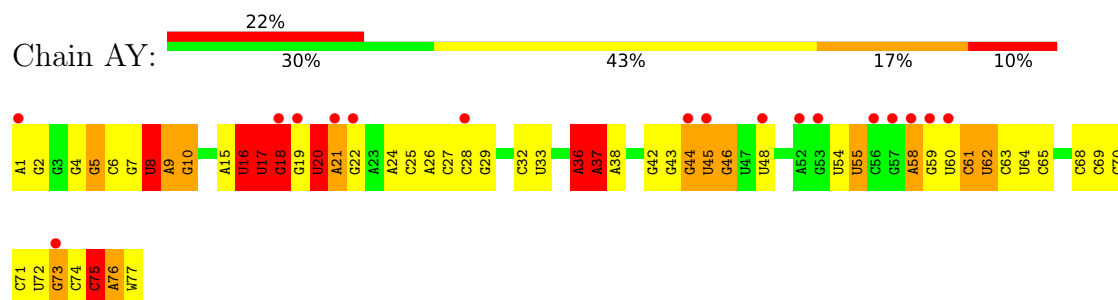
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



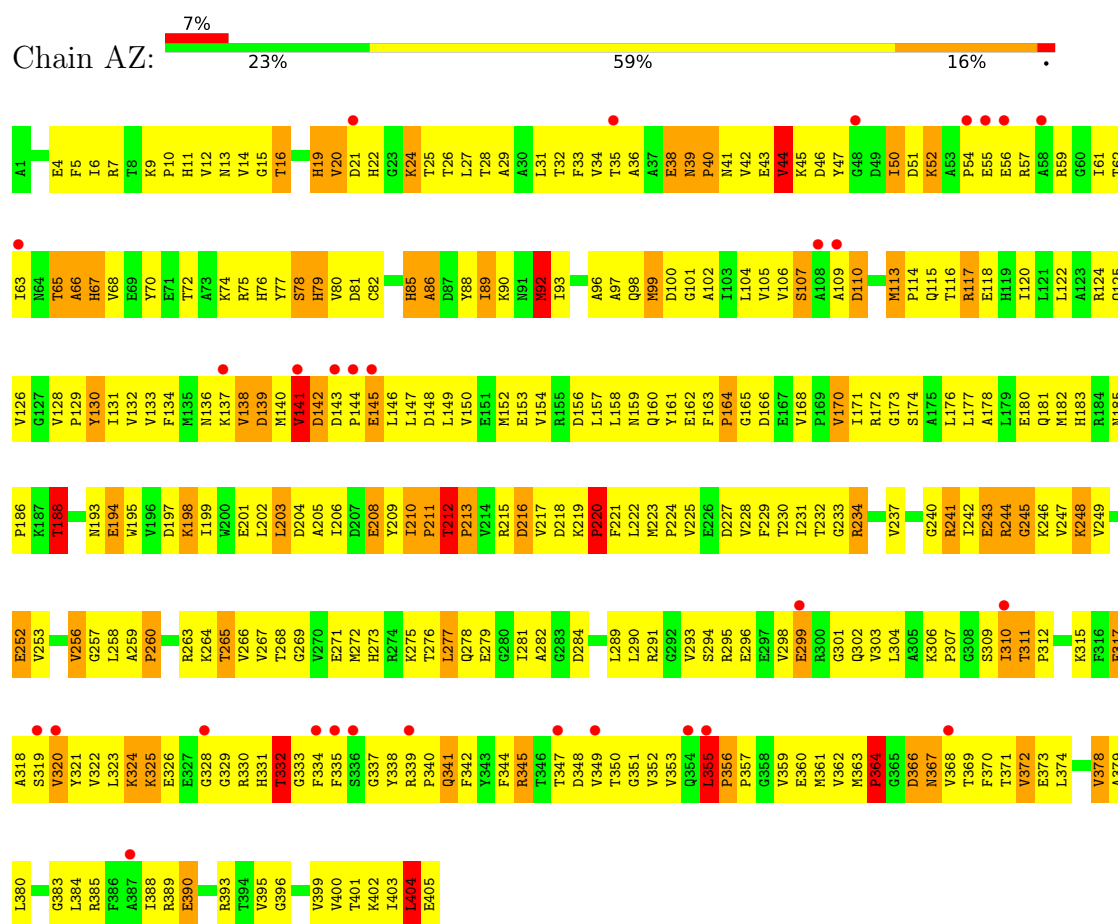
• Molecule 23: MRNA



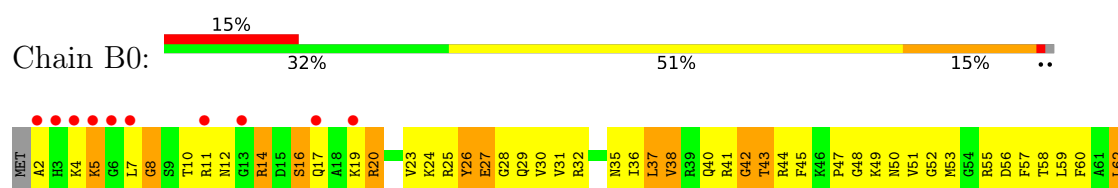
• Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

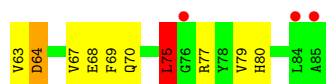


• Molecule 25: ELONGATION FACTOR TU

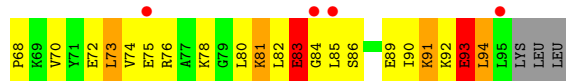


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

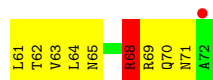




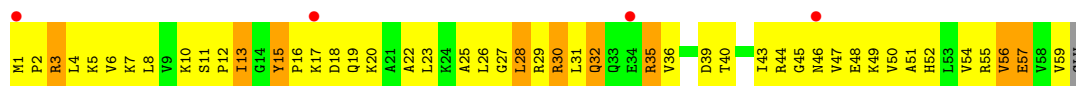
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



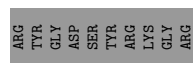
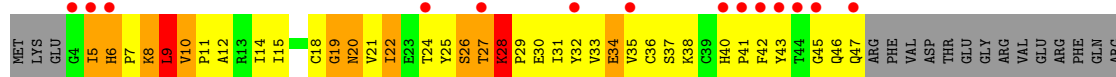
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



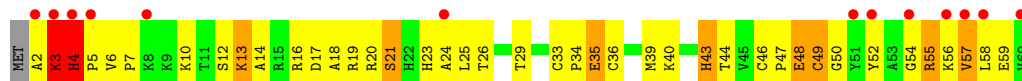
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



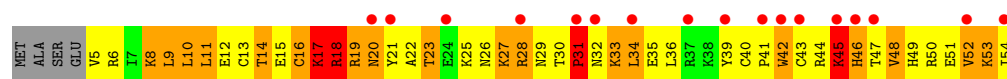
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



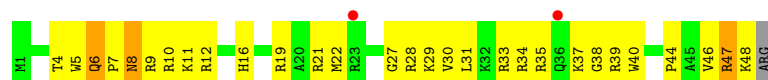
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



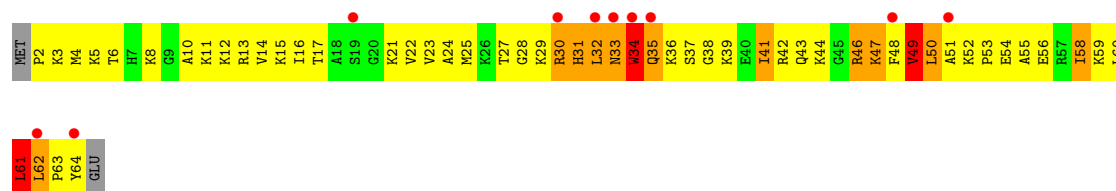
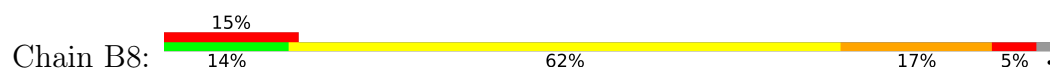
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



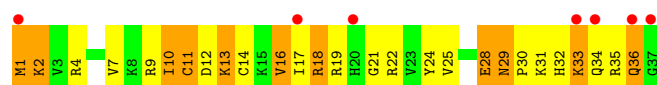
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



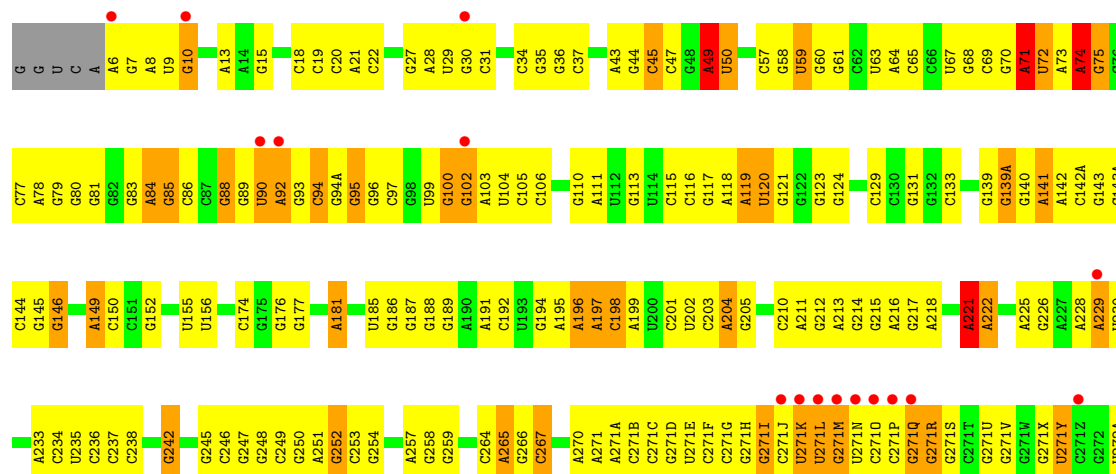
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

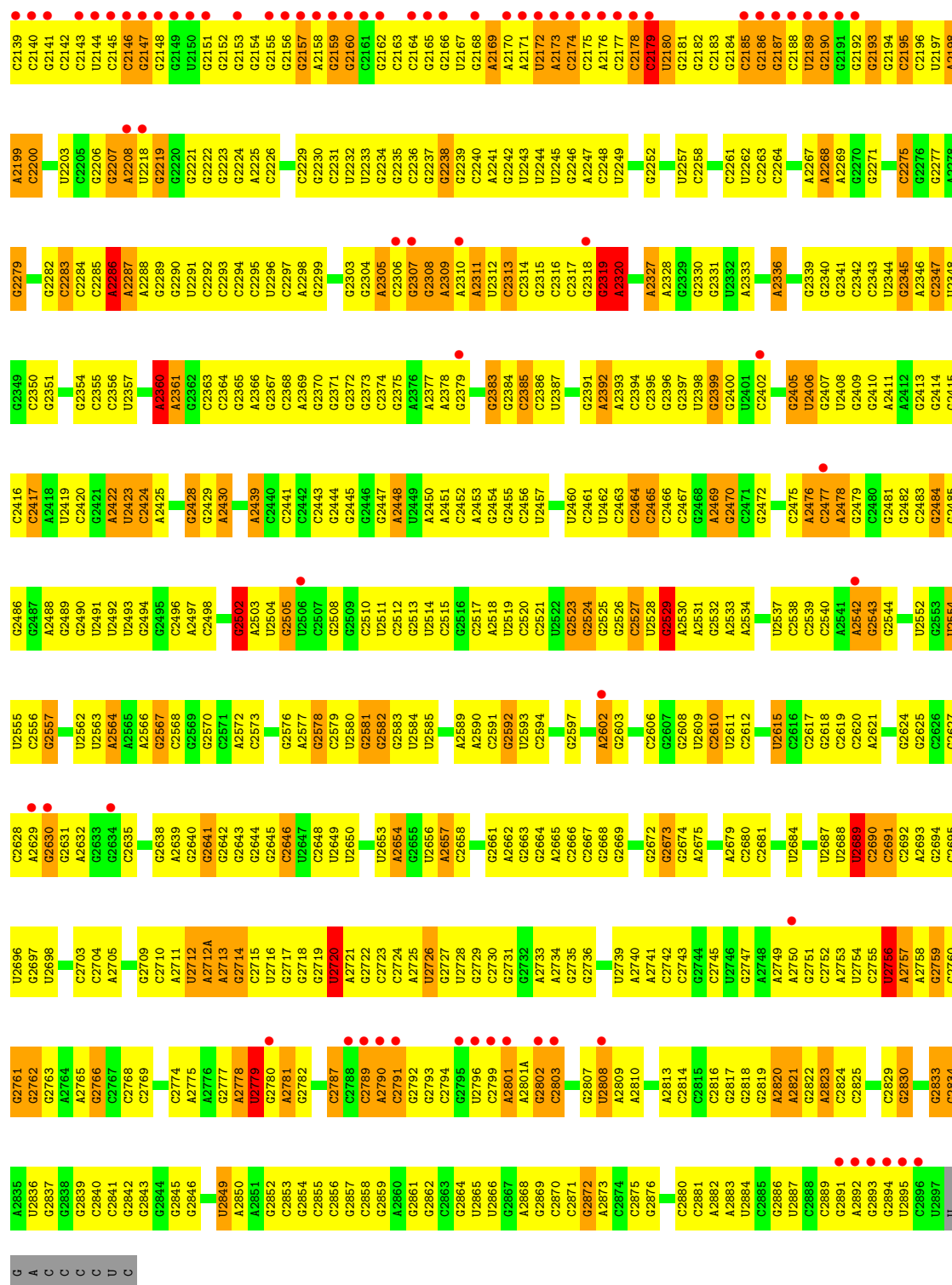


- Molecule 36: 23S RIBOSOMAL RNA

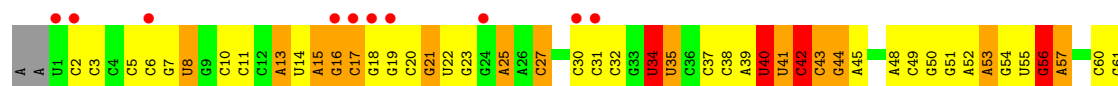


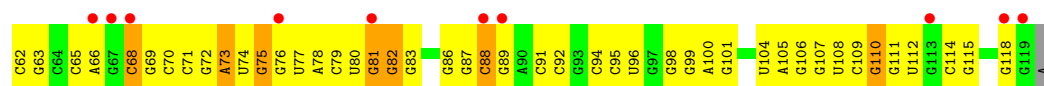
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A1142A	U1078	U1012	U943	A878	U803	C730	A654U	G613	G552	C487	G406	C334	G272D
A1143	C1079	C1013	G944	G879	A804	C731	A654V	U614	G553		G407	C335	
G1144	C1080	U1014	A945	G880	C805	G732	G656	U614B	U554	G491	G408	C336	C272H
C1145	U1081		G946	G881	C806	G733	G657	A614C	U555	G492		C337	U272I
	U1082	C1018	G947	G882	U807		C658	G615	G556	G493		C338	C272J
	U1083	U1019	G948	G883	U810	C736	U657	G616	U557	G494		U339	G274
A1148	A1084	A1020	G949	G884	U811	C737	C659	G618	G558	G495	C414	A340	G275
G1149	A1085	A1021	G950	G885	U812	G738	C660	G619	G559	G496	A415	A276	G276
C1150	A1086	G1022	C951	C886	C812	G739	C661	G620	G560	A497	C416	C342	C277
C1152	G1087	U1023	G952	A887	U813	U740	G662	G621	G561	G498		C343	
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G1154	U1090	U1026	G956	A890	C816	G743	G669	G623	C564	A501	U421	G348	C286
A1155	A1091	A1027	A957	G892	G744	G744	A670	C624	U566	A502		G349	C287
A1156	U1092	A1028	G958	C893	A819	G745	C671	G625	A567	C426		G352	C288
G1157	G1093	C994	A959	C894	A820	G746	C672	U626	U568	U427		G353	A289
C1158	U1094	A821	A960	U895	A822	U747	C673	A627	U569	A428		G354	G290
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G1160	C997		G962	C998	U827	A752	A675	G629	A571	A507		G356	U293
C1161	U1097	C1038	U963	C999	U828	C753	A676	G630	A572	C508	G438	A357	G295
G1162	G1098	G1039	C964	A999	A829	C754		A631	G573	G509	G440	G358	A294
G1163	U1099	C1040	C965	C903	G830	C755		A632	C574	C510	U441	A359	G296
U1165	U1101	G1041	G968	C904	G831	U757		C634	U576	U511	A443	G380	C297
C1166	C1102	G1042	U969	U905	G832		G686	C635	G577	A513	C444	G361	G298
U1167	A1103	C1043	G970	G906	U833	G760	C687	G636	A578	A514	C445	U362	A299
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G1171	U1107	G1047	C974	A910	C840	G764			G582	G518	U449		U303
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A1174	C1109	C1049	A981	C912	C846	G768	C692	A646	C584	G520	C451	A363F	U305
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A1181	C1116	A1056	G988	G919	U852	G777	G707	A654	G592	A528	U459		G313
G1182	G1117	G1057	G989	G920	C853	A777	G708	G654A	G593	A529	G463	U380	A314
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C1185	C1121	C1060	C991	C923	C857	A781	G710	G654D	G596	G532	A466		G317
G1186	U1122	U1061		C924	U858	A782	G711	G654E	U597	G533		C385	C318
C1187	G1123	G1062	C995	C925	G859	A783		G654F	U598	G534	G469	G386	C319
U1188	C1124	G1063	A996	A926	U860	G785	U714	C654G	C535	U534	A470	U387	A320
A1189	G1125	C1064	G997	G927	A861	G786	G715	G654H	G599	A536	A471	G388	G321
G1190		U1065	C998	G928	C862	U788	A716	G654I	G600	C537	A472	G389	A322
C1191	U1129	U1066	U999		A863	U787	G717	C654J	C601	G538	C473	A390	G323
G1192	U1130	A1067	A1000	G932	G864	A788	A718	G654K	G602	G539		G391	A324
G1193	G1131	G1068	A1001	A933	C865	A789	C719	C654L	A603	G598	A478	C392	G325
A1194	A1132	A1069	G1002	G934	A866	G790	G719	G654M	G604	C540		C393	G326
G1195	U1133	C1070	C936	C935		G791	G721	G654N	C605		A479	G327	
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G1196	G1136	C1072	U937	U937	A870	A793	G723	G654P	U607	G544	G481	G396	U328
G1197	G1137	A1073	G938	G938	U871		U724	C654Q	A608	C545	A482	A402	G329
	G1138	G1074	G939	G939	U871	C796		C654R	A609	A547	A483	A403	A330
	G1139	C1075	G940	G940	G875	C797	A727		G610	A548	C484		A331

U2074	G2010	G1934	A1847	U1779	A1889	A1608	U1640	C1474	U1405	G1334	A1285	G1203
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	A2013	A1937	C1783	C1784	G1696	G1611	C1543	G1479	C1408	G1337	A1268	G1206
	A2014	A1938	A1785	A1786	G1697	G1612	A1544	G1480	C1409	G1338	A1269	C1207
	A2015	U1939	A1787	A1788	G1698	G1613	C1545	U1481	C1410	G1339	C1270	G1208
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	A2020					A1618	C1550	A1486	U1415	G1345	A1275	
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	C2022					G1626	A1553	A1490	C1417	A1349	G1215	G1216
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	G2025						C1556	C1493	U1420	U1352	G1286	G1219
	U2026						A1557	A1494	C1421	A1353	A1287	G1220
	G2027						A1558	A1495		A1354	U1288	G1221
	C2028						G1559	A1496	G1425	G1355	C1289	C1221A
	U2029							U1497	G1426		G1297	C1222
	G2030						A1566	C1498	A1427	A1359	C1298	G1223
	A2031						A1567	C1499	C1428	A1360	C1299	G1224
	G2032						G1568	G1500	G1429	G1361	C1291	U1292
	A2033						A1569	C1501	C1430	C1362	C1293	G1225
	U2034						A1570	G1502	U1431	C1363	A1295	A1226
	G2035						A1571	U1503	C1432	G1364	G1227	G1228
	C2036						A1572	C1504	U1433	A1365	C1298	G1229
	G2037						G1573	C1505	A1434	G1368	C1299	G1230
	U2038						C1574		G1435	G1369	U1300	G1231
	G2039						C1575	C1509	C1437	A1301	G1302	G1232
	A2042						U1576	A1509A		A1373	A1303	C1233
	C2043						C1577	A1509B	A1445	G1374	G1304	U1234
	G2044						A1578	C1511	C1445A	C1375	G1305	G1235
	U2045						A1579	U1512	C1446	G1376	G1377	G1236
	G2046						A1580	G1515	G1447	A1378	G1238	G1239
	U2047						G1581	C1516	G1448	A1379	U1240	A1241
	G2048						C1582	G1517	A1449	G1380	G1310	A1242
	C2049						A1583	U1518	G1450	G1381	G1311	G1243
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	G2052						A1587	U1521	U1452	A1384	C1314	A1246
	C2053						C1588	G1522	G1453	G1385	C1315	A1247
	A2054						G1589	U1523	G1455	C1386	U1316	G1248
	C2055						U1590	G1525		C1387	G1317	C1251
	G2056						G1591	C1526	C1458	G1388	C1318	G1252
	U2057						C1592	G1527	G1459	G1389	G1319	A1253
	C2058						G1593	A1528	A1460	U1390	C1320	A1254
	A2059						G1594	C1528A	G1461	G1395	A1321	U1255
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	G2063						C1598	G1532	C1467	C1399	U1329	G1259
	C2064						C1599	C1533	G1468	G1400	C1330	G1260
	U2065						U1602	G1534	C1469	G1401	A1331	U1263
	A2066						A1603	U1535	A1469	C1402	G1332	G1264
	G2067						C1604	C1536	G1470	G1333		
	U2068						G1605	G1537	A1471	C1403		
	A2069						G1606	U1538	A1472	G1404		
	C2070						U1607	G1539	G1473			
	U2072											
	C2073											

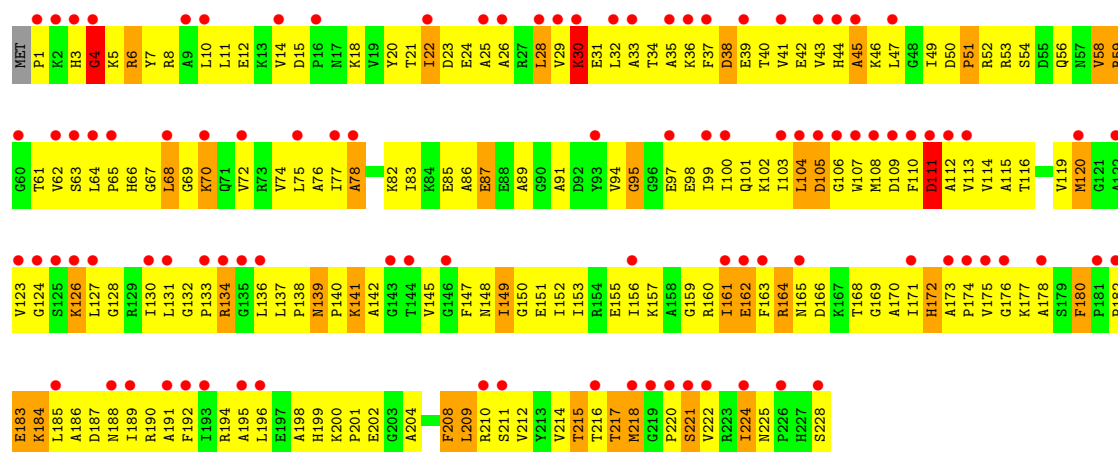


Molecule 37: 5S RIBOSOMAL RNA

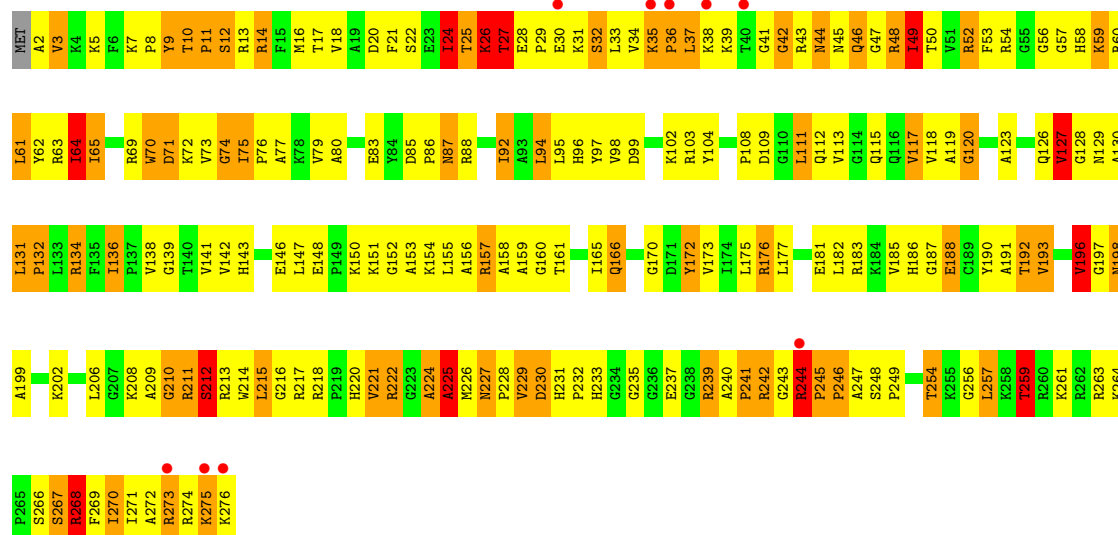




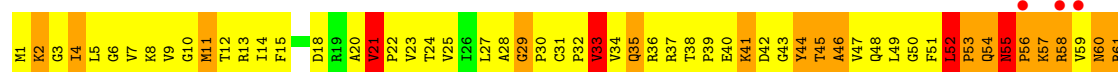
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

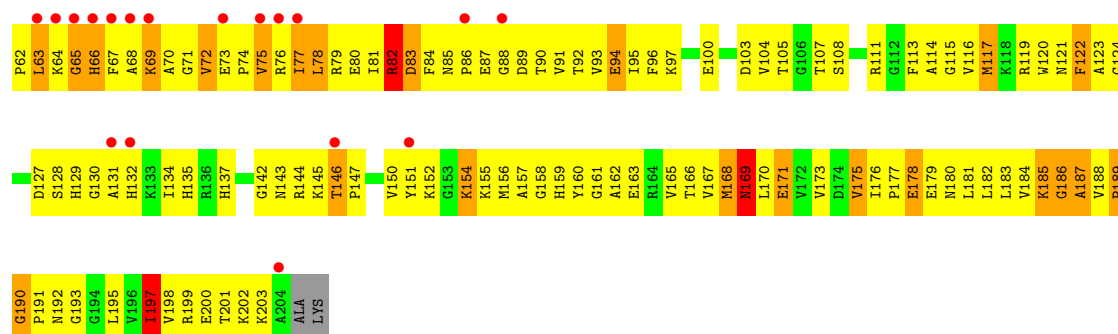


• Molecule 39: 50S RIBOSOMAL PROTEIN L2



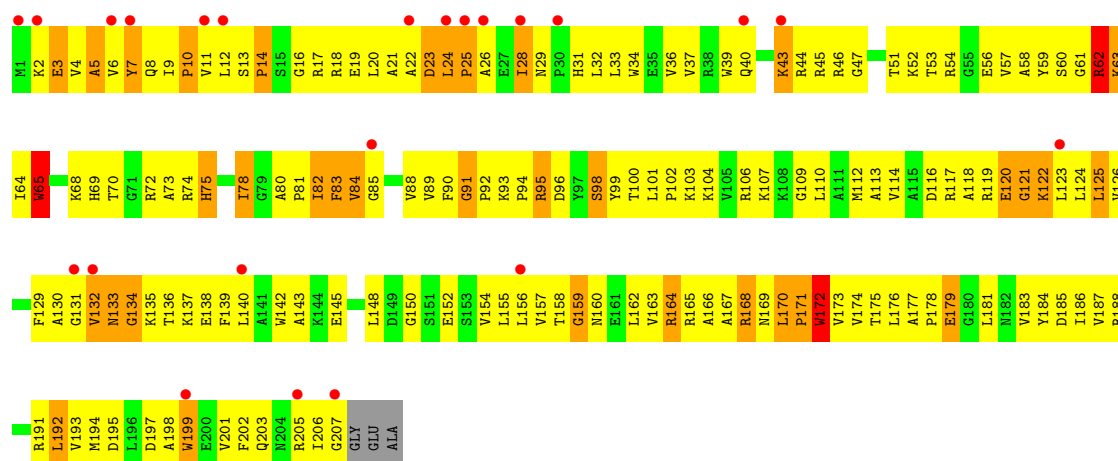
• Molecule 40: 50S RIBOSOMAL PROTEIN L3





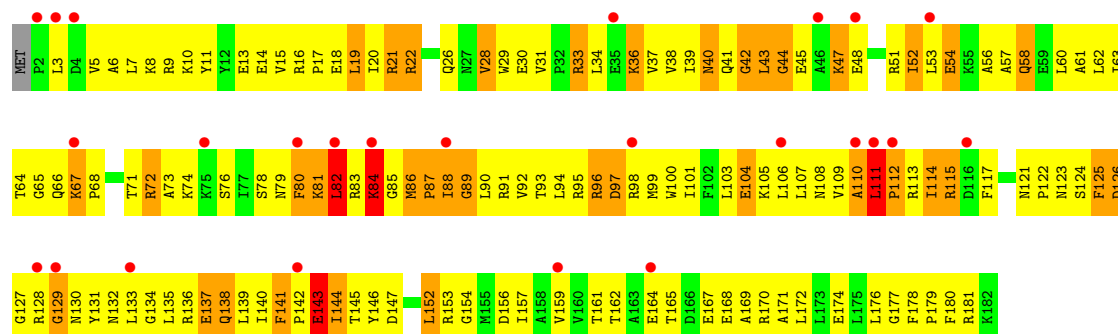
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF: 11% 20% 61% 16% ..



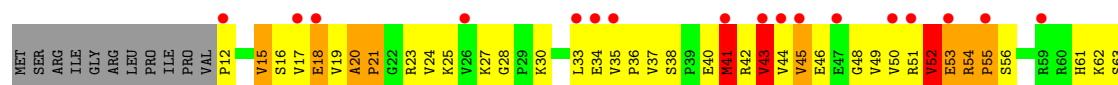
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

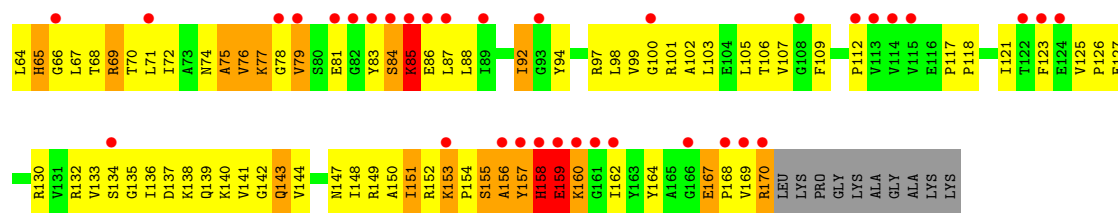
Chain BG: 14% 19% 58% 20% ..



• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain BH: 29% 24% 47% 14% 12%





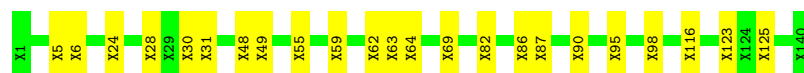
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 81% 19%



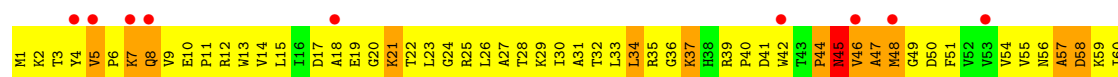
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 84% 16%



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 11% 12% 65% 19% ..



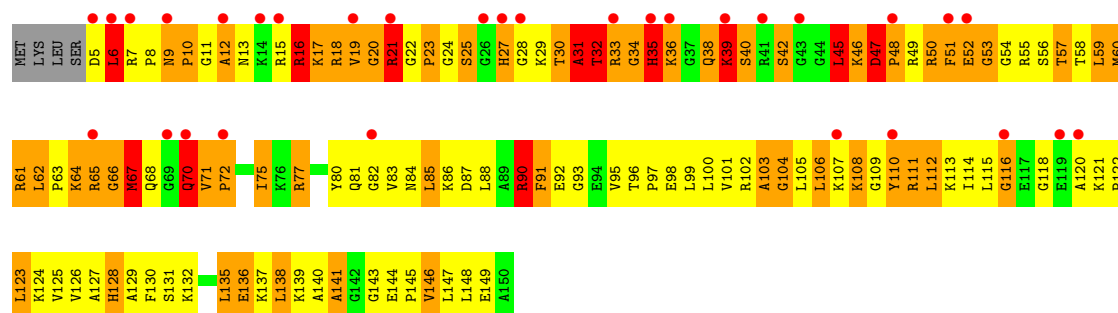
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 36% 48% 15% .

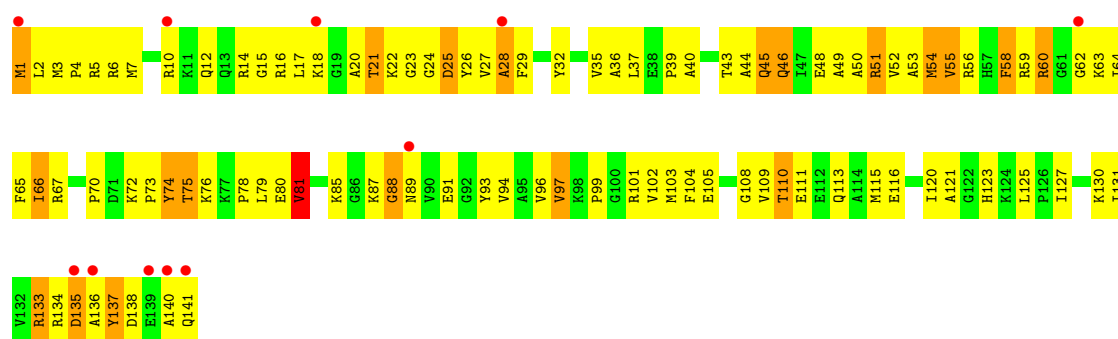
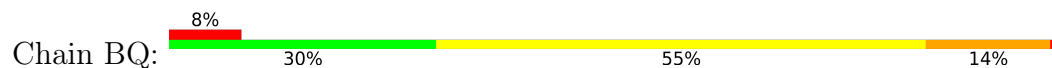


• Molecule 48: 50S RIBOSOMAL PROTEIN L15

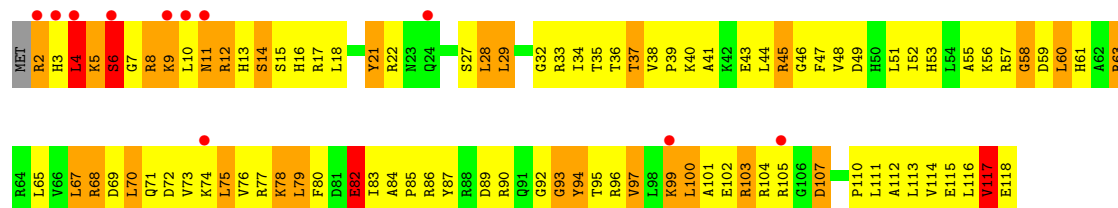
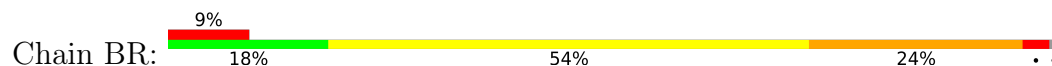
Chain BP: 21% 13% 41% 35% 8% .



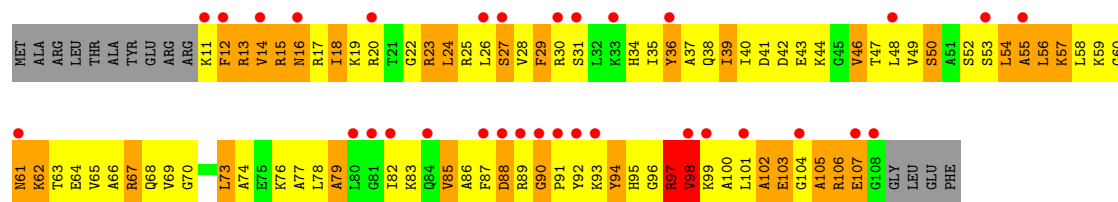
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



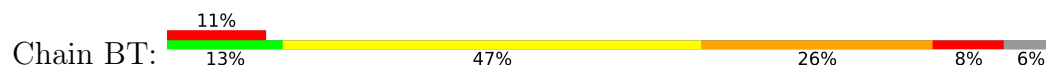
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

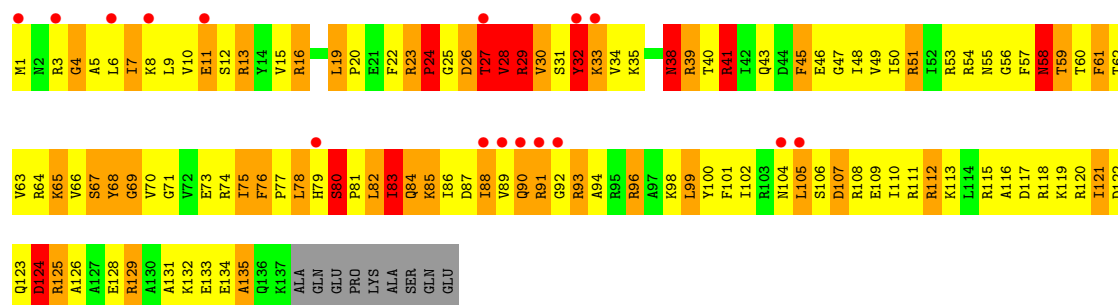


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

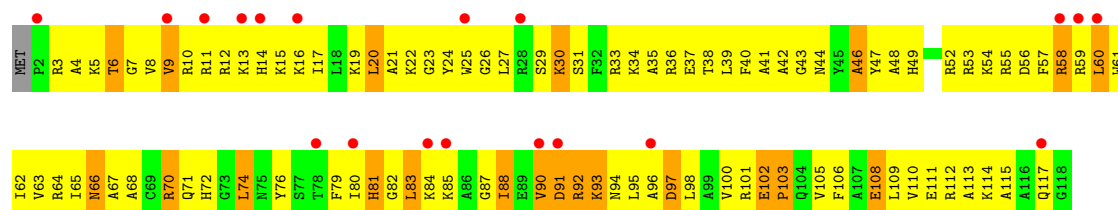


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

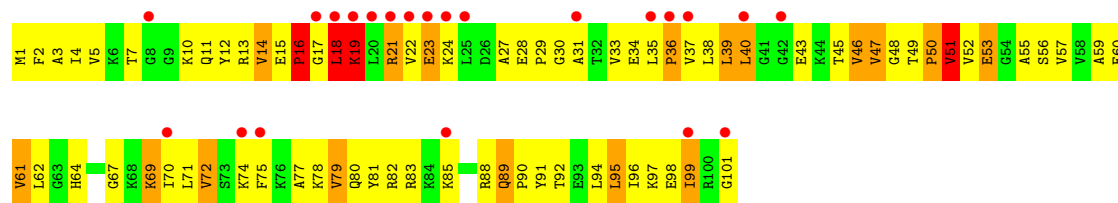




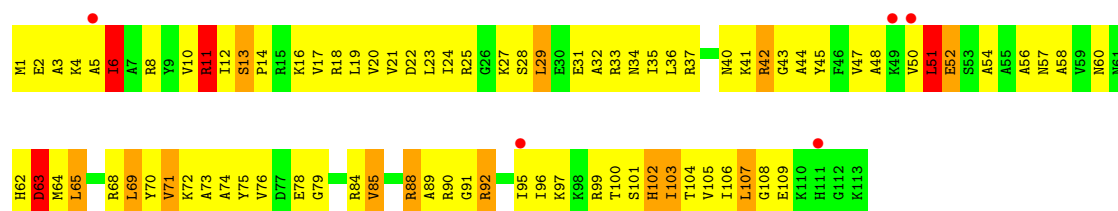
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



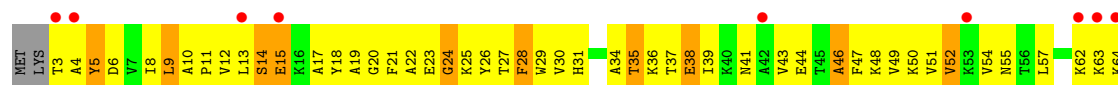
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

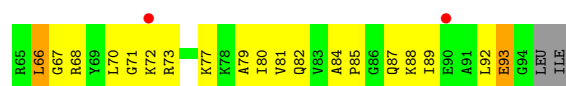


• Molecule 55: 50S RIBOSOMAL PROTEIN L22

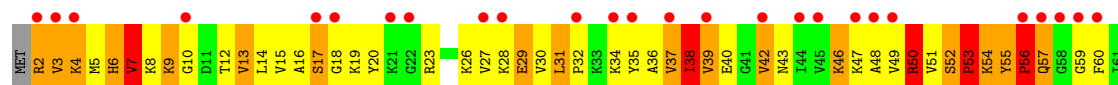
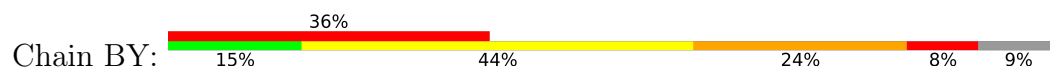


• Molecule 56: 50S RIBOSOMAL PROTEIN L23

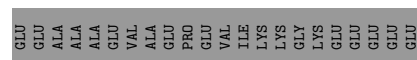
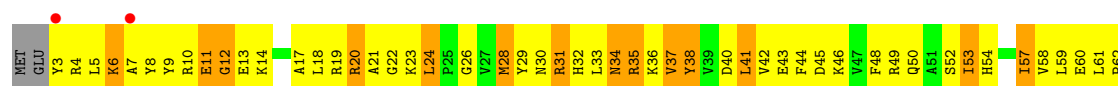
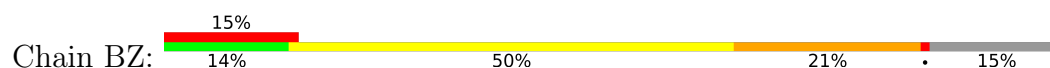




● Molecule 57: 50S RIBOSOMAL PROTEIN L24



● Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	197.60Å 274.93Å 282.46Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.10) 98.8 (50.00-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.268 0.232 , 0.267	Depositor DCC
R_{free} test set	28503 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k 0.019 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	153628	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 7MG, OMC, PSU, PAR, MIA, H2U, 4SU, GCP, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.47	3/36190 (0.0%)	0.75	74/56486 (0.1%)
2	AB	0.56	0/1935	1.13	14/2609 (0.5%)
3	AC	0.62	1/1636 (0.1%)	1.12	12/2205 (0.5%)
4	AD	0.52	0/1733	1.09	14/2318 (0.6%)
5	AE	0.68	0/1162	1.13	5/1564 (0.3%)
6	AF	0.53	0/856	1.02	4/1154 (0.3%)
7	AG	0.53	0/1276	1.04	6/1709 (0.4%)
8	AH	0.58	0/1136	1.13	11/1527 (0.7%)
9	AI	0.53	0/1029	0.98	3/1378 (0.2%)
10	AJ	0.61	0/807	1.18	12/1085 (1.1%)
11	AK	0.59	0/900	1.16	7/1213 (0.6%)
12	AL	0.69	0/986	1.33	15/1320 (1.1%)
13	AM	0.54	0/998	1.18	9/1336 (0.7%)
14	AN	0.63	0/501	1.12	2/664 (0.3%)
15	AO	0.52	0/745	0.96	0/992
16	AP	0.53	0/716	1.10	7/963 (0.7%)
17	AQ	0.49	0/836	1.05	5/1117 (0.4%)
18	AR	0.57	0/579	1.09	4/768 (0.5%)
19	AS	0.50	0/642	1.08	5/865 (0.6%)
20	AT	0.47	0/765	1.14	9/1007 (0.9%)
21	AU	0.51	0/212	0.99	0/277
22	AV	0.45	0/1809	0.68	0/2819
22	AW	0.45	0/1809	0.64	3/2819 (0.1%)
23	AX	0.51	0/334	0.82	2/519 (0.4%)
24	AY	0.45	1/1618 (0.1%)	0.77	6/2514 (0.2%)
25	AZ	0.50	0/3203	1.03	18/4346 (0.4%)
26	B0	0.48	0/671	1.00	1/892 (0.1%)
27	B1	0.57	0/738	1.11	5/981 (0.5%)
28	B2	0.42	0/600	1.04	2/793 (0.3%)
29	B3	0.46	0/472	1.04	2/634 (0.3%)
30	B4	0.52	0/349	0.88	0/474
31	B5	0.53	0/473	1.06	4/639 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B6	0.75	0/440	1.28	4/586 (0.7%)
33	B7	0.54	0/426	1.07	3/561 (0.5%)
34	B8	0.57	0/515	1.14	5/679 (0.7%)
35	B9	0.57	0/310	0.90	0/407
36	BA	0.45	0/69976	0.70	68/109244 (0.1%)
37	BB	0.41	0/2853	0.68	3/4451 (0.1%)
38	BC	0.57	4/1774 (0.2%)	1.08	11/2391 (0.5%)
39	BD	0.73	2/2195 (0.1%)	1.37	34/2955 (1.2%)
40	BE	0.55	0/1596	1.11	15/2153 (0.7%)
41	BF	0.46	0/1658	1.09	11/2244 (0.5%)
42	BG	0.44	0/1499	1.05	11/2016 (0.5%)
43	BH	0.49	0/1245	1.10	9/1682 (0.5%)
46	BN	0.45	0/1131	1.06	5/1525 (0.3%)
47	BO	0.61	0/943	1.10	6/1269 (0.5%)
48	BP	0.64	1/1131 (0.1%)	1.44	22/1504 (1.5%)
49	BQ	0.52	0/1143	1.02	5/1527 (0.3%)
50	BR	0.47	0/974	1.04	4/1302 (0.3%)
51	BS	0.50	0/778	1.06	5/1036 (0.5%)
52	BT	0.55	0/1155	1.28	21/1542 (1.4%)
53	BU	0.45	0/975	1.08	8/1297 (0.6%)
54	BV	0.43	0/790	0.96	3/1057 (0.3%)
55	BW	0.49	0/907	1.04	9/1216 (0.7%)
56	BX	0.50	0/739	1.01	4/993 (0.4%)
57	BY	0.48	0/788	1.13	8/1051 (0.8%)
58	BZ	0.48	0/1435	0.95	2/1949 (0.1%)
All	All	0.48	12/165092 (0.0%)	0.84	537/246624 (0.2%)

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
1	AA	3	51
23	AX	0	1
24	AY	2	1
36	BA	4	70
37	BB	0	2
All	All	9	125

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	BD	64	ILE	CA-CB	7.20	1.62	1.53
38	BC	120	MET	CG-SD	6.78	1.97	1.80
48	BP	38	GLN	CA-C	6.64	1.55	1.52
39	BD	221	VAL	CA-CB	6.07	1.61	1.54
1	AA	1125	U	O5'-C5'	5.84	1.51	1.42

The worst 5 of 537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	15.02	132.03	109.50
1	AA	508	C	C2'-C3'-O3'	14.90	131.85	109.50
24	AY	75	C	C2'-C3'-O3'	13.79	130.19	109.50
36	BA	1799	G	C2'-C3'-O3'	13.73	130.09	109.50
1	AA	1504	G	C2'-C3'-O3'	13.37	129.55	109.50

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
24	AY	36	A	C3'
24	AY	75	C	C3'

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	198	G	Sidechain
1	AA	250	A	Sidechain
1	AA	50	A	Sidechain
1	AA	62	U	Sidechain
1	AA	7	G	Sidechain

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	AA	32329	0	16318	1086	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1900	0	1951	273	0
3	AC	1612	0	1677	148	0
4	AD	1703	0	1764	159	0
5	AE	1146	0	1207	106	0
6	AF	843	0	857	54	0
7	AG	1257	0	1296	124	0
8	AH	1116	0	1177	94	0
9	AI	1011	0	1043	138	0
10	AJ	794	0	840	138	0
11	AK	885	0	904	79	0
12	AL	970	0	1057	112	0
13	AM	987	0	1059	142	0
14	AN	492	0	529	66	0
15	AO	734	0	771	68	0
16	AP	700	0	720	70	0
17	AQ	823	0	891	90	0
18	AR	574	0	644	39	0
19	AS	629	0	652	128	0
20	AT	763	0	861	116	0
21	AU	208	0	221	29	0
22	AV	1619	0	822	61	0
22	AW	1619	0	822	85	0
23	AX	298	0	152	25	0
24	AY	1644	0	853	68	0
25	AZ	3142	0	3152	401	0
26	B0	662	0	688	107	0
27	B1	731	0	808	86	0
28	B2	598	0	653	78	0
29	B3	467	0	523	61	0
30	B4	340	0	337	57	0
31	B5	459	0	480	82	0
32	B6	433	0	461	137	0
33	B7	418	0	467	31	0
34	B8	507	0	576	110	0
35	B9	307	0	335	52	0
36	BA	62477	0	31497	2449	2
37	BB	2551	0	1295	117	0
38	BC	1742	0	1800	360	0
39	BD	2145	0	2234	332	0
40	BE	1563	0	1629	279	0
41	BF	1623	0	1677	263	0
42	BG	1474	0	1535	242	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BH	1222	0	1282	176	0
44	BJ	651	0	152	15	0
45	BK	700	0	166	13	0
46	BN	1104	0	1180	194	0
47	BO	933	0	996	93	0
48	BP	1114	0	1187	308	0
49	BQ	1122	0	1179	154	0
50	BR	960	0	1021	153	0
51	BS	770	0	832	176	0
52	BT	1141	0	1202	255	0
53	BU	958	0	1015	163	0
54	BV	779	0	852	130	0
55	BW	896	0	953	110	0
56	BX	725	0	778	101	0
57	BY	775	0	870	199	0
58	BZ	1403	0	1432	253	0
59	AA	42	0	45	2	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
61	AZ	32	0	14	5	0
62	AZ	1	0	0	0	0
63	AZ	1	0	0	0	0
All	All	153628	0	104391	10252	2

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 40.

The worst 5 of 10252 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)
36:BA:1899:G:N2	36:BA:1902:C:H41	1.36	1.21
36:BA:2833:G:H3'	36:BA:2834:G:H5''	1.24	1.20
24:AY:1:A:H5'	25:AZ:90:LYS:HZ2	1.06	1.17
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.22	1.17
55:BW:14:PRO:HG2	55:BW:78:GLU:HG3	1.22	1.17

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1267:C:O5'	36:BA:654(I):C:O4'[2_746]	1.83	0.37
1:AA:1266:G:O3'	36:BA:654(I):C:O4'[2_746]	2.16	0.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	163 (70%)	41 (18%)	28 (12%)	0	1
3	AC	204/239 (85%)	155 (76%)	33 (16%)	16 (8%)	1	4
4	AD	206/209 (99%)	157 (76%)	34 (16%)	15 (7%)	1	5
5	AE	148/162 (91%)	125 (84%)	16 (11%)	7 (5%)	2	11
6	AF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	5
7	AG	153/156 (98%)	118 (77%)	25 (16%)	10 (6%)	1	6
8	AH	136/138 (99%)	118 (87%)	16 (12%)	2 (2%)	8	32
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	0	2
10	AJ	96/105 (91%)	67 (70%)	17 (18%)	12 (12%)	0	1
11	AK	117/129 (91%)	94 (80%)	19 (16%)	4 (3%)	3	16
12	AL	122/135 (90%)	89 (73%)	20 (16%)	13 (11%)	0	2
13	AM	122/126 (97%)	74 (61%)	27 (22%)	21 (17%)	0	0
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	0
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	2	11
16	AP	81/88 (92%)	62 (76%)	14 (17%)	5 (6%)	1	7
17	AQ	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	1	10
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	1	5
19	AS	76/93 (82%)	41 (54%)	21 (28%)	14 (18%)	0	0
20	AT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	0	4
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	AZ	403/405 (100%)	285 (71%)	83 (21%)	35 (9%)	0	4
26	B0	82/85 (96%)	65 (79%)	12 (15%)	5 (6%)	1	7
27	B1	91/98 (93%)	73 (80%)	9 (10%)	9 (10%)	0	3
28	B2	69/72 (96%)	46 (67%)	15 (22%)	8 (12%)	0	1
29	B3	57/60 (95%)	40 (70%)	9 (16%)	8 (14%)	0	1
30	B4	42/71 (59%)	23 (55%)	11 (26%)	8 (19%)	0	0
31	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	1
32	B6	48/54 (89%)	23 (48%)	12 (25%)	13 (27%)	0	0
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	34 (56%)	17 (28%)	10 (16%)	0	0
35	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	1
38	BC	226/229 (99%)	161 (71%)	46 (20%)	19 (8%)	0	4
39	BD	273/276 (99%)	219 (80%)	28 (10%)	26 (10%)	0	3
40	BE	202/206 (98%)	116 (57%)	53 (26%)	33 (16%)	0	0
41	BF	205/210 (98%)	144 (70%)	35 (17%)	26 (13%)	0	1
42	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	1
43	BH	157/180 (87%)	96 (61%)	42 (27%)	19 (12%)	0	1
46	BN	136/140 (97%)	93 (68%)	21 (15%)	22 (16%)	0	0
47	BO	120/122 (98%)	97 (81%)	16 (13%)	7 (6%)	1	8
48	BP	144/150 (96%)	74 (51%)	36 (25%)	34 (24%)	0	0
49	BQ	139/141 (99%)	108 (78%)	24 (17%)	7 (5%)	1	11
50	BR	115/118 (98%)	72 (63%)	28 (24%)	15 (13%)	0	1
51	BS	96/112 (86%)	37 (38%)	37 (38%)	22 (23%)	0	0
52	BT	135/146 (92%)	85 (63%)	27 (20%)	23 (17%)	0	0
53	BU	115/118 (98%)	72 (63%)	34 (30%)	9 (8%)	1	4
54	BV	99/101 (98%)	69 (70%)	13 (13%)	17 (17%)	0	0
55	BW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	4
56	BX	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	0	3
57	BY	98/110 (89%)	45 (46%)	26 (26%)	27 (28%)	0	0
58	BZ	174/206 (84%)	108 (62%)	39 (22%)	27 (16%)	0	0
All	All	6150/6553 (94%)	4274 (70%)	1193 (19%)	683 (11%)	0	2

5 of 683 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	191	ASP
2	AB	194	PRO
2	AB	195	ASP
3	AC	146	ALA
4	AD	4	TYR

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	168 (83%)	34 (17%)	2	10
3	AC	160/188 (85%)	137 (86%)	23 (14%)	3	14
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	24
5	AE	115/123 (94%)	94 (82%)	21 (18%)	2	8
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6	24
7	AG	126/127 (99%)	117 (93%)	9 (7%)	13	41
8	AH	119/119 (100%)	104 (87%)	15 (13%)	4	19
9	AI	98/99 (99%)	86 (88%)	12 (12%)	5	20
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	23
11	AK	90/99 (91%)	78 (87%)	12 (13%)	4	17
12	AL	104/111 (94%)	90 (86%)	14 (14%)	4	16
13	AM	99/101 (98%)	87 (88%)	12 (12%)	5	20
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	11
15	AO	79/80 (99%)	74 (94%)	5 (6%)	16	45
16	AP	72/74 (97%)	63 (88%)	9 (12%)	4	19
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	40
18	AR	61/77 (79%)	55 (90%)	6 (10%)	7	29
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	5
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	51
25	AZ	339/339 (100%)	286 (84%)	53 (16%)	2	12
26	B0	66/67 (98%)	56 (85%)	10 (15%)	3	13
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
28	B2	66/67 (98%)	61 (92%)	5 (8%)	12	39
29	B3	51/52 (98%)	48 (94%)	3 (6%)	18	48
30	B4	39/63 (62%)	30 (77%)	9 (23%)	1	4
31	B5	51/52 (98%)	46 (90%)	5 (10%)	7	29
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	4
33	B7	41/42 (98%)	36 (88%)	5 (12%)	5	20
34	B8	53/55 (96%)	44 (83%)	9 (17%)	2	10
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	9
38	BC	180/181 (99%)	163 (91%)	17 (9%)	8	31
39	BD	217/218 (100%)	177 (82%)	40 (18%)	1	8
40	BE	165/166 (99%)	146 (88%)	19 (12%)	5	23
41	BF	165/166 (99%)	153 (93%)	12 (7%)	13	40
42	BG	155/156 (99%)	133 (86%)	22 (14%)	3	14
43	BH	132/148 (89%)	122 (92%)	10 (8%)	12	39
46	BN	117/119 (98%)	106 (91%)	11 (9%)	8	31
47	BO	100/100 (100%)	90 (90%)	10 (10%)	7	29
48	BP	112/116 (97%)	87 (78%)	25 (22%)	1	4
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	19
50	BR	100/101 (99%)	82 (82%)	18 (18%)	2	8
51	BS	77/88 (88%)	65 (84%)	12 (16%)	2	12
52	BT	120/127 (94%)	93 (78%)	27 (22%)	1	4
53	BU	92/94 (98%)	80 (87%)	12 (13%)	4	18
54	BV	82/82 (100%)	72 (88%)	10 (12%)	5	20
55	BW	91/92 (99%)	80 (88%)	11 (12%)	5	20
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	30
57	BY	84/91 (92%)	68 (81%)	16 (19%)	1	7
58	BZ	155/179 (87%)	128 (83%)	27 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5186/5431 (96%)	4486 (86%)	700 (14%)	4 16

5 of 700 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BF	125	LEU
50	BR	94	TYR
42	BG	58	GLN
41	BF	122	LYS
47	BO	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
41	BF	40	GLN
50	BR	71	GLN
41	BF	160	ASN
47	BO	89	ASN
53	BU	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	249 (16%)	56 (3%)
22	AV	75/76 (98%)	22 (29%)	0
22	AW	75/76 (98%)	17 (22%)	0
23	AX	13/14 (92%)	3 (23%)	1 (7%)
24	AY	75/77 (97%)	23 (30%)	2 (2%)
36	BA	2900/2915 (99%)	550 (18%)	52 (1%)
37	BB	118/122 (96%)	24 (20%)	2 (1%)
All	All	4759/4802 (99%)	888 (18%)	113 (2%)

5 of 888 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	AY	18	G
36	BA	2762	G
36	BA	614(C)	A
36	BA	2756	U
36	BA	2126	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
24	4SU	AY	8	24	18,21,22	0.43	0	25,30,33	0.87	2 (8%)
24	7MG	AY	46	24	23,26,27	2.57	3 (13%)	27,39,42	1.76	3 (11%)
24	OMC	AY	32	24	19,22,23	0.34	0	25,31,34	0.65	1 (4%)
24	MIA	AY	37	24	28,31,32	0.83	2 (7%)	38,44,47	0.99	1 (2%)
24	H2U	AY	16	24	18,21,22	0.84	0	19,30,33	1.72	4 (21%)
24	PSU	AY	55	24	18,21,22	0.93	2 (11%)	21,30,33	1.92	5 (23%)
24	H2U	AY	20	24	18,21,22	0.90	0	19,30,33	1.81	5 (26%)
24	H2U	AY	17	24	18,21,22	0.94	1 (5%)	19,30,33	1.56	3 (15%)
24	5MU	AY	54	24	19,22,23	0.40	0	27,32,35	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	4SU	AY	8	24	-	0/7/25/26	0/2/2/2
24	7MG	AY	46	24	-	5/7/37/38	0/3/3/3
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MIA	AY	37	24	-	3/15/33/34	0/3/3/3
24	H2U	AY	16	24	-	1/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2
24	H2U	AY	20	24	-	4/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	3/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-11.62	1.38	1.45
24	AY	46	7MG	C5-N7	3.11	1.39	1.35
24	AY	55	PSU	C6-C5	2.66	1.38	1.35
24	AY	37	MIA	C12-N6	-2.36	1.40	1.45
24	AY	46	7MG	C8-N7	-2.36	1.30	1.42

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	46	7MG	N9-C8-N7	6.96	113.23	103.37
24	AY	37	MIA	C11-S10-C2	4.91	105.94	102.25
24	AY	55	PSU	N1-C2-N3	4.64	120.06	115.17
24	AY	16	H2U	N3-C2-N1	4.56	121.23	116.65
24	AY	46	7MG	C4-C5-N7	4.54	110.74	105.38

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C1'-N1-C6
24	AY	37	MIA	C5-C6-N6-C12
24	AY	20	H2U	O4'-C1'-N1-C2
24	AY	46	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	8	4SU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	37	MIA	2	0
24	AY	16	H2U	1	0
24	AY	55	PSU	1	0
24	AY	20	H2U	3	0
24	AY	17	H2U	1	0
24	AY	54	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GCP	AZ	501	62	32,34,34	1.68	6 (18%)	49,54,54	1.26	7 (14%)
59	PAR	AA	1601	-	44,45,45	1.39	6 (13%)	63,67,67	1.24	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GCP	AZ	501	62	-	11/19/38/38	0/3/3/3
59	PAR	AA	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	PA-O3A	-4.19	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	PG-O2G	-4.05	1.45	1.55
61	AZ	501	GCP	C5-N7	-3.68	1.31	1.39
59	AA	1601	PAR	C52-C42	3.47	1.59	1.52
61	AZ	501	GCP	C6-N1	3.28	1.45	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AA	1601	PAR	O33-C14-C24	5.11	116.45	108.08
59	AA	1601	PAR	O54-C54-C64	3.73	113.23	106.07
59	AA	1601	PAR	C14-O54-C54	3.57	120.69	113.72
61	AZ	501	GCP	C2-N1-C6	-3.25	119.21	125.11
61	AZ	501	GCP	O3G-PG-O2G	3.01	116.55	107.96

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AA	1601	PAR	C44-C54-C64-N64
59	AA	1601	PAR	O54-C54-C64-N64
61	AZ	501	GCP	PB-C3B-PG-O1G
61	AZ	501	GCP	PB-C3B-PG-O2G
61	AZ	501	GCP	PG-C3B-PB-O1B

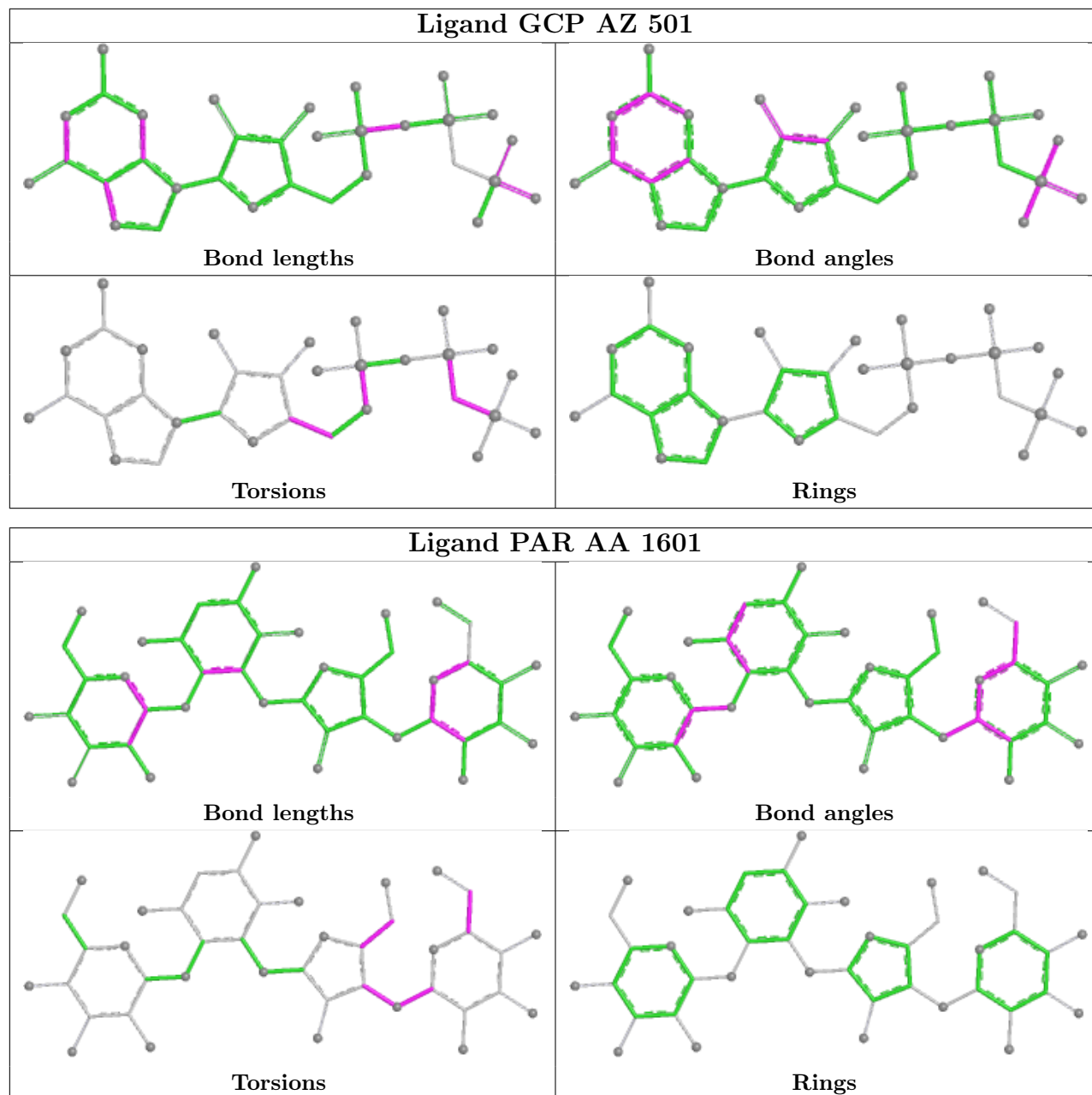
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AZ	501	GCP	5	0
59	AA	1601	PAR	2	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.11	75 (4%) 34 18	24, 58, 149, 200	0
2	AB	234/256 (91%)	0.58	16 (6%) 23 12	35, 74, 133, 147	0
3	AC	206/239 (86%)	0.04	3 (1%) 72 52	34, 57, 91, 103	0
4	AD	208/209 (99%)	0.42	9 (4%) 40 22	44, 68, 96, 102	0
5	AE	150/162 (92%)	0.03	3 (2%) 65 44	33, 52, 82, 102	0
6	AF	101/101 (100%)	0.29	0 100 100	52, 74, 89, 100	0
7	AG	155/156 (99%)	0.33	7 (4%) 38 20	46, 71, 96, 119	0
8	AH	138/138 (100%)	-0.01	3 (2%) 62 41	38, 58, 78, 87	0
9	AI	127/128 (99%)	0.56	6 (4%) 36 19	41, 74, 103, 112	0
10	AJ	98/105 (93%)	0.92	11 (11%) 10 5	35, 75, 111, 117	0
11	AK	119/129 (92%)	0.22	1 (0%) 82 65	39, 59, 95, 117	0
12	AL	124/135 (91%)	0.18	6 (4%) 35 19	36, 48, 77, 112	0
13	AM	124/126 (98%)	0.93	15 (12%) 8 5	50, 80, 107, 132	0
14	AN	60/61 (98%)	0.18	1 (1%) 69 48	32, 48, 76, 83	0
15	AO	88/89 (98%)	0.23	0 100 100	42, 64, 89, 93	0
16	AP	83/88 (94%)	0.35	1 (1%) 76 58	50, 65, 85, 114	0
17	AQ	99/105 (94%)	0.32	5 (5%) 33 18	45, 70, 95, 97	0
18	AR	70/88 (79%)	0.22	1 (1%) 73 53	46, 65, 97, 111	0
19	AS	78/93 (83%)	0.99	10 (12%) 7 4	58, 84, 115, 123	0
20	AT	99/106 (93%)	0.84	8 (8%) 18 10	56, 86, 128, 131	0
21	AU	24/27 (88%)	0.71	3 (12%) 8 5	52, 64, 79, 91	0
22	AV	76/76 (100%)	1.06	12 (15%) 5 2	35, 127, 168, 176	0
22	AW	76/76 (100%)	2.17	45 (59%) 0 0	60, 175, 200, 200	0
23	AX	14/14 (100%)	0.84	5 (35%) 1 0	34, 57, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	AY	68/77 (88%)	1.50	17 (25%) 2 1	47, 110, 160, 196	0
25	AZ	405/405 (100%)	0.77	30 (7%) 20 11	57, 100, 135, 143	0
26	B0	84/85 (98%)	0.84	13 (15%) 5 2	59, 75, 116, 136	0
27	B1	93/98 (94%)	0.59	5 (5%) 31 17	44, 65, 106, 114	0
28	B2	71/72 (98%)	1.04	6 (8%) 16 9	75, 108, 124, 146	0
29	B3	59/60 (98%)	0.90	4 (6%) 23 12	72, 93, 110, 135	0
30	B4	44/71 (61%)	1.67	14 (31%) 1 0	103, 134, 142, 149	0
31	B5	59/60 (98%)	1.38	13 (22%) 2 1	57, 89, 151, 155	0
32	B6	50/54 (92%)	1.67	17 (34%) 1 0	52, 81, 99, 108	0
33	B7	48/49 (97%)	0.49	2 (4%) 40 22	49, 59, 99, 117	0
34	B8	63/65 (96%)	1.24	10 (15%) 5 2	53, 73, 91, 106	0
35	B9	37/37 (100%)	1.28	7 (18%) 3 1	61, 82, 96, 97	0
36	BA	2901/2915 (99%)	0.61	277 (9%) 14 7	28, 76, 190, 200	0
37	BB	119/122 (97%)	1.14	20 (16%) 4 2	74, 103, 134, 150	0
38	BC	228/229 (99%)	2.02	99 (43%) 0 0	125, 160, 177, 186	0
39	BD	275/276 (99%)	0.00	9 (3%) 49 29	24, 45, 71, 93	0
40	BE	204/206 (99%)	0.83	21 (10%) 12 6	50, 77, 128, 135	0
41	BF	207/210 (98%)	0.99	23 (11%) 10 5	47, 97, 149, 155	0
42	BG	181/182 (99%)	1.01	25 (13%) 6 4	79, 101, 126, 137	0
43	BH	159/180 (88%)	1.65	52 (32%) 1 0	80, 119, 144, 150	0
44	BJ	0/130	-	-	-	-
45	BK	0/140	-	-	-	-
46	BN	138/140 (98%)	0.94	15 (10%) 10 5	68, 93, 127, 132	0
47	BO	122/122 (100%)	-0.00	0 100 100	42, 59, 72, 83	0
48	BP	146/150 (97%)	1.38	31 (21%) 2 1	55, 90, 121, 146	0
49	BQ	141/141 (100%)	0.69	11 (7%) 19 10	50, 68, 100, 134	0
50	BR	117/118 (99%)	0.88	11 (9%) 14 8	58, 81, 100, 105	0
51	BS	98/112 (87%)	1.54	32 (32%) 1 0	70, 93, 121, 126	0
52	BT	137/146 (93%)	0.87	16 (11%) 9 5	54, 80, 139, 161	0
53	BU	117/118 (99%)	1.13	19 (16%) 4 2	68, 88, 113, 120	0
54	BV	101/101 (100%)	1.41	22 (21%) 2 1	67, 117, 132, 137	0
55	BW	113/113 (100%)	0.79	5 (4%) 39 21	65, 88, 115, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BX	92/96 (95%)	1.06	11 (11%) 9 5	65, 85, 101, 107	0
57	BY	100/110 (90%)	1.87	40 (40%) 1 0	94, 125, 149, 158	0
58	BZ	176/206 (85%)	1.30	31 (17%) 4 2	69, 102, 125, 134	0
All	All	11008/11625 (94%)	0.66	1154 (10%) 11 6	24, 77, 158, 200	0

The worst 5 of 1154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	BQ	140	ALA	10.3
31	B5	2	ALA	8.0
36	BA	654(L)	G	8.0
32	B6	42	TRP	7.9
36	BA	271(N)	U	7.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	PSU	AY	55	20/21	0.42	0.16	154,158,159,160	0
24	H2U	AY	20	20/21	0.53	0.21	185,187,191,191	0
24	H2U	AY	16	20/21	0.55	0.18	171,185,187,190	0
24	H2U	AY	17	20/21	0.55	0.25	191,199,200,200	0
24	5MU	AY	54	21/22	0.62	0.19	145,152,154,155	0
24	4SU	AY	8	20/21	0.79	0.19	104,105,107,108	0
24	7MG	AY	46	24/25	0.84	0.17	112,114,120,121	0
24	OMC	AY	32	21/22	0.90	0.15	76,80,87,88	0
24	MIA	AY	37	29/30	0.92	0.16	48,63,74,86	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

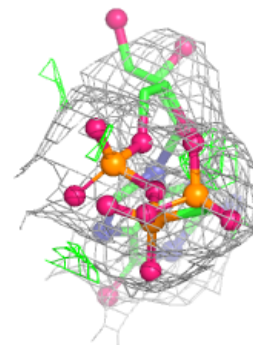
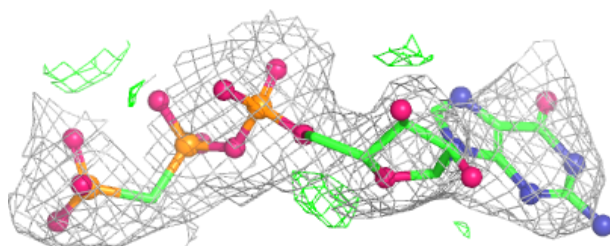
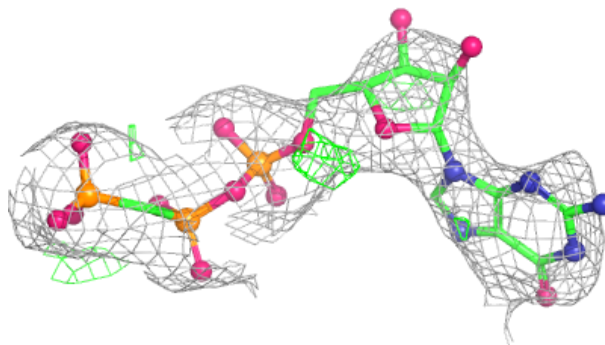
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	AZ	502	1/1	0.85	0.15	55,55,55,55	0
61	GCP	AZ	501	32/32	0.91	0.15	89,110,116,117	0
59	PAR	AA	1601	42/42	0.93	0.13	33,42,58,62	0
60	ZN	AD	301	1/1	0.97	0.20	58,58,58,58	0
60	ZN	B4	101	1/1	0.97	0.07	132,132,132,132	0
60	ZN	AN	101	1/1	1.00	0.04	45,45,45,45	0
60	ZN	B9	101	1/1	1.00	0.04	92,92,92,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

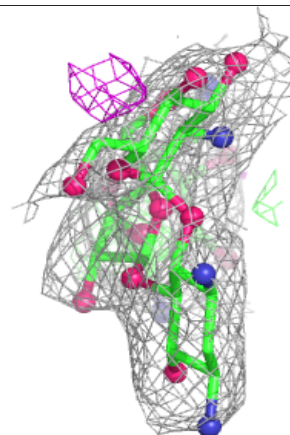
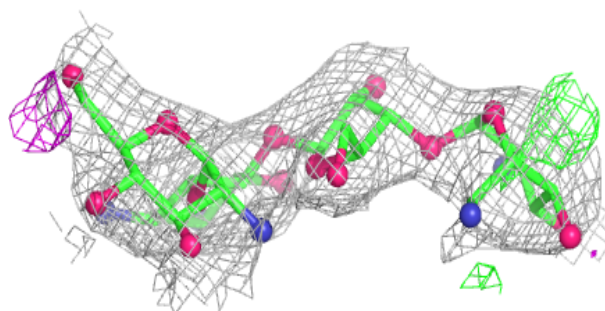
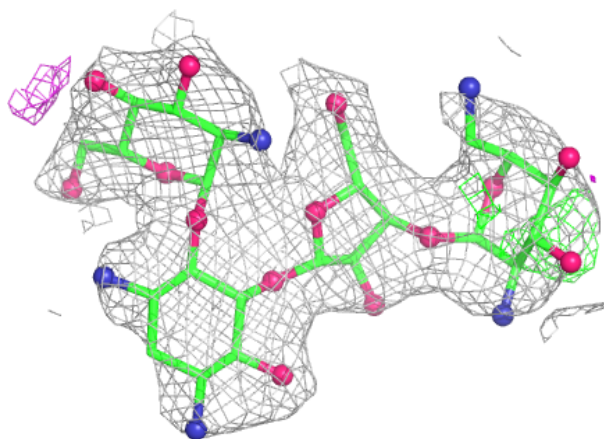
Electron density around GCP AZ 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR AA 1601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.