



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 4V90 / pdb_00004v90
Title : Thermus thermophilus Ribosome
Authors : Chen, Y.; Feng, S.; Kumar, V.; Ero, R.; Gao, Y.G.
Deposited on : 2014-02-22
Resolution : 2.95 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

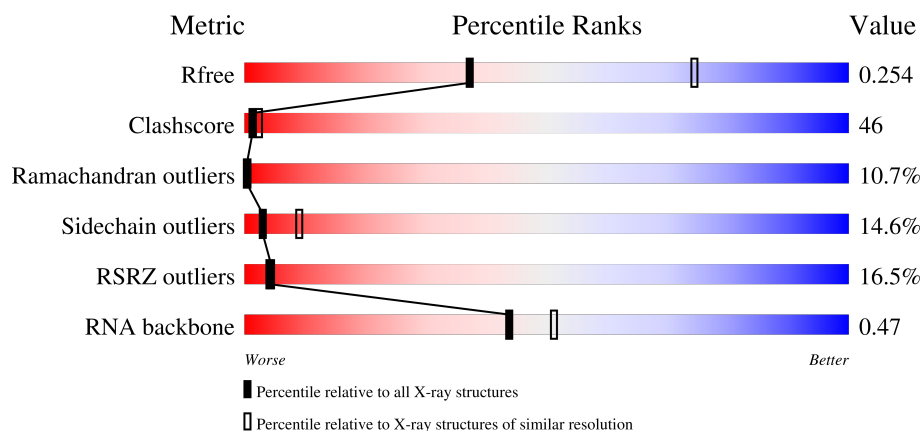
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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	1519	
2	AB	256	
3	AC	239	
4	AD	209	

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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	132	
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	
23	AX	9	
24	AY	691	
25	B0	84	
26	B1	97	
27	B2	71	
28	B3	60	
29	B4	71	

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Mol	Chain	Length	Quality of chain
30	B5	59	
31	B6	53	
32	B7	48	
33	B8	64	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	228	
38	BD	275	
39	BE	206	
40	BF	210	
41	BG	181	
42	BH	180	
43	BJ	130	
44	BK	140	
45	BL	71	
46	BN	140	
47	BO	122	
48	BP	149	
49	BQ	141	
50	BR	117	
51	BS	111	
52	BT	146	
53	BU	117	
54	BV	101	

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Mol	Chain	Length	Quality of chain
55	BW	113	
56	BX	95	
57	BY	109	
58	BZ	205	

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
59	MG	AA	1607	-	-	-	X
59	MG	AA	1620	-	-	-	X
59	MG	AA	1666	-	-	-	X
59	MG	AA	1684	-	-	-	X
59	MG	AA	1703	-	-	-	X
59	MG	AA	1740	-	-	-	X
59	MG	AA	1772	-	-	-	X
59	MG	B0	101	-	-	-	X
59	MG	BA	3130	-	-	-	X
59	MG	BA	3239	-	-	-	X
59	MG	BA	3253	-	-	-	X
59	MG	BA	3268	-	-	-	X
59	MG	BA	3280	-	-	-	X
59	MG	BA	3281	-	-	-	X
61	GCP	AY	701	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153829 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1507	Total	C	N	O	P	0	0	0
			32391	14418	6002	10465	1506			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1030	C	-	insertion	GB 48256
AA	1034	G	-	insertion	GB 48256
AA	1245	A	-	insertion	GB 48256
AA	1246	C	-	insertion	GB 48256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	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	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

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

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	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	88	Total	C	N	O	S	0	0	1
			692	440	128	122	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	25	Total	C	N	O		0	0	1
			209	128	51	30				

- Molecule 22 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	291	530	75			

- Molecule 23 is a RNA chain called 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			188	86	34	60	8			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	687	Total	C	N	O	S	0	0	1
			5376	3412	922	1022	20			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62476	27807	11683	20086	2900			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	2155	G	A	conflict	GB 55771382

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	227	Total	C	N	O	S	0	0	0
			1735	1096	318	318	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	179	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	176	Total	C	N	O	S	0	0	1
			1345	853	253	237	2			

- Molecule 43 is a protein called CHAIN J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	130	Total	C	N	O	0	0	0
			654	393	130	131			

- Molecule 44 is a protein called CHAIN K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	0	0	0
			701	420	140	141			

- Molecule 45 is a protein called CHAIN L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BL	71	Total	C	N	O	0	0	0
			356	213	71	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	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		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	99	Total	C	N	O		0	0	1
			771	486	155	130				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	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	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	198	Total	Mg	0	0
			198	198		
59	AY	1	Total	Mg	0	0
			1	1		
59	B0	1	Total	Mg	0	0
			1	1		

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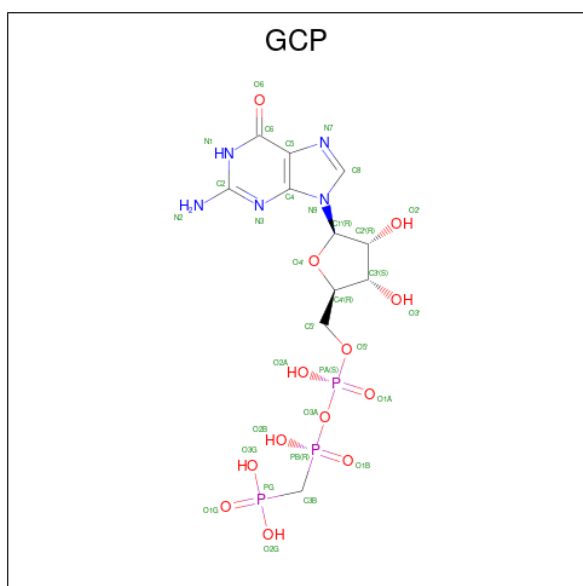
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Mg	0	0
			1	1		
59	BA	320	Total	Mg	0	0
			320	320		
59	BC	1	Total	Mg	0	0
			1	1		
59	BU	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



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

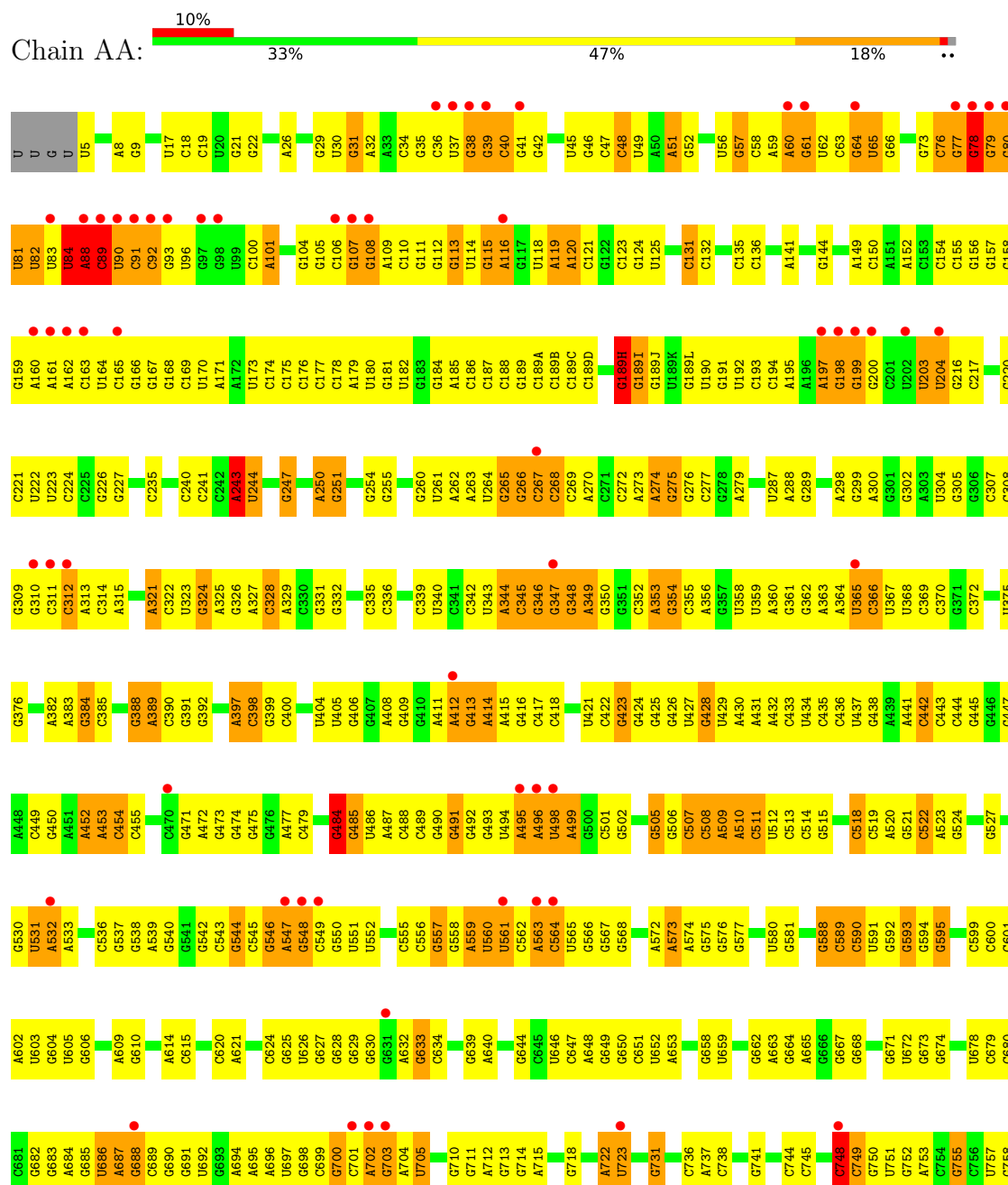
- Molecule 62 is water.

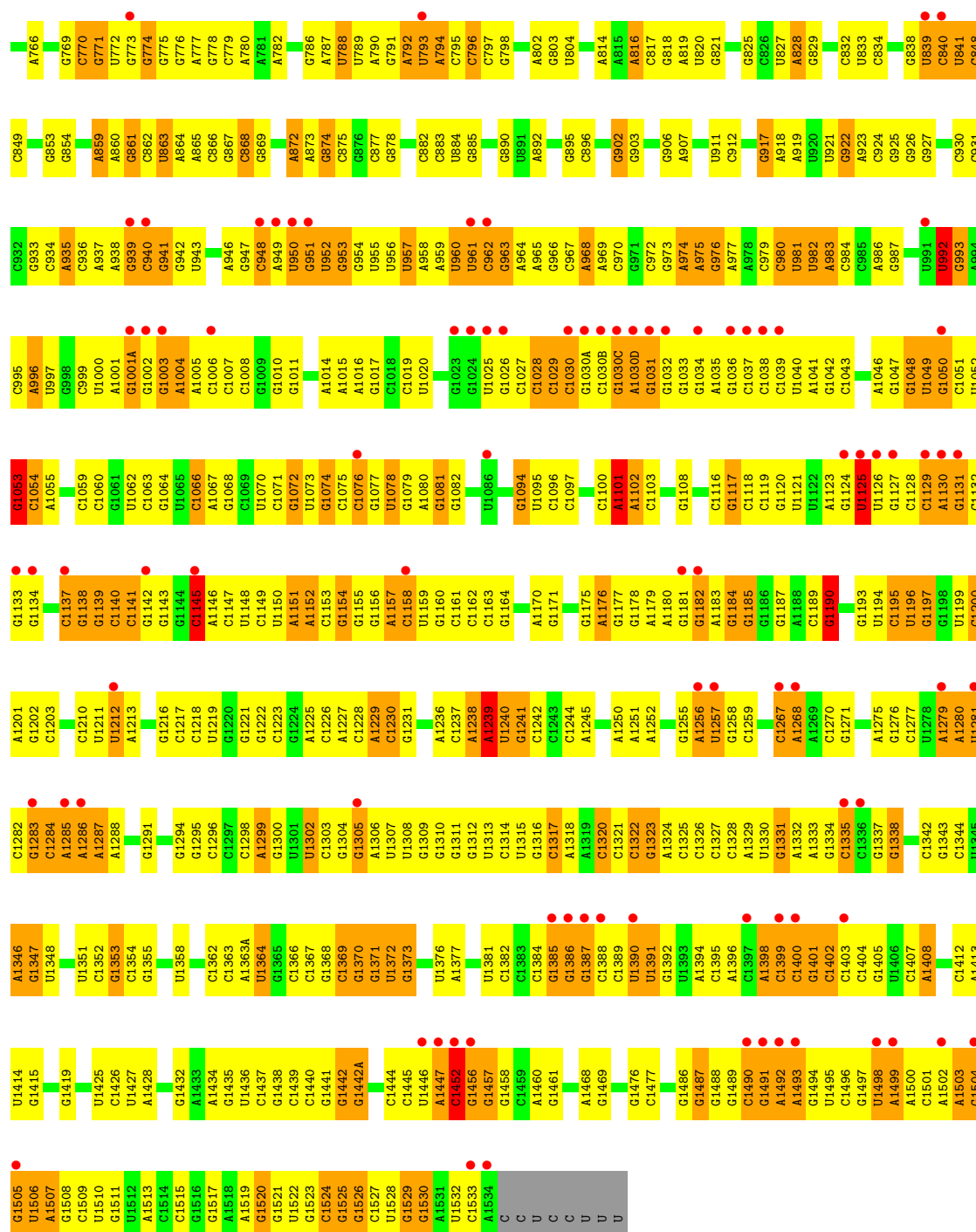
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	2	Total	O	0	0
			2	2		

3 Residue-property plots

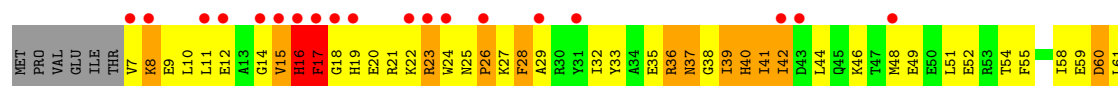
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

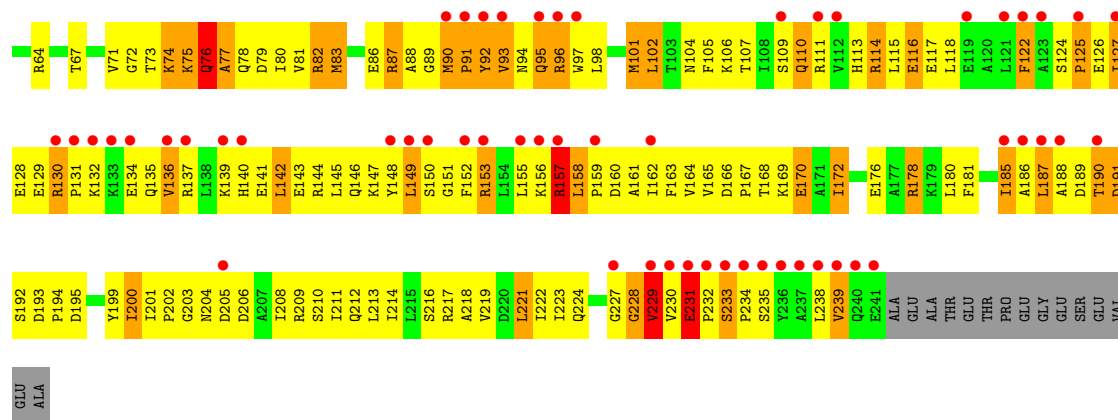
• Molecule 1: 16S RIBOSOMAL RNA



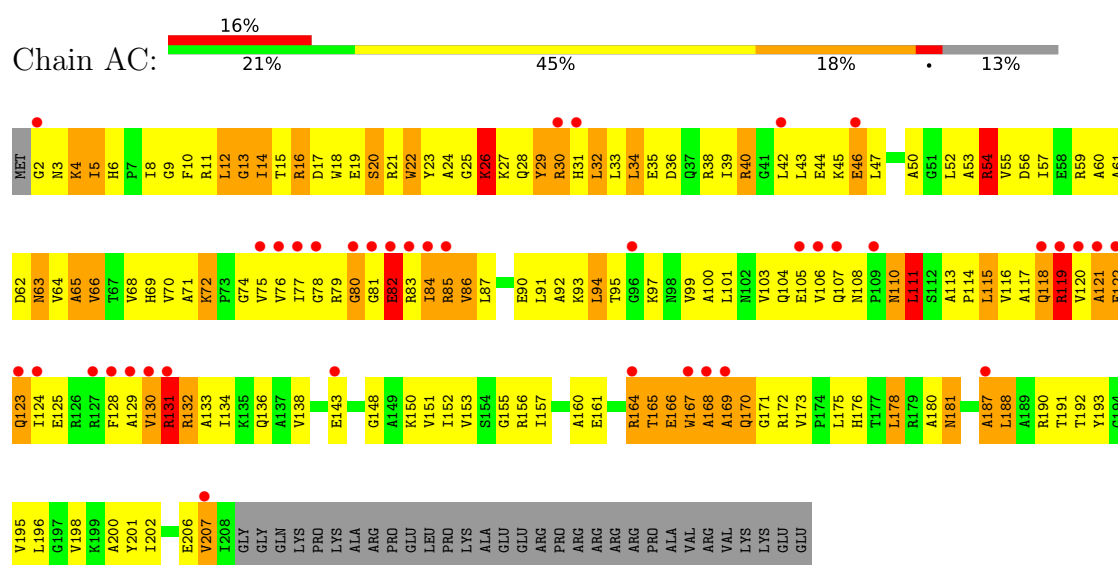


● Molecule 2: 30S RIBOSOMAL PROTEIN S2

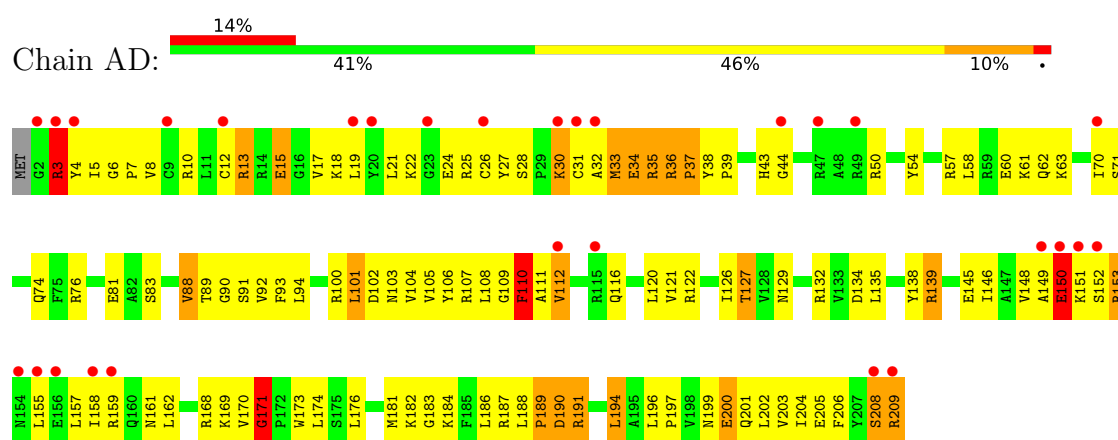




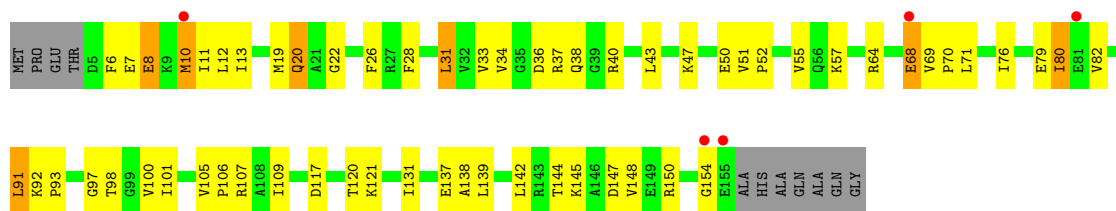
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



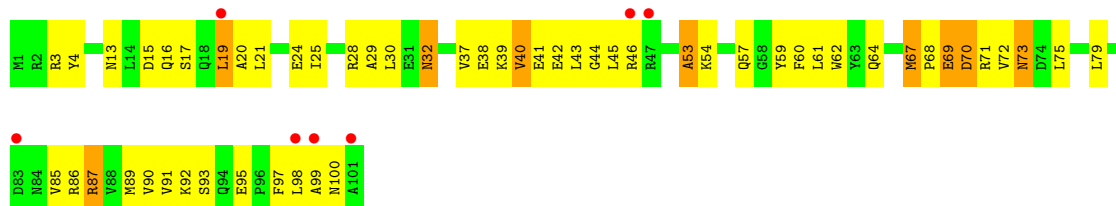
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



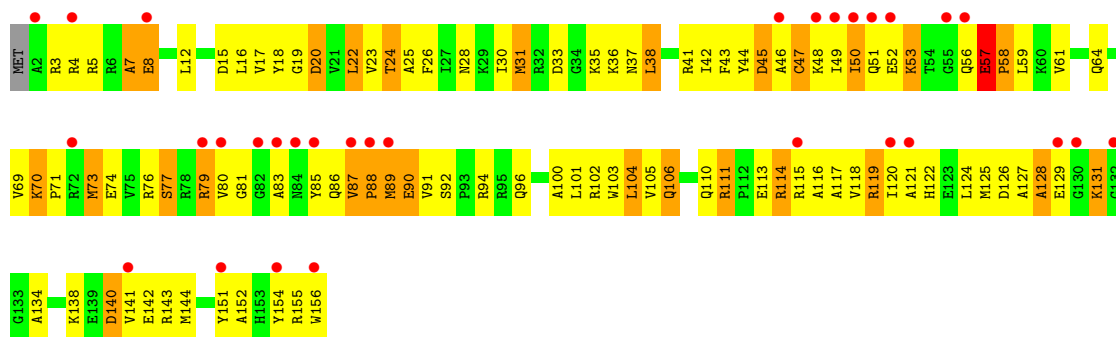
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



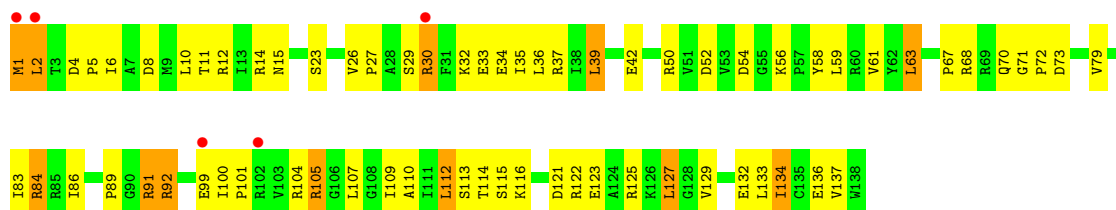
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



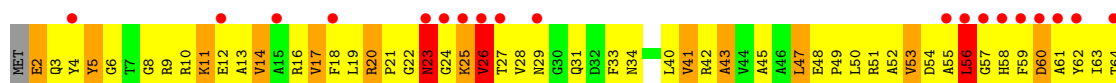
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

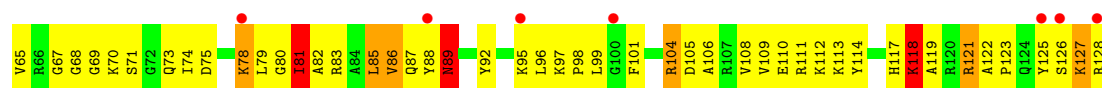


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

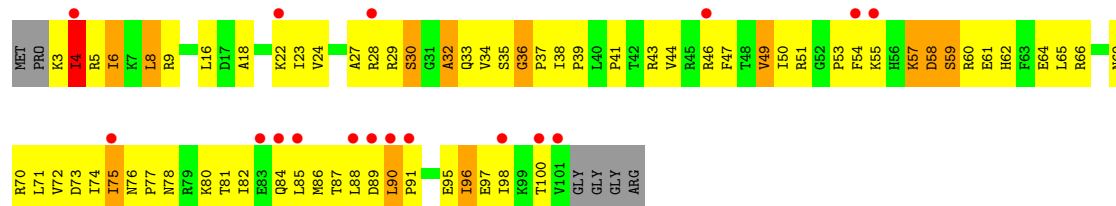


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

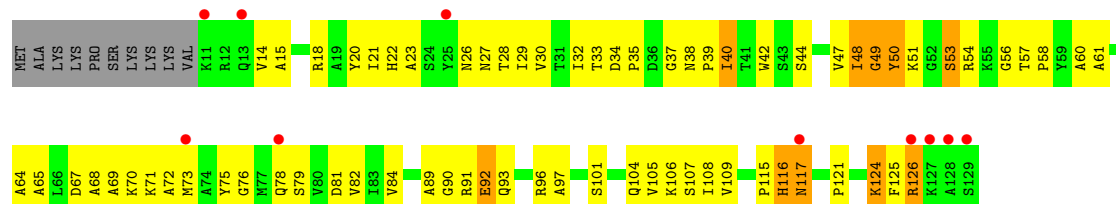




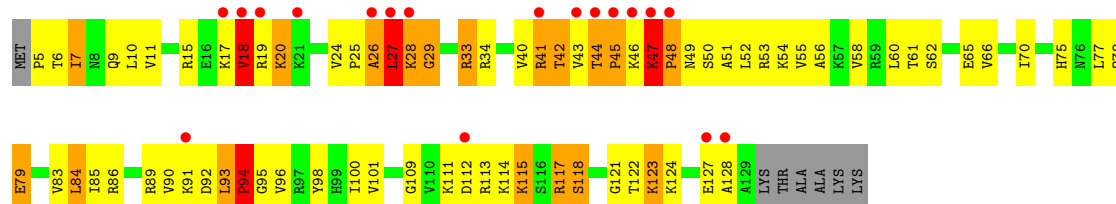
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



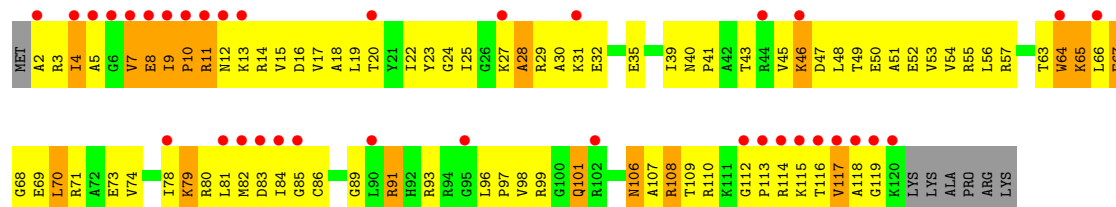
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

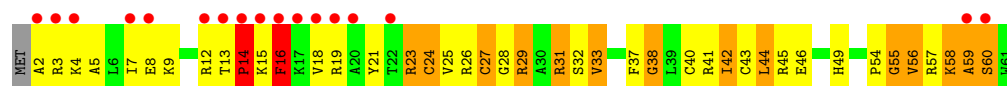


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

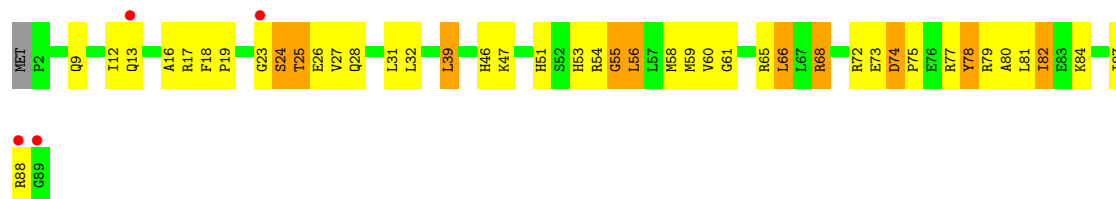


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

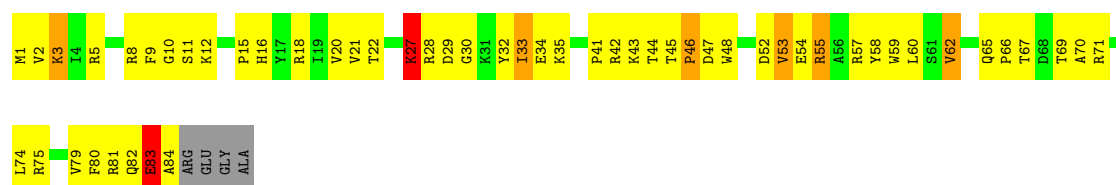




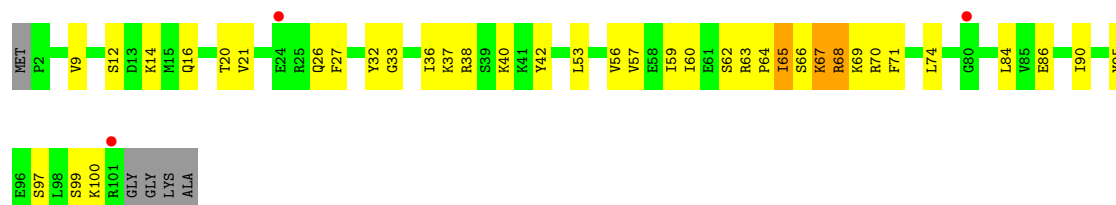
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



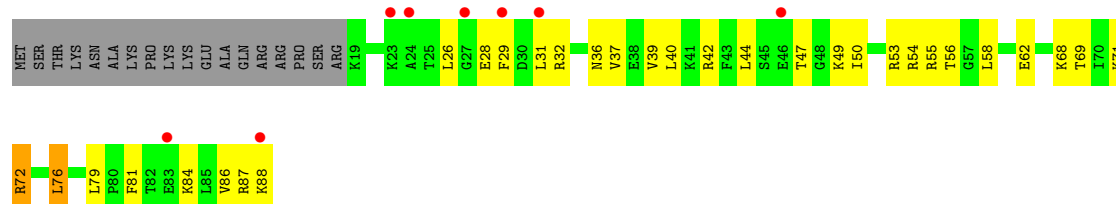
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

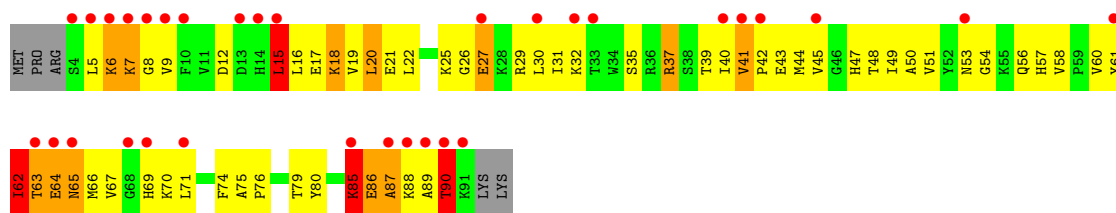


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

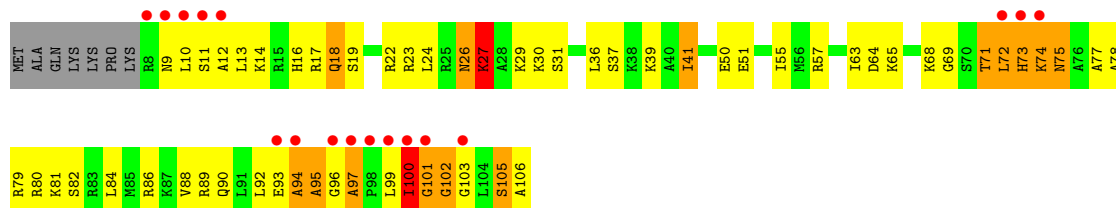


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

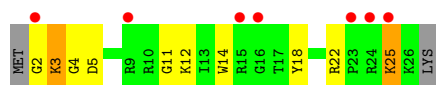




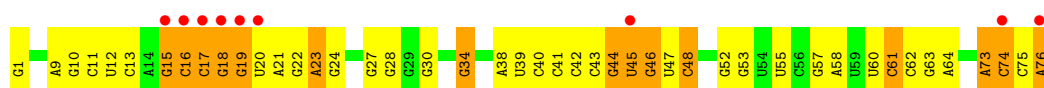
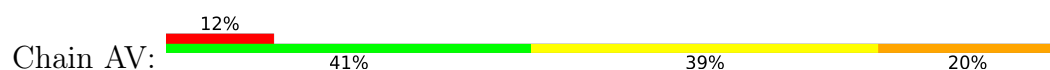
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



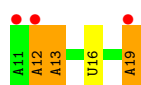
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



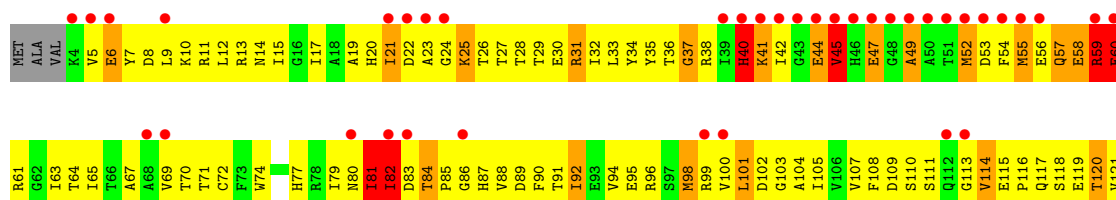
• Molecule 22: RNA (77-MER)

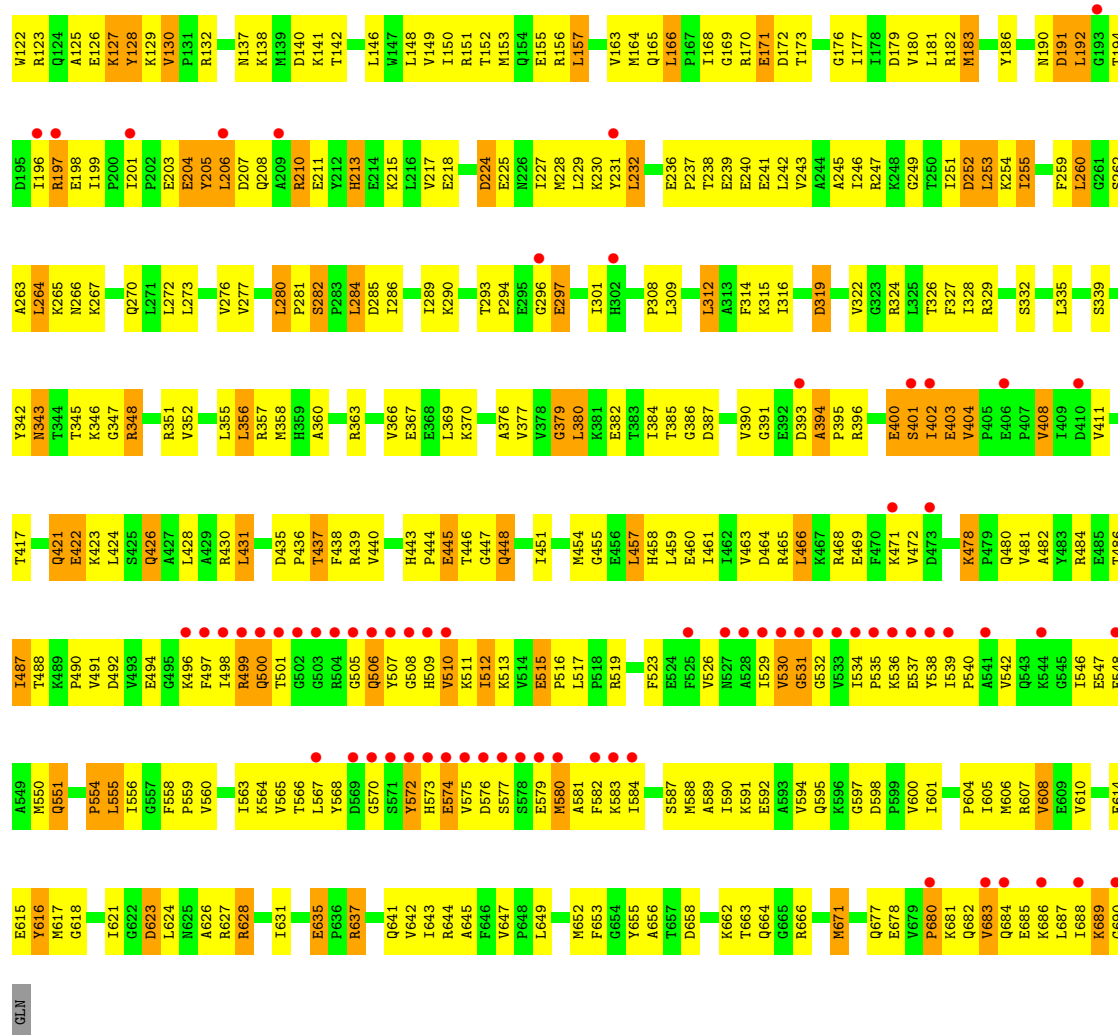


• Molecule 23: 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

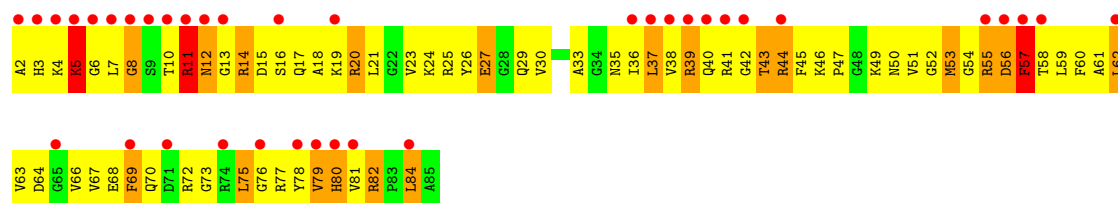
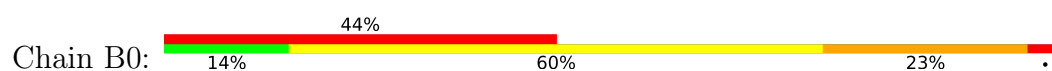


• Molecule 24: ELONGATION FACTOR G



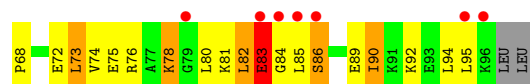


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

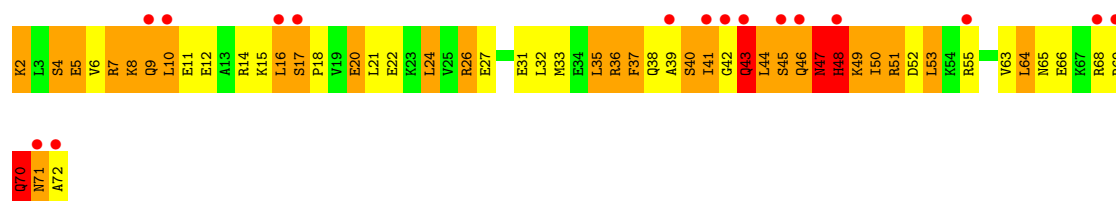
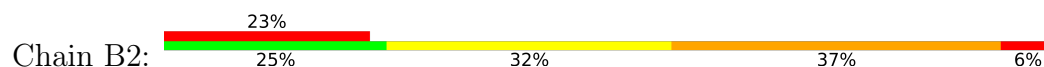


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

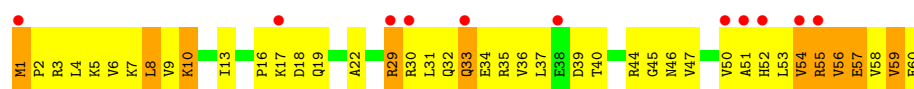




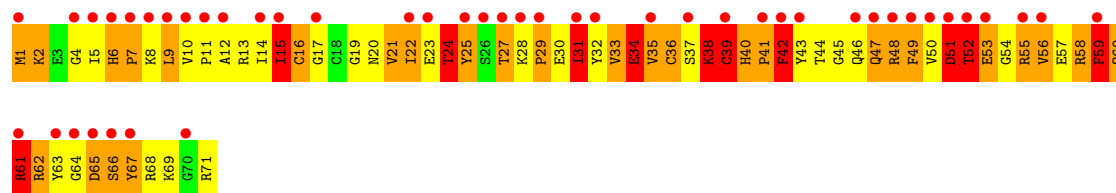
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



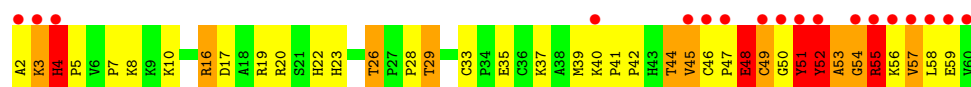
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

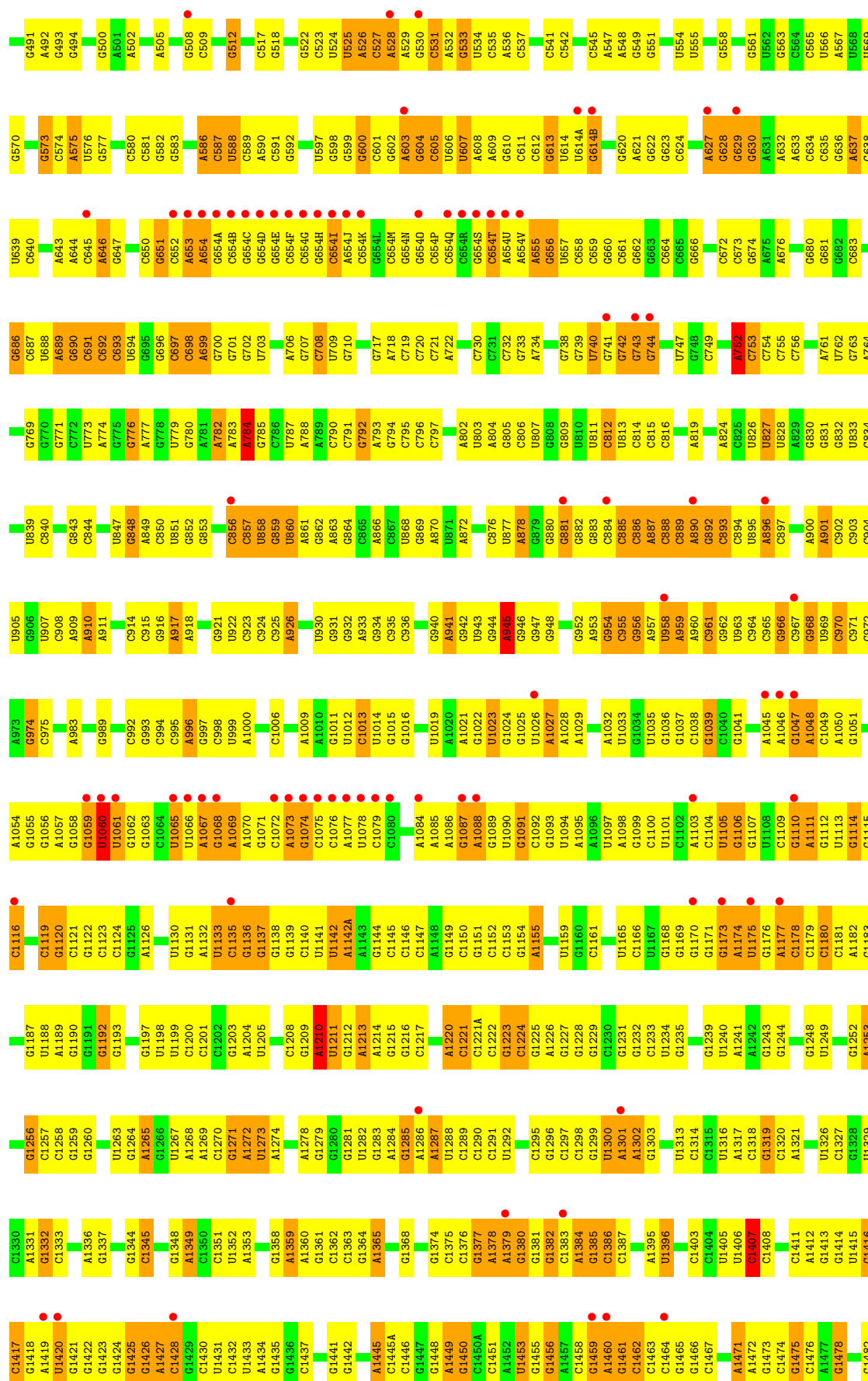


• Molecule 31: 50S RIBOSOMAL PROTEIN L33

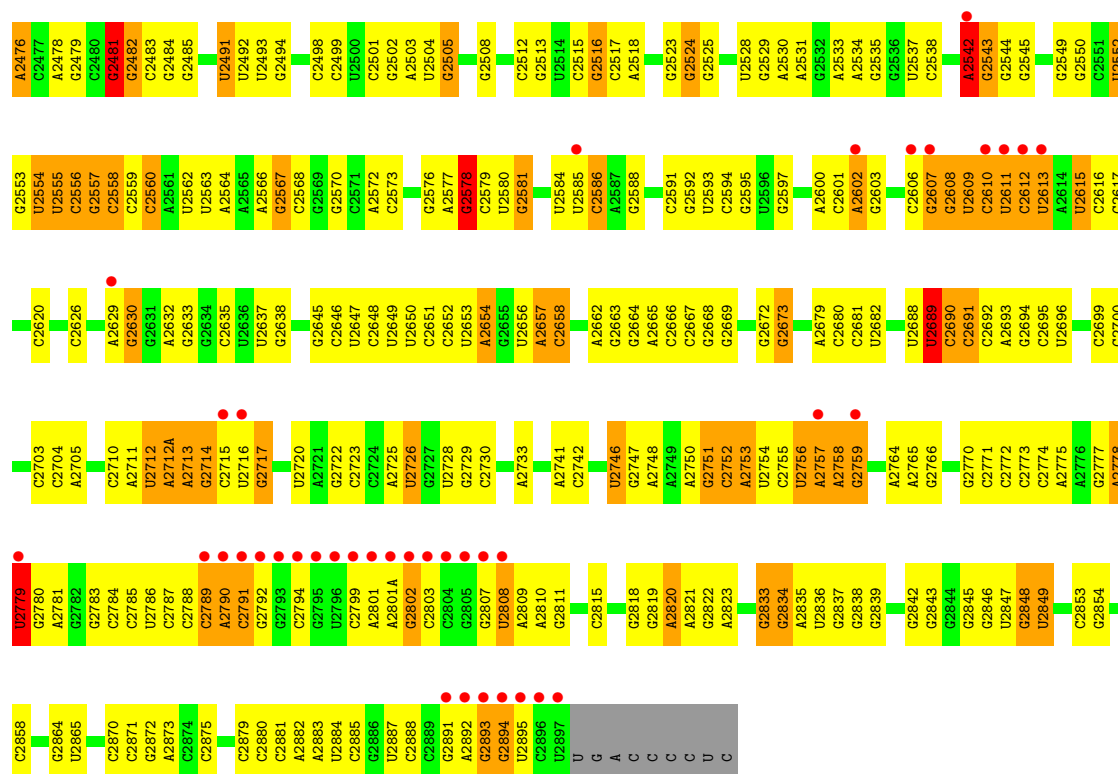


• Molecule 32: 50S RIBOSOMAL PROTEIN L34

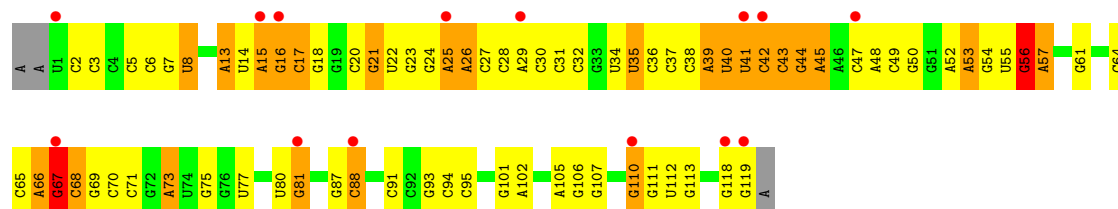




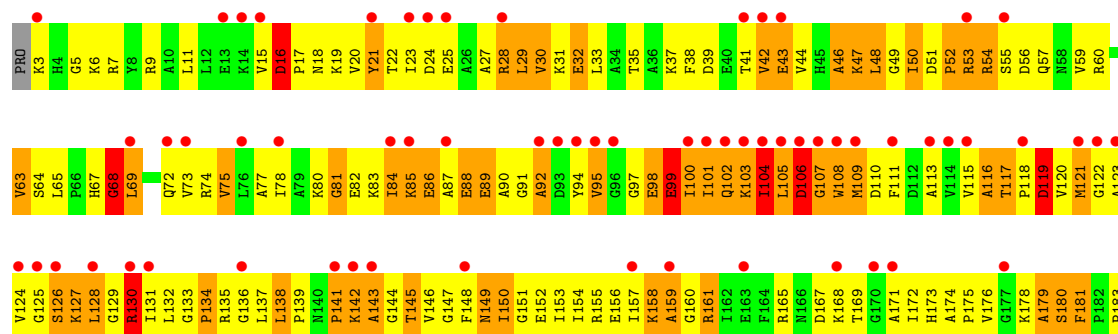
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C2334	A2335	A2336	G2337	G2338	G2339	G2340	G2341	C2342	C2343	U2344	G2345	A2346	C2347	C2350	A2351	C2352	G2353	C2354	C2355	C2356	U2357	C2358	C2359	A2360	A2361	G2362	C2363	C2364	G2365	A2369	G2373	C2374	G2375	A2376	A2377	G2378	G2379	C2380	C2381	G2382	C2383	C2384	C2385	C2386	U2387	C2388	G2389	U2390	G2391	A2392	A2393	C2394	C2395	C2396	U2397	C2398		
C2261	U2262	C2263	A2267	A2268	A2269	G2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2282	C2283	C2284	C2285	C2286	A2287	A2288	U2291	C2292	C2293	G2297	A2298	G2299	G2300	G2304	A2305	C2306	G2307	G2308	A2309	A2310	A2311	U2312	C2313	C2314	G2315	C2316	C2317	G2318	C2319	A2320	C2321	A2327	A2328	C2329	G2330	C2331	U2332	A2333					
G2186	G2187	C2188	U2189	G2190	G2191	G2192	G2193	G2194	C2195	C2196	U2197	A2198	A2199	C2200	C2201	U2203	C2205	G2206	G2207	A2208	U2218	G2219	G2220	G2221	G2222	G2223	G2224	A2225	C2226	G2230	C2231	U2232	U2233	G2234	G2235	C2236	G2237	G2238	G2239	C2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2252	G2253	U2257	C2258	G2259				
G2116	A2117	U2118	G2123	G2124	G2125	A2126	G2127	C2128	C2129	U2130	G2131	U2132	A2133	A2134	C2135	C2136	C2137	C2138	C2139	G2140	G2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	A2157	A2158	C2159	C2163	A2169	A2170	A2171	U2172	U2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	G2181	G2182	C2183	G2184	C2185			
A1969	A1970	A1971	A1972	G1973	C1974	G1980	A1981	C1982	C1983	G1984	G1985	A1986	G1987	G1988	G1989	C1990	U1991	G1992	U1993	C1994	U1995	C1996	G1997	G1998	C1999	G2000	A2001	G2002	C2006	C2007	C2008	G2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	U2098	A2020	C2021	U2022	G2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034
A1890	G1891	C1892	C1893	C1894	G1899	A1900	A1901	G1902	G1903	G1906	G1907	A1912	A1913	C1914	U1915	A1916	A1918	A1919	C1920	G1921	C1922	U1923	C1924	G1925	U1926	A1927	G1930	U1931	A1932	G1933	A1936	A1937	A1938	A1939	C1941	C1942	G1945	U1946	C1947	G1954	U1955	U1956	C1961	C1962	U1963	G1964	C1965	A1966	G1967	C1968								
G1811	A1812	G1813	G1816	G1817	U1818	A1819	U1820	A1821	G1822	G1823	G1824	C1827	G1828	A1829	U1833	U1834	G1835	C1836	C1837	C1838	G1839	G1840	U1841	G1842	C1843	C1844	G1845	G1846	A1847	U1848	G1849	A1853	A1854	G1855	G1856	G1857	G1858	A1859	U1864	G1865	C1866	A1876	A1877	G1878	G1881	C1882	G1883	A1884	A1885	C1886	C1887	G1888	A1889					
C1745A	G1746	G1747	G1747A	G1748	G1749	G1750	C1751	G1754	A1762	G1763	G1764	G1765	U1766	C1767	U1768	G1769	G1770	C1771	A1772	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	C1781	C1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	A1791	U1794	C1795	U1796	C1797	U1798	G1799	C1800	G1801	A1802	A1803	C1804	U1805	A1806	G1807	U1808	A1809	A1810			
G1650	G1651	A1652	G1653	A1654	C1658	C1659	C1660	G1661	C1662	C1663	A1669	C1670	G1674	G1675	C1676	A1676	A1677	G1678	G1681	G1682	C1683	C1684	C1685	U1688	C1689	A1690	C1691	U1692	U1693	C1694	C1695	G1696	G1697	A1698	G1699	A1700	A1701	G1702	G1703	U1709	C1710	C1711	C1712	U1713	G1714	G1717	G1718	G1719	U1720	G1721	A1722	U1739	C1740	A1741				
C1564	C1565	G1568	G1568	A1569	A1570	A1571	A1572	C1577	U1578	A1579	A1580	G1581	C1584	A1586	A1587	C1588	C1589	C1591	C1592	G1593	G1594	G1595	A1596	A1597	C1598	C1599	C1600	G1601	U1602	C1607	A1608	A1609	C1533	A1610	A1616	C1617	A1618	C1625	G1626	C1636	C1637	C1638	U1639	C1640	A1641	G1642	C1643	C1644	C1645	C1646	G1647	C1648	C1649					
G1484	G1485	A1486	G1487	G1488	U1489	A1490	C1493	A1494	A1495	A1496	U1497	C1501	C1502	U1503	C1504	C1505	C1506	C1509	A1509A	A1509B	G1510	C1511	C1516	C1517	C1518	A1528	A1528A	G1529	C1530	C1531	C1532	C1533	U1534	A1535	C1536	C1537	C1538	G1539	U1540	G1541	A1542	C1543	A1544	A1545	C1546	C1547	C1548	C1549	A1554	A1558	G1559							

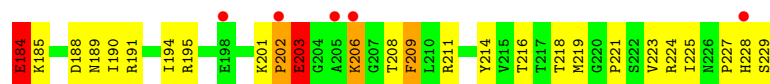


• Molecule 36: 5S RIBOSOMAL RNA

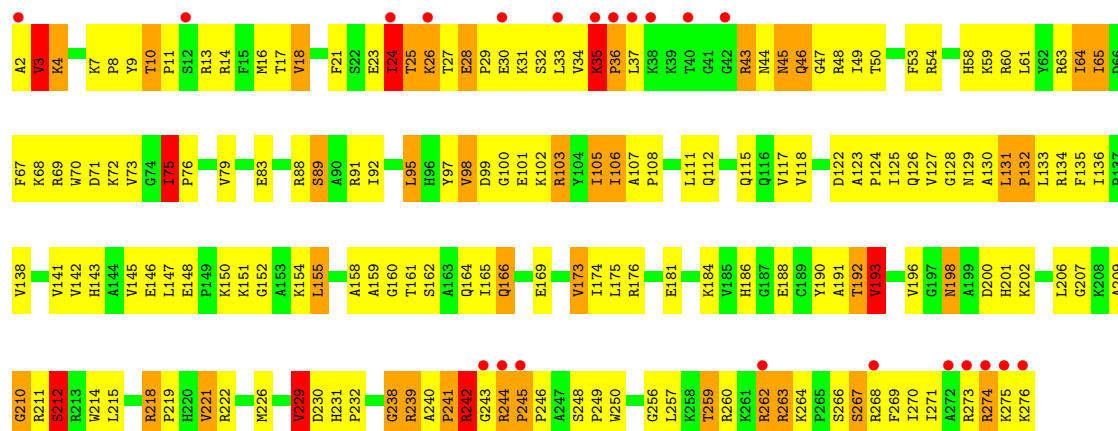


• Molecule 37: RIBOSOMAL PROTEIN L1

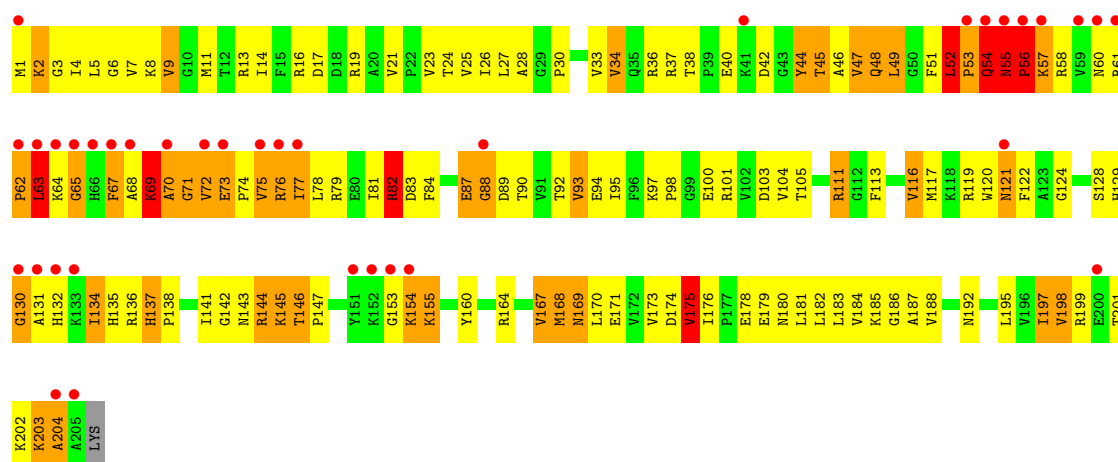




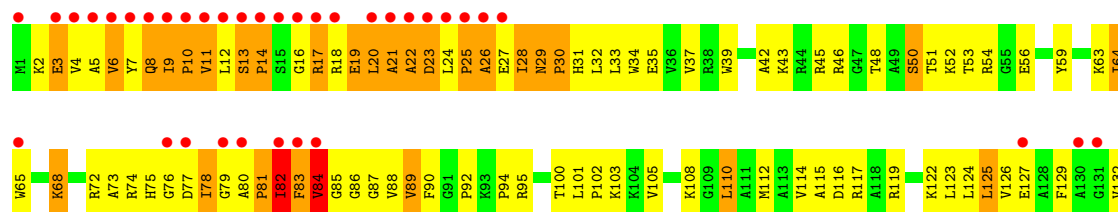
● Molecule 38: 50S RIBOSOMAL PROTEIN L2

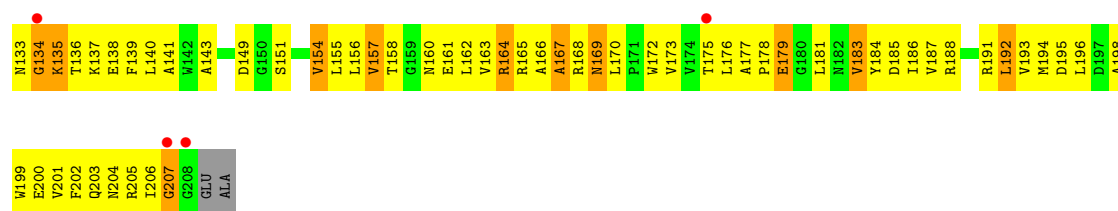


● Molecule 39: 50S RIBOSOMAL PROTEIN L3

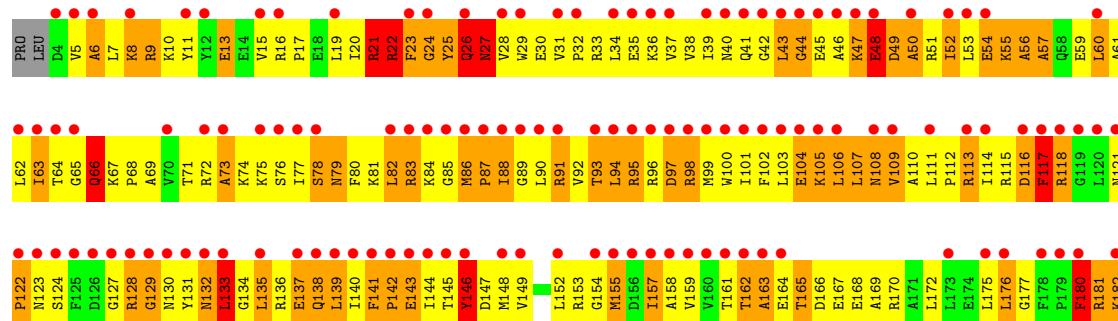


● Molecule 40: 50S RIBOSOMAL PROTEIN L4

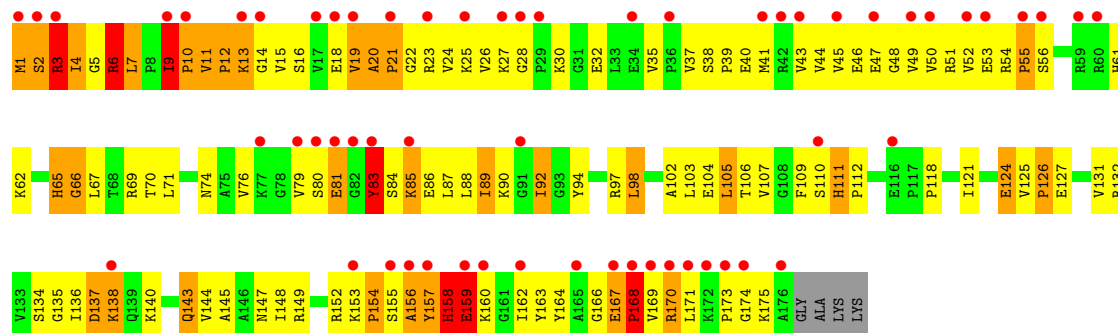




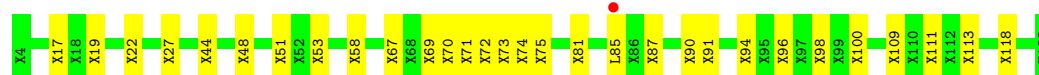
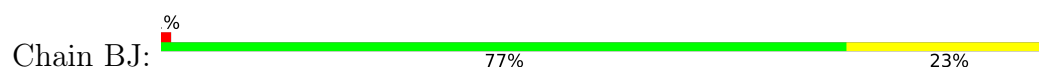
● Molecule 41: 50S RIBOSOMAL PROTEIN L5



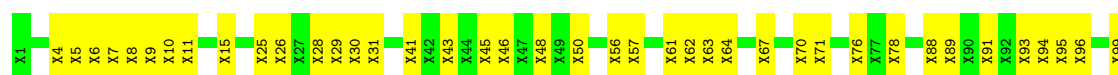
● Molecule 42: 50S RIBOSOMAL PROTEIN L6

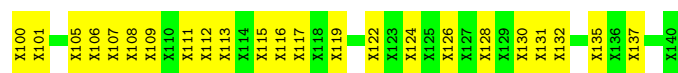


● Molecule 43: CHAIN J

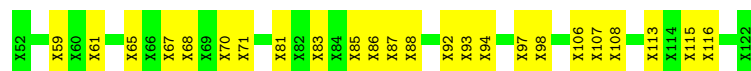


● Molecule 44: CHAIN K

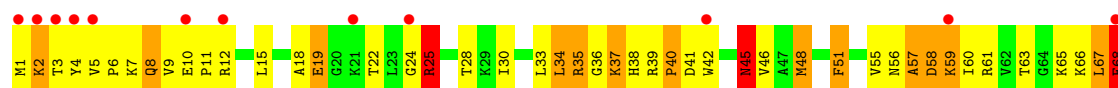




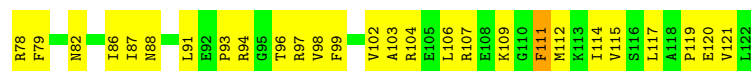
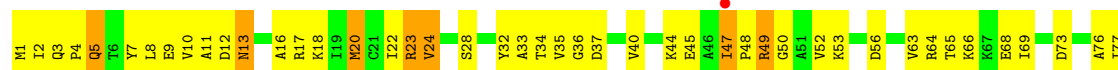
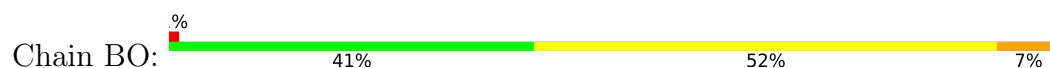
• Molecule 45: CHAIN L



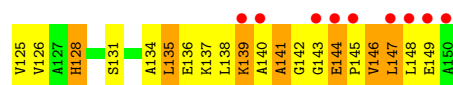
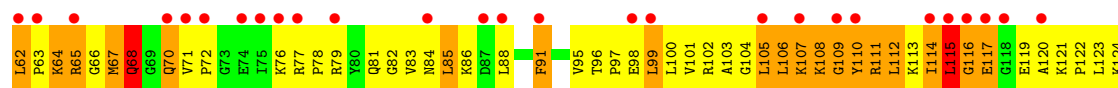
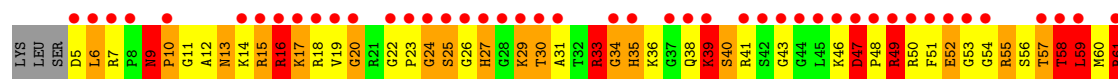
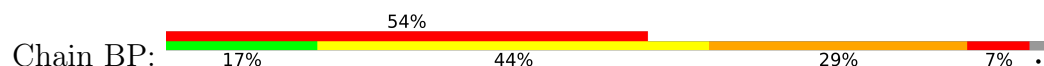
• Molecule 46: 50S RIBOSOMAL PROTEIN L13



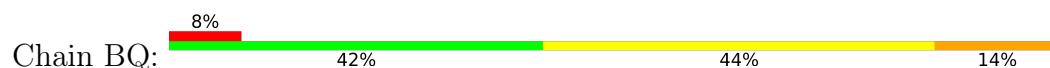
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

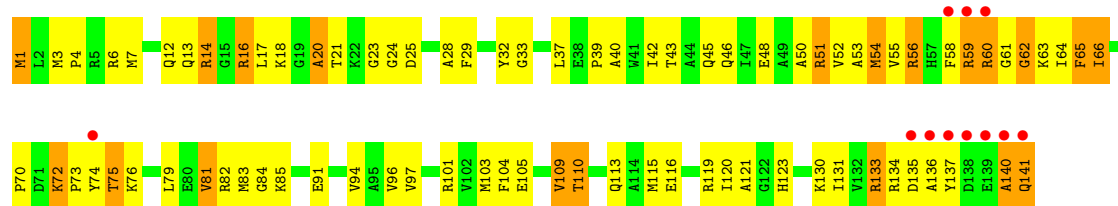


• Molecule 48: 50S RIBOSOMAL PROTEIN L15

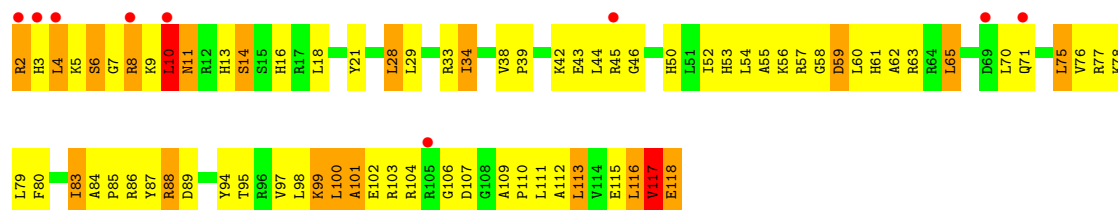


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

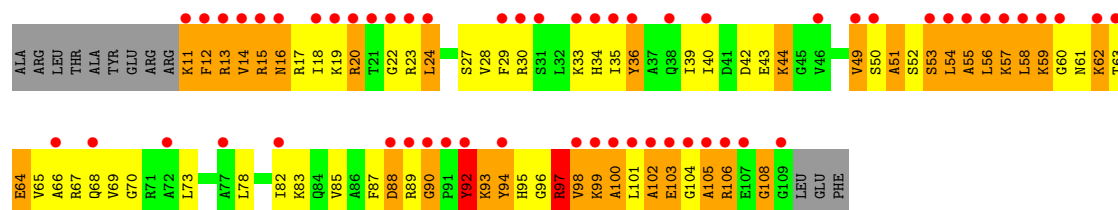
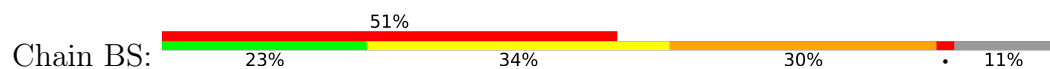




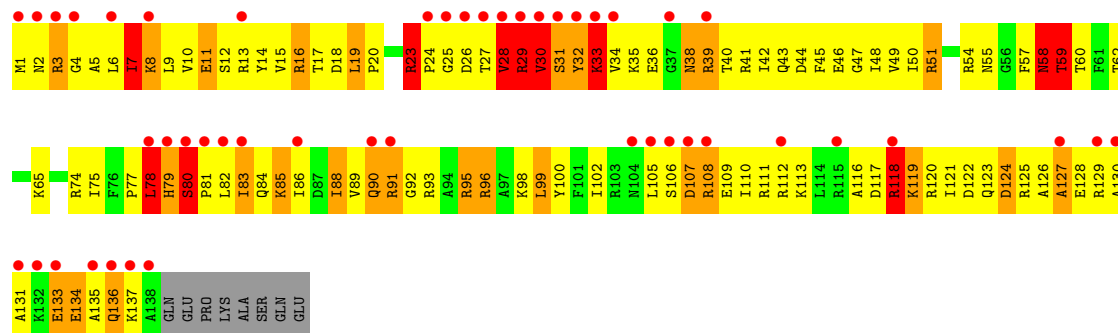
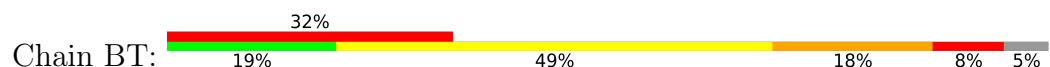
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



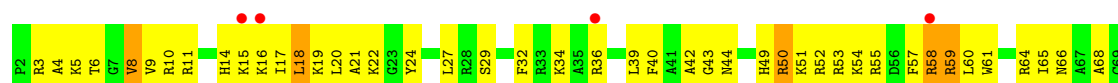
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

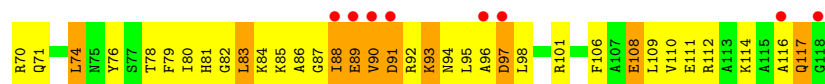


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

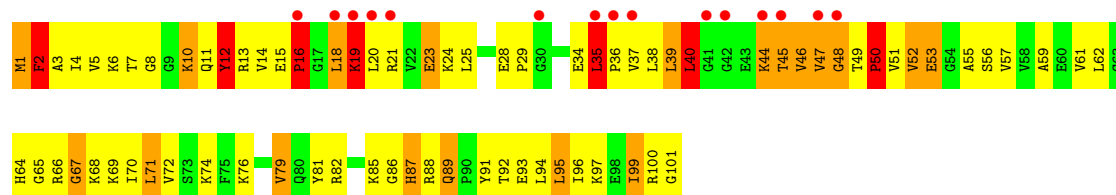


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

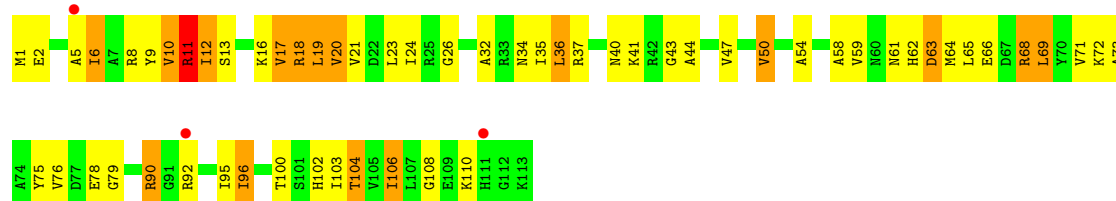




• Molecule 54: 50S RIBOSOMAL PROTEIN L21



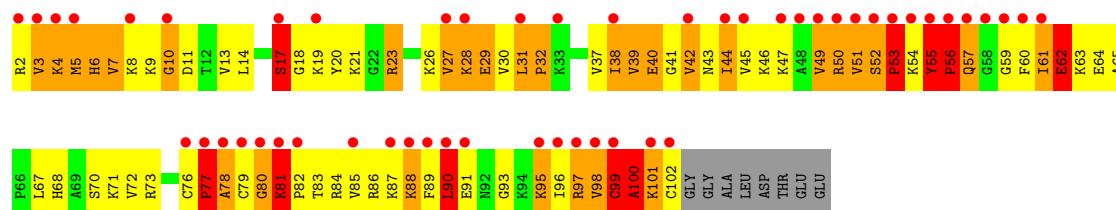
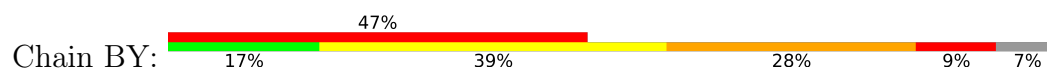
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



• Molecule 56: 50S RIBOSOMAL PROTEIN L23

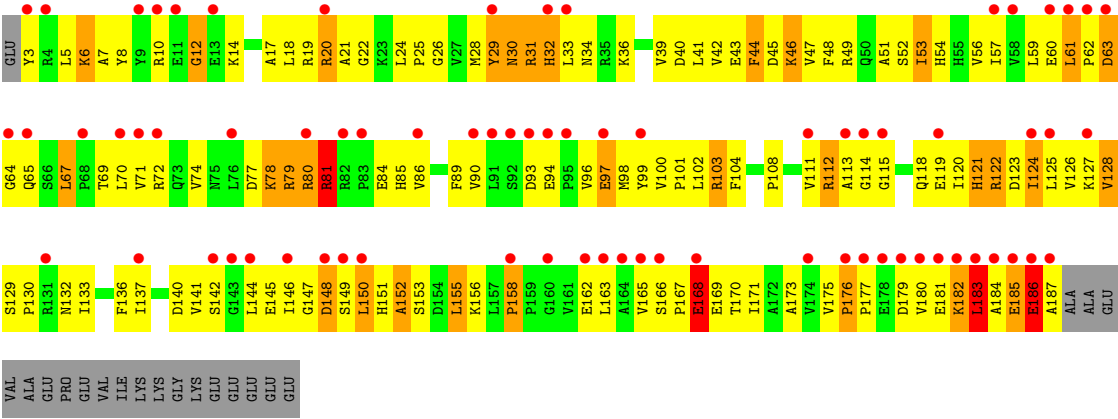


• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• 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	202.90Å 242.63Å 309.32Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	49.75 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-2.95) 100.0 (49.75-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.244 0.223 , 0.254	Depositor DCC
R_{free} test set	30895 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	153829	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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, GCP

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	0.38	1/36258 (0.0%)	0.62	18/56589 (0.0%)
2	AB	0.32	0/1936	0.73	2/2611 (0.1%)
3	AC	0.44	0/1637	0.92	6/2207 (0.3%)
4	AD	0.43	0/1733	0.94	8/2318 (0.3%)
5	AE	0.54	1/1163 (0.1%)	1.00	1/1566 (0.1%)
6	AF	0.43	0/856	0.91	1/1154 (0.1%)
7	AG	0.43	0/1276	1.03	10/1709 (0.6%)
8	AH	0.49	0/1136	1.04	7/1527 (0.5%)
9	AI	0.44	0/1029	1.01	7/1379 (0.5%)
10	AJ	0.52	1/808 (0.1%)	0.98	2/1087 (0.2%)
11	AK	0.48	0/900	1.03	6/1213 (0.5%)
12	AL	0.50	1/987 (0.1%)	1.10	5/1322 (0.4%)
13	AM	0.43	1/948 (0.1%)	0.90	1/1272 (0.1%)
14	AN	0.50	0/501	1.11	4/664 (0.6%)
15	AO	0.45	0/745	0.95	3/992 (0.3%)
16	AP	0.50	1/717 (0.1%)	1.07	6/965 (0.6%)
17	AQ	0.49	1/837 (0.1%)	1.00	3/1119 (0.3%)
18	AR	0.41	0/579	0.89	2/768 (0.3%)
19	AS	0.47	1/706 (0.1%)	1.07	6/950 (0.6%)
20	AT	0.53	1/765 (0.1%)	1.19	7/1007 (0.7%)
21	AU	0.56	1/213 (0.5%)	0.91	0/279
22	AV	0.44	0/1809	0.60	0/2819
23	AX	0.53	0/210	0.59	0/325
24	AY	0.42	1/5477 (0.0%)	0.93	20/7415 (0.3%)
25	B0	0.30	0/671	0.68	2/892 (0.2%)
26	B1	0.49	1/739 (0.1%)	0.85	3/983 (0.3%)
27	B2	10.01	1/600 (0.2%)	0.68	0/793
28	B3	0.44	1/473 (0.2%)	0.82	1/636 (0.2%)
29	B4	0.30	0/594	0.57	0/795
30	B5	0.53	0/473	1.07	2/639 (0.3%)
31	B6	0.55	0/440	1.16	5/586 (0.9%)
32	B7	0.53	0/427	0.98	1/561 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.62	1/516 (0.2%)	1.20	3/681 (0.4%)
34	B9	0.55	0/310	1.08	2/407 (0.5%)
35	BA	0.40	1/69972 (0.0%)	0.66	43/109230 (0.0%)
36	BB	0.39	0/2853	0.67	4/4451 (0.1%)
37	BC	0.39	0/1766	0.90	8/2380 (0.3%)
38	BD	0.59	0/2195	1.20	20/2955 (0.7%)
39	BE	0.52	1/1597 (0.1%)	1.08	9/2155 (0.4%)
40	BF	0.48	1/1659 (0.1%)	1.06	12/2246 (0.5%)
41	BG	0.54	0/1483	1.12	11/1994 (0.6%)
42	BH	0.57	2/1371 (0.1%)	1.04	7/1853 (0.4%)
43	BJ	0.16	0/7	0.49	0/8
46	BN	0.56	1/1132 (0.1%)	1.14	9/1527 (0.6%)
47	BO	0.55	0/943	1.05	2/1269 (0.2%)
48	BP	0.57	0/1131	1.25	16/1504 (1.1%)
49	BQ	0.49	0/1143	0.99	3/1527 (0.2%)
50	BR	0.57	0/974	1.06	5/1302 (0.4%)
51	BS	0.44	1/779 (0.1%)	0.97	4/1038 (0.4%)
52	BT	0.51	1/1156 (0.1%)	1.04	14/1544 (0.9%)
53	BU	0.53	0/975	1.06	3/1297 (0.2%)
54	BV	0.52	0/790	0.99	3/1057 (0.3%)
55	BW	0.53	0/907	1.01	5/1216 (0.4%)
56	BX	0.56	1/740 (0.1%)	0.98	3/995 (0.3%)
57	BY	0.68	1/789 (0.1%)	1.34	12/1053 (1.1%)
58	BZ	0.40	0/1500	0.97	6/2037 (0.3%)
All	All	0.74	25/164331 (0.0%)	0.77	343/244868 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
24	AY	0	1
35	BA	0	19
36	BB	0	2
All	All	0	23

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B2	72	ALA	C-OXT	245.06	6.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1453	U	O3'-P	-13.64	1.40	1.61
42	BH	1	MET	SD-CE	9.83	2.04	1.79
57	BY	101	LYS	C-N	-5.94	1.25	1.33
51	BS	108	GLY	C-N	-5.77	1.25	1.33

The worst 5 of 343 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	26	ALA	N-CA-C	-14.90	97.17	112.97
48	BP	24	GLY	N-CA-C	12.72	126.98	110.45
3	AC	122	GLU	N-CA-C	-11.75	99.42	113.88
20	AT	12	ALA	N-CA-C	-11.41	98.02	113.30
53	BU	58	ARG	N-CA-C	-10.14	99.06	111.33

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(H)	G	Sidechain
24	AY	499	ARG	Sidechain
35	BA	271(H)	G	Sidechain
35	BA	271(Q)	G	Sidechain
35	BA	271(Y)	U	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	32391	0	16349	1986	0
2	AB	1901	0	1947	332	1
3	AC	1613	0	1677	229	28
4	AD	1703	0	1765	138	0
5	AE	1147	0	1207	57	0
6	AF	843	0	857	59	0
7	AG	1257	0	1296	147	0
8	AH	1116	0	1177	67	0
9	AI	1010	0	1037	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	117	0
11	AK	885	0	904	58	0
12	AL	971	0	1057	115	0
13	AM	938	0	995	131	0
14	AN	492	0	529	71	0
15	AO	734	0	771	53	0
16	AP	701	0	720	60	0
17	AQ	824	0	891	50	0
18	AR	574	0	644	27	0
19	AS	692	0	714	117	0
20	AT	763	0	861	73	11
21	AU	209	0	221	13	0
22	AV	1619	0	823	59	0
23	AX	188	0	98	7	0
24	AY	5376	0	5433	584	0
25	B0	662	0	688	165	0
26	B1	732	0	808	117	0
27	B2	598	0	651	130	11
28	B3	468	0	523	68	0
29	B4	581	0	577	216	0
30	B5	459	0	478	78	0
31	B6	433	0	461	132	0
32	B7	419	0	467	29	0
33	B8	508	0	576	115	0
34	B9	307	0	335	34	0
35	BA	62476	0	31499	3272	28
36	BB	2551	0	1295	106	0
37	BC	1735	0	1790	289	1
38	BD	2145	0	2234	263	0
39	BE	1564	0	1629	239	0
40	BF	1624	0	1677	232	0
41	BG	1459	0	1516	402	0
42	BH	1345	0	1430	194	0
43	BJ	654	0	156	22	0
44	BK	701	0	168	46	0
45	BL	356	0	86	20	0
46	BN	1105	0	1180	120	0
47	BO	933	0	996	74	0
48	BP	1114	0	1186	316	0
49	BQ	1122	0	1179	116	0
50	BR	960	0	1021	107	0
51	BS	771	0	832	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	BT	1142	0	1200	234	0
53	BU	958	0	1015	128	0
54	BV	779	0	852	153	0
55	BW	896	0	953	60	0
56	BX	726	0	778	49	0
57	BY	776	0	870	169	0
58	BZ	1468	0	1492	225	0
59	AA	198	0	0	0	0
59	AY	1	0	0	0	0
59	B0	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	320	0	0	0	0
59	BC	1	0	0	0	0
59	BU	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
61	AY	32	0	14	11	0
62	AY	2	0	0	2	0
All	All	153829	0	105425	11884	40

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 46.

The worst 5 of 11884 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)
30:B5:46:CYS:SG	30:B5:47:PRO:HD2	1.41	1.57
29:B4:12:ALA:H	29:B4:24:THR:CG2	1.16	1.56
9:AI:18:PHE:C	9:AI:61:ALA:HB1	1.27	1.54
9:AI:19:LEU:HA	9:AI:61:ALA:CB	1.39	1.53
52:BT:80:SER:HB3	52:BT:81:PRO:CD	1.40	1.51

The worst 5 of 40 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)
20:AT:100:ILE:CG1	27:B2:43:GLN:CD[2_554]	0.34	1.86
20:AT:100:ILE:CD1	27:B2:43:GLN:NE2[2_554]	0.69	1.51
3:AC:79:ARG:CD	35:BA:2139:C:C4[2_555]	0.83	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:79:ARG:CD	35:BA:2139:C:C5[2_555]	0.87	1.33
3:AC:79:ARG:CG	35:BA:2139:C:C6[2_555]	0.96	1.24

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	233/256 (91%)	163 (70%)	44 (19%)	26 (11%)	0	0
3	AC	205/239 (86%)	145 (71%)	32 (16%)	28 (14%)	0	0
4	AD	206/209 (99%)	160 (78%)	35 (17%)	11 (5%)	1	3
5	AE	149/162 (92%)	134 (90%)	12 (8%)	3 (2%)	6	16
6	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	1	2
7	AG	153/156 (98%)	113 (74%)	26 (17%)	14 (9%)	0	1
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	18	40
9	AI	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	0	1
10	AJ	97/105 (92%)	73 (75%)	15 (16%)	9 (9%)	0	1
11	AK	117/129 (91%)	95 (81%)	19 (16%)	3 (3%)	4	12
12	AL	123/132 (93%)	101 (82%)	11 (9%)	11 (9%)	0	1
13	AM	117/126 (93%)	74 (63%)	32 (27%)	11 (9%)	0	1
14	AN	58/61 (95%)	44 (76%)	7 (12%)	7 (12%)	0	0
15	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	28
16	AP	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	4	13
17	AQ	98/105 (93%)	86 (88%)	10 (10%)	2 (2%)	6	16
18	AR	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	3	10
19	AS	86/93 (92%)	53 (62%)	21 (24%)	12 (14%)	0	0
20	AT	97/106 (92%)	79 (81%)	10 (10%)	8 (8%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	0	1
24	AY	685/691 (99%)	537 (78%)	99 (14%)	49 (7%)	1	1
25	B0	82/84 (98%)	56 (68%)	19 (23%)	7 (8%)	0	1
26	B1	92/97 (95%)	73 (79%)	14 (15%)	5 (5%)	1	3
27	B2	69/71 (97%)	45 (65%)	11 (16%)	13 (19%)	0	0
28	B3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	7	20
29	B4	69/71 (97%)	16 (23%)	17 (25%)	36 (52%)	0	0
30	B5	57/59 (97%)	45 (79%)	3 (5%)	9 (16%)	0	0
31	B6	48/53 (91%)	22 (46%)	11 (23%)	15 (31%)	0	0
32	B7	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
33	B8	62/64 (97%)	42 (68%)	8 (13%)	12 (19%)	0	0
34	B9	35/37 (95%)	23 (66%)	9 (26%)	3 (9%)	0	1
37	BC	225/228 (99%)	121 (54%)	56 (25%)	48 (21%)	0	0
38	BD	273/275 (99%)	222 (81%)	33 (12%)	18 (7%)	1	1
39	BE	203/206 (98%)	145 (71%)	34 (17%)	24 (12%)	0	0
40	BF	206/210 (98%)	165 (80%)	19 (9%)	22 (11%)	0	0
41	BG	177/181 (98%)	78 (44%)	49 (28%)	50 (28%)	0	0
42	BH	174/180 (97%)	112 (64%)	31 (18%)	31 (18%)	0	0
43	BJ	1/130 (1%)	0	1 (100%)	0	100	100
46	BN	137/140 (98%)	110 (80%)	15 (11%)	12 (9%)	0	1
47	BO	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	4	13
48	BP	144/149 (97%)	84 (58%)	23 (16%)	37 (26%)	0	0
49	BQ	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	2	4
50	BR	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	1
51	BS	97/111 (87%)	52 (54%)	25 (26%)	20 (21%)	0	0
52	BT	136/146 (93%)	90 (66%)	25 (18%)	21 (15%)	0	0
53	BU	115/117 (98%)	87 (76%)	22 (19%)	6 (5%)	1	3
54	BV	99/101 (98%)	73 (74%)	11 (11%)	15 (15%)	0	0
55	BW	111/113 (98%)	93 (84%)	14 (13%)	4 (4%)	2	6
56	BX	91/95 (96%)	79 (87%)	11 (12%)	1 (1%)	11	29
57	BY	99/109 (91%)	54 (54%)	17 (17%)	28 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	BZ	183/205 (89%)	131 (72%)	30 (16%)	22 (12%)	0	0
All	All	6506/6949 (94%)	4803 (74%)	1007 (16%)	696 (11%)	0	0

5 of 696 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	26	PRO
2	AB	37	ASN
2	AB	76	GLN
2	AB	77	ALA

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%)	160 (79%)	42 (21%)	1	3
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	3
4	AD	180/181 (99%)	155 (86%)	25 (14%)	3	10
5	AE	115/123 (94%)	109 (95%)	6 (5%)	21	46
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	24
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	19
8	AH	119/119 (100%)	105 (88%)	14 (12%)	5	15
9	AI	98/99 (99%)	83 (85%)	15 (15%)	3	8
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	11	28
11	AK	90/99 (91%)	85 (94%)	5 (6%)	19	43
12	AL	104/109 (95%)	88 (85%)	16 (15%)	2	8
13	AM	94/101 (93%)	83 (88%)	11 (12%)	5	16
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	9
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	20
16	AP	72/74 (97%)	68 (94%)	4 (6%)	19	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	34	59
18	AR	61/77 (79%)	55 (90%)	6 (10%)	7	21
19	AS	74/80 (92%)	65 (88%)	9 (12%)	5	14
20	AT	76/82 (93%)	67 (88%)	9 (12%)	5	15
21	AU	19/22 (86%)	19 (100%)	0	100	100
24	AY	579/582 (100%)	508 (88%)	71 (12%)	4	14
25	B0	66/66 (100%)	46 (70%)	20 (30%)	0	0
26	B1	78/82 (95%)	61 (78%)	17 (22%)	1	2
27	B2	66/66 (100%)	41 (62%)	25 (38%)	0	0
28	B3	51/52 (98%)	41 (80%)	10 (20%)	1	3
29	B4	63/63 (100%)	46 (73%)	17 (27%)	0	0
30	B5	51/51 (100%)	40 (78%)	11 (22%)	1	2
31	B6	49/51 (96%)	36 (74%)	13 (26%)	0	1
32	B7	41/41 (100%)	38 (93%)	3 (7%)	13	33
33	B8	53/54 (98%)	40 (76%)	13 (24%)	1	1
34	B9	34/34 (100%)	30 (88%)	4 (12%)	5	15
37	BC	179/180 (99%)	155 (87%)	24 (13%)	4	11
38	BD	217/217 (100%)	183 (84%)	34 (16%)	2	8
39	BE	165/166 (99%)	132 (80%)	33 (20%)	1	3
40	BF	165/166 (99%)	147 (89%)	18 (11%)	6	18
41	BG	153/155 (99%)	127 (83%)	26 (17%)	2	5
42	BH	146/148 (99%)	132 (90%)	14 (10%)	8	22
43	BJ	1/1 (100%)	1 (100%)	0	100	100
46	BN	117/119 (98%)	101 (86%)	16 (14%)	3	11
47	BO	100/100 (100%)	93 (93%)	7 (7%)	14	34
48	BP	112/115 (97%)	87 (78%)	25 (22%)	1	2
49	BQ	111/111 (100%)	93 (84%)	18 (16%)	2	7
50	BR	100/100 (100%)	83 (83%)	17 (17%)	2	5
51	BS	77/87 (88%)	62 (80%)	15 (20%)	1	3
52	BT	120/127 (94%)	95 (79%)	25 (21%)	1	3
53	BU	92/93 (99%)	84 (91%)	8 (9%)	9	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BV	82/82 (100%)	65 (79%)	17 (21%)	1	3
55	BW	91/92 (99%)	76 (84%)	15 (16%)	2	7
56	BX	74/77 (96%)	68 (92%)	6 (8%)	11	28
57	BY	84/90 (93%)	68 (81%)	16 (19%)	1	3
58	BZ	162/178 (91%)	140 (86%)	22 (14%)	3	11
All	All	5469/5656 (97%)	4668 (85%)	801 (15%)	3	9

5 of 801 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BC	138	LEU
41	BG	133	LEU
58	BZ	185	GLU
38	BD	46	GLN
37	BC	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
38	BD	201	HIS
47	BO	13	ASN
39	BE	129	HIS
41	BG	40	ASN
48	BP	128	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1519 (99%)	323 (21%)	51 (3%)
22	AV	75/76 (98%)	24 (32%)	2 (2%)
23	AX	8/9 (88%)	3 (37%)	0
35	BA	2900/2915 (99%)	669 (23%)	60 (2%)
36	BB	118/122 (96%)	26 (22%)	2 (1%)
All	All	4607/4641 (99%)	1045 (22%)	115 (2%)

5 of 1045 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	38	G
1	AA	39	G

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	221	A
35	BA	2689	U
35	BA	1060	U
35	BA	2610	C
35	BA	2157	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 527 ligands modelled in this entry, 526 are monoatomic - leaving 1 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	AY	701	59	32,34,34	1.56	6 (18%)	49,54,54	1.89	15 (30%)

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	AY	701	59	-	7/19/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GCP	PG-O3G	-3.45	1.47	1.55
61	AY	701	GCP	PB-O2B	-3.32	1.48	1.56
61	AY	701	GCP	C5-C6	-3.00	1.33	1.44
61	AY	701	GCP	PG-O2G	-2.94	1.48	1.55
61	AY	701	GCP	C5-N7	-2.74	1.33	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GCP	C2-N3-C4	4.86	120.68	112.30
61	AY	701	GCP	C5-C4-N3	-4.57	121.11	128.39
61	AY	701	GCP	PB-O3A-PA	-3.80	119.98	132.37
61	AY	701	GCP	C2-N1-C6	-3.78	118.26	125.11
61	AY	701	GCP	O1G-PG-C3B	-3.37	104.02	111.37

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	GCP	PG-C3B-PB-O2B
61	AY	701	GCP	PG-C3B-PB-O3A
61	AY	701	GCP	O4'-C4'-C5'-O5'
61	AY	701	GCP	PB-O3A-PA-O2A
61	AY	701	GCP	PG-C3B-PB-O1B

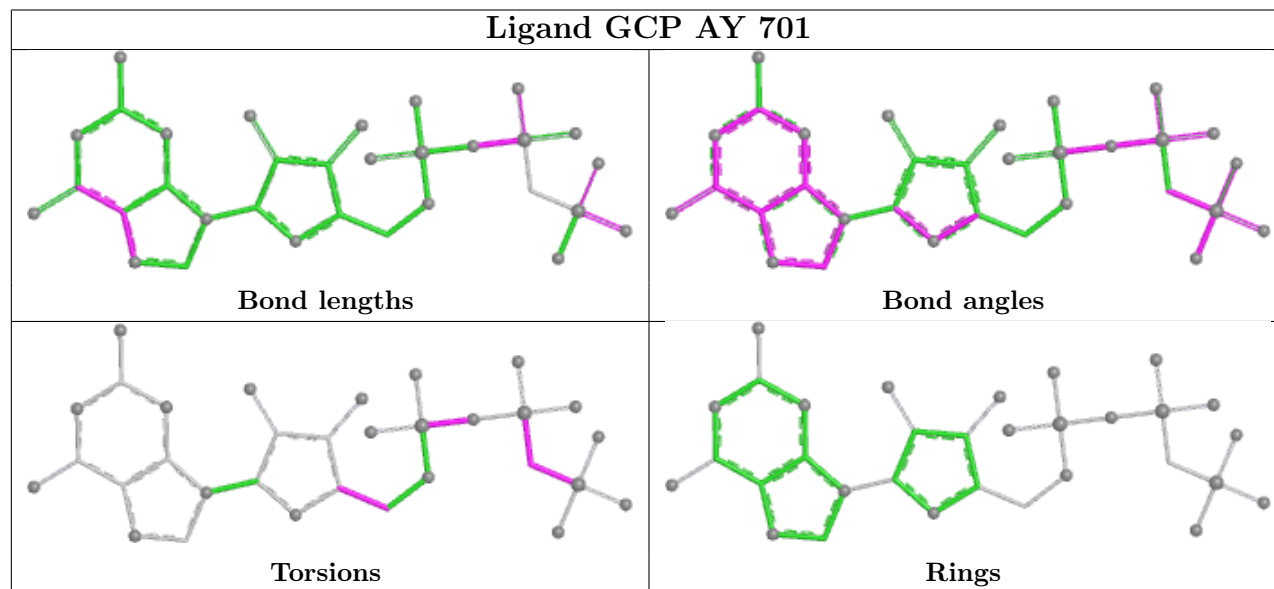
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GCP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	BA	3
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	496:A	O3'	498:U	P	3.07
1	BA	45:C	O3'	47:C	P	2.97
1	BA	1133:U	O3'	1135:C	P	2.48
1	BA	2203:U	O3'	2205:C	P	2.42

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	1507/1519 (99%)	0.44	149 (9%) 13 11	24, 47, 125, 239	0
2	AB	235/256 (91%)	1.47	74 (31%) 1 1	34, 61, 112, 122	0
3	AC	207/239 (86%)	1.20	39 (18%) 3 3	30, 54, 84, 102	0
4	AD	208/209 (99%)	0.94	29 (13%) 6 6	36, 57, 80, 89	0
5	AE	151/162 (93%)	0.15	5 (3%) 49 42	29, 40, 59, 81	0
6	AF	101/101 (100%)	0.76	7 (6%) 23 19	41, 68, 86, 99	0
7	AG	155/156 (99%)	1.22	31 (20%) 3 3	44, 66, 112, 126	0
8	AH	138/138 (100%)	0.21	5 (3%) 46 38	32, 45, 63, 74	0
9	AI	127/128 (99%)	1.23	26 (20%) 2 2	33, 61, 81, 90	0
10	AJ	99/105 (94%)	1.21	17 (17%) 4 3	38, 58, 100, 104	0
11	AK	119/129 (92%)	0.74	10 (8%) 17 15	26, 53, 76, 94	0
12	AL	125/132 (94%)	0.81	18 (14%) 6 5	27, 45, 64, 96	0
13	AM	119/126 (94%)	1.86	36 (30%) 1 1	46, 83, 107, 117	0
14	AN	60/61 (98%)	1.34	17 (28%) 1 1	35, 48, 83, 91	0
15	AO	88/89 (98%)	0.61	4 (4%) 38 31	33, 51, 75, 85	0
16	AP	84/88 (95%)	0.60	0 100 100	37, 47, 70, 95	0
17	AQ	100/105 (95%)	0.34	3 (3%) 52 45	27, 44, 62, 65	0
18	AR	70/88 (79%)	0.78	8 (11%) 10 9	36, 57, 94, 95	0
19	AS	88/93 (94%)	1.78	32 (36%) 1 1	59, 82, 103, 109	0
20	AT	99/106 (93%)	0.87	17 (17%) 4 3	33, 45, 68, 73	0
21	AU	25/27 (92%)	1.45	7 (28%) 1 1	43, 59, 79, 81	0
22	AV	76/76 (100%)	0.79	9 (11%) 9 8	33, 74, 111, 145	0
23	AX	9/9 (100%)	1.26	3 (33%) 1 1	28, 51, 122, 134	0
24	AY	687/691 (99%)	1.11	108 (15%) 5 5	39, 67, 119, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
25	B0	84/84 (100%)	2.26	37 (44%)	0	0	43, 56, 121, 140	0
26	B1	94/97 (96%)	1.31	24 (25%)	1	1	26, 47, 76, 88	0
27	B2	71/71 (100%)	1.33	16 (22%)	2	2	41, 57, 88, 112	0
28	B3	60/60 (100%)	1.14	11 (18%)	3	3	35, 56, 75, 100	0
29	B4	71/71 (100%)	2.54	46 (64%)	0	0	129, 151, 159, 159	0
30	B5	59/59 (100%)	1.30	18 (30%)	1	1	20, 42, 109, 122	0
31	B6	50/53 (94%)	3.00	36 (72%)	0	0	41, 72, 91, 98	0
32	B7	48/48 (100%)	0.30	6 (12%)	8	7	18, 30, 60, 86	0
33	B8	64/64 (100%)	1.85	24 (37%)	1	1	32, 49, 70, 87	0
34	B9	37/37 (100%)	1.19	7 (18%)	3	3	40, 52, 62, 76	0
35	BA	2901/2915 (99%)	0.26	226 (7%)	19	17	18, 42, 116, 244	0
36	BB	119/122 (97%)	1.02	14 (11%)	9	8	42, 88, 115, 130	0
37	BC	227/228 (99%)	1.63	68 (29%)	1	1	25, 78, 124, 135	0
38	BD	275/275 (100%)	0.42	22 (8%)	18	16	18, 32, 58, 93	0
39	BE	205/206 (99%)	0.85	36 (17%)	4	3	23, 42, 78, 86	0
40	BF	208/210 (99%)	1.11	40 (19%)	3	3	17, 52, 104, 121	0
41	BG	179/181 (98%)	2.63	125 (69%)	0	0	94, 122, 138, 144	0
42	BH	176/180 (97%)	1.78	59 (33%)	1	1	52, 75, 96, 108	0
43	BJ	1/130 (0%)	3.51	1 (100%)	0	0	121, 121, 121, 121	0
44	BK	0/140	-	-	-	-	-	-
45	BL	0/71	-	-	-	-	-	-
46	BN	139/140 (99%)	0.88	21 (15%)	5	5	31, 45, 72, 93	0
47	BO	122/122 (100%)	0.12	1 (0%)	82	78	25, 39, 54, 63	0
48	BP	146/149 (97%)	2.30	81 (55%)	0	0	34, 67, 96, 118	0
49	BQ	141/141 (100%)	0.84	11 (7%)	19	17	32, 49, 75, 115	0
50	BR	117/117 (100%)	0.59	9 (7%)	19	17	23, 40, 59, 67	0
51	BS	99/111 (89%)	2.39	57 (57%)	0	0	68, 91, 113, 122	0
52	BT	138/146 (94%)	1.69	47 (34%)	1	1	32, 53, 122, 144	0
53	BU	117/117 (100%)	0.60	12 (10%)	12	11	28, 42, 69, 85	0
54	BV	101/101 (100%)	1.05	15 (14%)	5	5	25, 62, 83, 87	0
55	BW	113/113 (100%)	0.32	3 (2%)	56	48	26, 38, 69, 104	0
56	BX	93/95 (97%)	0.43	4 (4%)	40	32	30, 41, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	101/109 (92%)	2.20	51 (50%) 0 0	37, 61, 118, 127	0
58	BZ	185/205 (90%)	1.87	73 (39%) 1 0	25, 81, 96, 109	0
All	All	11218/11801 (95%)	0.84	1855 (16%) 4 4	17, 52, 116, 244	0

The worst 5 of 1855 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	B0	2	ALA	11.0
24	AY	50	ALA	10.6
24	AY	48	GLY	10.5
49	BQ	141	GLN	10.4
57	BY	51	VAL	10.2

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

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

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
59	MG	BA	3280	1/1	0.38	0.41	87,87,87,87	0
59	MG	AA	1712	1/1	0.39	0.21	66,66,66,66	0
59	MG	BA	3247	1/1	0.45	0.28	49,49,49,49	0
59	MG	BA	3179	1/1	0.48	0.32	87,87,87,87	0
59	MG	AA	1601	1/1	0.50	0.39	97,97,97,97	0
59	MG	BA	3215	1/1	0.51	0.27	81,81,81,81	0
59	MG	AA	1780	1/1	0.52	0.16	54,54,54,54	0
59	MG	AA	1666	1/1	0.53	0.48	83,83,83,83	0
59	MG	BC	301	1/1	0.56	0.17	115,115,115,115	0
59	MG	AA	1677	1/1	0.57	0.37	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3204	1/1	0.57	0.29	60,60,60,60	0
59	MG	AA	1703	1/1	0.57	0.46	81,81,81,81	0
59	MG	BA	3252	1/1	0.58	0.18	50,50,50,50	0
59	MG	AA	1756	1/1	0.59	0.27	54,54,54,54	0
59	MG	AA	1716	1/1	0.63	0.38	71,71,71,71	0
59	MG	AA	1607	1/1	0.63	0.44	97,97,97,97	0
59	MG	AA	1758	1/1	0.64	0.35	75,75,75,75	0
59	MG	AA	1754	1/1	0.65	0.36	75,75,75,75	0
59	MG	BA	3275	1/1	0.65	0.29	52,52,52,52	0
59	MG	BA	3142	1/1	0.65	0.17	48,48,48,48	0
59	MG	AA	1767	1/1	0.65	0.33	60,60,60,60	0
59	MG	BA	3182	1/1	0.66	0.29	73,73,73,73	0
59	MG	BA	3194	1/1	0.66	0.14	74,74,74,74	0
59	MG	BA	3175	1/1	0.66	0.21	62,62,62,62	0
59	MG	BA	3226	1/1	0.67	0.24	56,56,56,56	0
59	MG	BA	3026	1/1	0.67	0.29	67,67,67,67	0
59	MG	BA	3282	1/1	0.67	0.24	67,67,67,67	0
59	MG	AA	1781	1/1	0.67	0.14	54,54,54,54	0
59	MG	AA	1744	1/1	0.68	0.24	90,90,90,90	0
59	MG	AA	1740	1/1	0.68	0.48	79,79,79,79	0
59	MG	AA	1635	1/1	0.69	0.12	65,65,65,65	0
59	MG	AA	1639	1/1	0.69	0.17	55,55,55,55	0
59	MG	BA	3236	1/1	0.69	0.18	52,52,52,52	0
59	MG	AA	1689	1/1	0.70	0.40	79,79,79,79	0
59	MG	AA	1620	1/1	0.70	0.41	75,75,75,75	0
59	MG	BA	3239	1/1	0.70	0.42	87,87,87,87	0
59	MG	BA	3163	1/1	0.71	0.16	55,55,55,55	0
59	MG	BA	3023	1/1	0.71	0.33	87,87,87,87	0
59	MG	BA	3261	1/1	0.71	0.22	67,67,67,67	0
59	MG	AA	1753	1/1	0.71	0.30	89,89,89,89	0
59	MG	BA	3090	1/1	0.71	0.25	56,56,56,56	0
59	MG	BA	3237	1/1	0.71	0.36	94,94,94,94	0
59	MG	AA	1773	1/1	0.71	0.40	60,60,60,60	0
59	MG	AA	1775	1/1	0.72	0.09	45,45,45,45	0
59	MG	AA	1707	1/1	0.73	0.23	60,60,60,60	0
59	MG	AA	1627	1/1	0.73	0.20	74,74,74,74	0
59	MG	B0	101	1/1	0.73	0.45	72,72,72,72	0
59	MG	BA	3266	1/1	0.73	0.24	71,71,71,71	0
59	MG	BA	3032	1/1	0.74	0.31	73,73,73,73	0
59	MG	BA	3301	1/1	0.74	0.30	45,45,45,45	0
59	MG	BA	3315	1/1	0.74	0.22	52,52,52,52	0
59	MG	AA	1772	1/1	0.74	0.46	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3240	1/1	0.75	0.32	60,60,60,60	0
59	MG	BA	3260	1/1	0.75	0.39	72,72,72,72	0
59	MG	BA	3279	1/1	0.75	0.38	63,63,63,63	0
59	MG	BA	3041	1/1	0.75	0.25	75,75,75,75	0
59	MG	BA	3055	1/1	0.76	0.20	33,33,33,33	0
59	MG	AA	1652	1/1	0.76	0.29	41,41,41,41	0
59	MG	BA	3281	1/1	0.76	0.40	79,79,79,79	0
59	MG	AA	1613	1/1	0.76	0.26	65,65,65,65	0
59	MG	AA	1632	1/1	0.76	0.27	56,56,56,56	0
59	MG	BA	3012	1/1	0.76	0.38	79,79,79,79	0
59	MG	BA	3241	1/1	0.76	0.25	65,65,65,65	0
59	MG	AA	1733	1/1	0.77	0.12	67,67,67,67	0
59	MG	BA	3134	1/1	0.77	0.22	65,65,65,65	0
59	MG	AA	1738	1/1	0.77	0.17	53,53,53,53	0
59	MG	AA	1674	1/1	0.77	0.39	74,74,74,74	0
59	MG	BA	3253	1/1	0.77	0.53	98,98,98,98	0
59	MG	AA	1697	1/1	0.77	0.17	61,61,61,61	0
59	MG	AA	1790	1/1	0.77	0.27	57,57,57,57	0
59	MG	AA	1640	1/1	0.77	0.26	74,74,74,74	0
59	MG	BA	3130	1/1	0.78	0.42	56,56,56,56	0
59	MG	BA	3183	1/1	0.78	0.11	58,58,58,58	0
59	MG	BA	3166	1/1	0.78	0.28	68,68,68,68	0
59	MG	BA	3304	1/1	0.78	0.21	32,32,32,32	0
59	MG	BA	3060	1/1	0.78	0.27	31,31,31,31	0
59	MG	BA	3040	1/1	0.78	0.30	71,71,71,71	0
59	MG	AA	1684	1/1	0.79	0.59	61,61,61,61	0
59	MG	BA	3265	1/1	0.79	0.31	65,65,65,65	0
59	MG	AA	1724	1/1	0.79	0.14	48,48,48,48	0
59	MG	BA	3268	1/1	0.79	0.41	85,85,85,85	0
59	MG	AA	1793	1/1	0.79	0.15	50,50,50,50	0
59	MG	BA	3278	1/1	0.79	0.24	91,91,91,91	0
59	MG	BA	3136	1/1	0.79	0.31	90,90,90,90	0
59	MG	AA	1743	1/1	0.79	0.23	38,38,38,38	0
59	MG	BA	3242	1/1	0.79	0.36	78,78,78,78	0
59	MG	AA	1626	1/1	0.79	0.34	59,59,59,59	0
59	MG	BA	3164	1/1	0.79	0.26	49,49,49,49	0
59	MG	BA	3216	1/1	0.79	0.18	54,54,54,54	0
59	MG	BA	3258	1/1	0.79	0.22	51,51,51,51	0
59	MG	AA	1762	1/1	0.79	0.28	100,100,100,100	0
59	MG	AA	1797	1/1	0.80	0.23	58,58,58,58	0
59	MG	BA	3075	1/1	0.80	0.23	31,31,31,31	0
59	MG	AA	1760	1/1	0.80	0.28	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3197	1/1	0.80	0.24	58,58,58,58	0
59	MG	BA	3106	1/1	0.80	0.20	47,47,47,47	0
59	MG	BA	3206	1/1	0.80	0.25	65,65,65,65	0
59	MG	BA	3212	1/1	0.80	0.26	46,46,46,46	0
59	MG	BA	3009	1/1	0.80	0.46	77,77,77,77	0
59	MG	BA	3132	1/1	0.80	0.32	59,59,59,59	0
59	MG	AA	1779	1/1	0.80	0.35	81,81,81,81	0
59	MG	BA	3230	1/1	0.80	0.22	40,40,40,40	0
59	MG	BA	3020	1/1	0.80	0.30	63,63,63,63	0
59	MG	AA	1704	1/1	0.80	0.24	25,25,25,25	0
59	MG	AA	1715	1/1	0.80	0.12	42,42,42,42	0
59	MG	AA	1788	1/1	0.80	0.31	73,73,73,73	0
59	MG	AA	1789	1/1	0.80	0.23	61,61,61,61	0
59	MG	AA	1611	1/1	0.80	0.33	75,75,75,75	0
59	MG	AA	1752	1/1	0.80	0.31	59,59,59,59	0
59	MG	AA	1676	1/1	0.81	0.23	62,62,62,62	0
59	MG	BA	3027	1/1	0.81	0.33	71,71,71,71	0
59	MG	AA	1644	1/1	0.81	0.23	60,60,60,60	0
59	MG	AA	1682	1/1	0.81	0.28	53,53,53,53	0
59	MG	BA	3269	1/1	0.81	0.18	48,48,48,48	0
59	MG	BA	3270	1/1	0.81	0.37	70,70,70,70	0
59	MG	AA	1730	1/1	0.81	0.17	62,62,62,62	0
59	MG	AA	1669	1/1	0.81	0.20	40,40,40,40	0
59	MG	BA	3147	1/1	0.81	0.31	119,119,119,119	0
59	MG	AA	1786	1/1	0.81	0.10	35,35,35,35	0
59	MG	BA	3251	1/1	0.81	0.29	44,44,44,44	0
59	MG	BA	3064	1/1	0.81	0.27	62,62,62,62	0
59	MG	BA	3300	1/1	0.81	0.32	65,65,65,65	0
59	MG	AA	1771	1/1	0.81	0.20	40,40,40,40	0
59	MG	BA	3255	1/1	0.81	0.26	35,35,35,35	0
59	MG	BA	3218	1/1	0.81	0.14	58,58,58,58	0
59	MG	AA	1638	1/1	0.81	0.11	38,38,38,38	0
59	MG	AA	1636	1/1	0.82	0.44	60,60,60,60	0
59	MG	BA	3213	1/1	0.82	0.29	31,31,31,31	0
59	MG	AA	1755	1/1	0.82	0.17	60,60,60,60	0
59	MG	BA	3190	1/1	0.82	0.27	81,81,81,81	0
59	MG	AA	1717	1/1	0.82	0.33	41,41,41,41	0
59	MG	BA	3283	1/1	0.82	0.20	73,73,73,73	0
59	MG	AA	1656	1/1	0.82	0.13	46,46,46,46	0
59	MG	BA	3200	1/1	0.82	0.31	71,71,71,71	0
59	MG	AA	1728	1/1	0.82	0.17	47,47,47,47	0
59	MG	BA	3095	1/1	0.82	0.32	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3276	1/1	0.82	0.30	46,46,46,46	0
61	GCP	AY	701	32/32	0.82	0.15	41,53,61,63	0
59	MG	BA	3259	1/1	0.83	0.11	39,39,39,39	0
59	MG	BA	3019	1/1	0.83	0.36	77,77,77,77	0
59	MG	BA	3187	1/1	0.83	0.32	68,68,68,68	0
59	MG	BA	3105	1/1	0.83	0.21	69,69,69,69	0
59	MG	BA	3244	1/1	0.83	0.17	41,41,41,41	0
59	MG	BA	3299	1/1	0.83	0.26	53,53,53,53	0
59	MG	BA	3030	1/1	0.83	0.45	86,86,86,86	0
59	MG	BA	3107	1/1	0.83	0.25	44,44,44,44	0
59	MG	AA	1651	1/1	0.83	0.27	68,68,68,68	0
59	MG	BA	3073	1/1	0.83	0.29	83,83,83,83	0
59	MG	AA	1650	1/1	0.83	0.20	36,36,36,36	0
59	MG	AA	1685	1/1	0.83	0.31	40,40,40,40	0
59	MG	BA	3198	1/1	0.84	0.23	63,63,63,63	0
59	MG	AA	1727	1/1	0.84	0.20	55,55,55,55	0
59	MG	BA	3202	1/1	0.84	0.24	43,43,43,43	0
59	MG	AA	1634	1/1	0.84	0.21	43,43,43,43	0
59	MG	BA	3016	1/1	0.84	0.35	77,77,77,77	0
59	MG	AA	1628	1/1	0.84	0.40	64,64,64,64	0
59	MG	AA	1696	1/1	0.84	0.27	35,35,35,35	0
59	MG	AA	1622	1/1	0.84	0.26	49,49,49,49	0
59	MG	AA	1726	1/1	0.84	0.17	45,45,45,45	0
59	MG	AA	1784	1/1	0.84	0.11	37,37,37,37	0
59	MG	BA	3184	1/1	0.84	0.22	40,40,40,40	0
59	MG	BA	3029	1/1	0.84	0.40	73,73,73,73	0
59	MG	BA	3138	1/1	0.84	0.37	57,57,57,57	0
59	MG	BA	3087	1/1	0.84	0.30	41,41,41,41	0
59	MG	BA	3238	1/1	0.84	0.16	42,42,42,42	0
59	MG	BA	3267	1/1	0.84	0.29	62,62,62,62	0
59	MG	BA	3144	1/1	0.84	0.17	28,28,28,28	0
59	MG	AA	1745	1/1	0.85	0.42	66,66,66,66	0
59	MG	AA	1637	1/1	0.85	0.30	65,65,65,65	0
59	MG	BA	3233	1/1	0.85	0.20	42,42,42,42	0
59	MG	BA	3234	1/1	0.85	0.18	63,63,63,63	0
59	MG	BA	3116	1/1	0.85	0.38	78,78,78,78	0
59	MG	BA	3121	1/1	0.85	0.30	33,33,33,33	0
59	MG	BA	3271	1/1	0.85	0.14	28,28,28,28	0
59	MG	BA	3025	1/1	0.85	0.28	42,42,42,42	0
59	MG	AA	1673	1/1	0.85	0.13	35,35,35,35	0
59	MG	BA	3193	1/1	0.85	0.43	64,64,64,64	0
59	MG	BA	3072	1/1	0.85	0.50	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	B5	101	1/1	0.85	0.22	47,47,47,47	0
59	MG	AA	1624	1/1	0.85	0.52	61,61,61,61	0
59	MG	BA	3079	1/1	0.85	0.21	34,34,34,34	0
59	MG	BA	3085	1/1	0.85	0.20	25,25,25,25	0
59	MG	BA	3284	1/1	0.85	0.33	61,61,61,61	0
59	MG	AA	1764	1/1	0.85	0.30	61,61,61,61	0
59	MG	BA	3148	1/1	0.85	0.17	53,53,53,53	0
59	MG	AA	1668	1/1	0.85	0.18	34,34,34,34	0
59	MG	BA	3093	1/1	0.85	0.41	69,69,69,69	0
59	MG	BA	3036	1/1	0.85	0.26	47,47,47,47	0
59	MG	BA	3174	1/1	0.85	0.34	97,97,97,97	0
59	MG	AA	1792	1/1	0.85	0.09	37,37,37,37	0
59	MG	AA	1658	1/1	0.86	0.15	25,25,25,25	0
59	MG	BA	3146	1/1	0.86	0.21	29,29,29,29	0
59	MG	BA	3028	1/1	0.86	0.30	60,60,60,60	0
59	MG	AA	1672	1/1	0.86	0.10	42,42,42,42	0
59	MG	BA	3152	1/1	0.86	0.32	64,64,64,64	0
59	MG	BA	3274	1/1	0.86	0.13	79,79,79,79	0
59	MG	BA	3160	1/1	0.86	0.17	55,55,55,55	0
59	MG	AA	1621	1/1	0.86	0.39	68,68,68,68	0
59	MG	AA	1709	1/1	0.86	0.10	41,41,41,41	0
59	MG	BA	3126	1/1	0.86	0.40	55,55,55,55	0
59	MG	BA	3167	1/1	0.86	0.25	61,61,61,61	0
59	MG	AA	1647	1/1	0.86	0.29	79,79,79,79	0
59	MG	BA	3039	1/1	0.86	0.26	38,38,38,38	0
59	MG	AA	1699	1/1	0.86	0.15	33,33,33,33	0
59	MG	AA	1731	1/1	0.86	0.11	48,48,48,48	0
59	MG	BA	3295	1/1	0.86	0.11	32,32,32,32	0
59	MG	BA	3297	1/1	0.86	0.10	39,39,39,39	0
59	MG	BA	3219	1/1	0.86	0.13	44,44,44,44	0
59	MG	BA	3225	1/1	0.86	0.17	44,44,44,44	0
59	MG	BA	3137	1/1	0.86	0.15	49,49,49,49	0
59	MG	BA	3302	1/1	0.86	0.30	52,52,52,52	0
59	MG	BA	3227	1/1	0.86	0.21	27,27,27,27	0
59	MG	BA	3263	1/1	0.86	0.24	63,63,63,63	0
59	MG	AA	1702	1/1	0.86	0.32	44,44,44,44	0
59	MG	BA	3059	1/1	0.86	0.38	45,45,45,45	0
59	MG	BA	3139	1/1	0.87	0.22	35,35,35,35	0
59	MG	BA	3140	1/1	0.87	0.14	45,45,45,45	0
59	MG	BA	3046	1/1	0.87	0.25	27,27,27,27	0
59	MG	AA	1695	1/1	0.87	0.35	50,50,50,50	0
59	MG	AA	1671	1/1	0.87	0.38	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1741	1/1	0.87	0.17	58,58,58,58	0
59	MG	AA	1708	1/1	0.87	0.28	57,57,57,57	0
59	MG	BA	3071	1/1	0.87	0.22	22,22,22,22	0
59	MG	BA	3201	1/1	0.87	0.32	64,64,64,64	0
59	MG	AA	1661	1/1	0.87	0.20	40,40,40,40	0
59	MG	BA	3161	1/1	0.87	0.29	30,30,30,30	0
59	MG	BA	3205	1/1	0.87	0.14	35,35,35,35	0
59	MG	AA	1643	1/1	0.87	0.13	38,38,38,38	0
59	MG	BA	3128	1/1	0.87	0.13	38,38,38,38	0
59	MG	BA	3292	1/1	0.87	0.21	64,64,64,64	0
59	MG	BA	3294	1/1	0.87	0.19	42,42,42,42	0
59	MG	BA	3129	1/1	0.87	0.20	51,51,51,51	0
59	MG	BA	3296	1/1	0.87	0.20	38,38,38,38	0
59	MG	BA	3257	1/1	0.87	0.24	43,43,43,43	0
59	MG	AA	1766	1/1	0.87	0.36	58,58,58,58	0
59	MG	BA	3168	1/1	0.87	0.14	58,58,58,58	0
59	MG	AA	1713	1/1	0.87	0.07	40,40,40,40	0
59	MG	BA	3082	1/1	0.87	0.30	23,23,23,23	0
59	MG	BA	3177	1/1	0.87	0.28	31,31,31,31	0
59	MG	BA	3308	1/1	0.87	0.17	58,58,58,58	0
59	MG	BA	3312	1/1	0.87	0.17	44,44,44,44	0
59	MG	AA	1606	1/1	0.87	0.31	60,60,60,60	0
59	MG	AA	1646	1/1	0.87	0.17	34,34,34,34	0
59	MG	AA	1791	1/1	0.87	0.09	57,57,57,57	0
59	MG	BA	3018	1/1	0.88	0.31	43,43,43,43	0
59	MG	AA	1729	1/1	0.88	0.26	45,45,45,45	0
59	MG	AA	1711	1/1	0.88	0.15	34,34,34,34	0
59	MG	AA	1604	1/1	0.88	0.31	59,59,59,59	0
59	MG	BA	3246	1/1	0.88	0.25	34,34,34,34	0
59	MG	BA	3264	1/1	0.88	0.35	77,77,77,77	0
59	MG	AA	1782	1/1	0.88	0.09	39,39,39,39	0
59	MG	BA	3133	1/1	0.88	0.17	39,39,39,39	0
59	MG	BA	3084	1/1	0.88	0.36	38,38,38,38	0
59	MG	BA	3112	1/1	0.88	0.44	51,51,51,51	0
59	MG	AA	1615	1/1	0.88	0.43	51,51,51,51	0
59	MG	BA	3290	1/1	0.88	0.25	43,43,43,43	0
59	MG	AA	1722	1/1	0.88	0.19	32,32,32,32	0
59	MG	BA	3293	1/1	0.88	0.39	76,76,76,76	0
59	MG	BA	3022	1/1	0.89	0.41	65,65,65,65	0
59	MG	AA	1735	1/1	0.89	0.40	62,62,62,62	0
59	MG	BA	3047	1/1	0.89	0.24	42,42,42,42	0
59	MG	AA	1737	1/1	0.89	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3248	1/1	0.89	0.20	58,58,58,58	0
59	MG	BA	3207	1/1	0.89	0.21	30,30,30,30	0
59	MG	BA	3056	1/1	0.89	0.25	38,38,38,38	0
59	MG	AA	1678	1/1	0.89	0.18	29,29,29,29	0
59	MG	BA	3176	1/1	0.89	0.30	23,23,23,23	0
59	MG	BA	3097	1/1	0.89	0.27	37,37,37,37	0
59	MG	AA	1679	1/1	0.89	0.24	32,32,32,32	0
59	MG	BA	3061	1/1	0.89	0.07	37,37,37,37	0
59	MG	BA	3220	1/1	0.89	0.30	56,56,56,56	0
59	MG	AA	1609	1/1	0.89	0.32	40,40,40,40	0
59	MG	BA	3111	1/1	0.89	0.19	30,30,30,30	0
59	MG	AA	1659	1/1	0.89	0.22	34,34,34,34	0
59	MG	BA	3188	1/1	0.89	0.26	34,34,34,34	0
59	MG	BA	3113	1/1	0.89	0.35	32,32,32,32	0
59	MG	BA	3191	1/1	0.89	0.37	72,72,72,72	0
59	MG	BA	3303	1/1	0.89	0.10	42,42,42,42	0
59	MG	AA	1655	1/1	0.89	0.26	30,30,30,30	0
59	MG	AA	1642	1/1	0.89	0.32	61,61,61,61	0
59	MG	BA	3158	1/1	0.89	0.20	27,27,27,27	0
59	MG	AA	1690	1/1	0.89	0.24	35,35,35,35	0
59	MG	AA	1691	1/1	0.89	0.21	65,65,65,65	0
59	MG	AA	1718	1/1	0.89	0.33	35,35,35,35	0
59	MG	AA	1759	1/1	0.90	0.21	37,37,37,37	0
59	MG	BA	3102	1/1	0.90	0.15	30,30,30,30	0
59	MG	BA	3068	1/1	0.90	0.15	33,33,33,33	0
59	MG	AA	1774	1/1	0.90	0.28	51,51,51,51	0
59	MG	AA	1663	1/1	0.90	0.28	37,37,37,37	0
59	MG	AA	1776	1/1	0.90	0.21	25,25,25,25	0
59	MG	BA	3217	1/1	0.90	0.12	35,35,35,35	0
59	MG	BA	3289	1/1	0.90	0.22	51,51,51,51	0
59	MG	AA	1777	1/1	0.90	0.13	40,40,40,40	0
59	MG	BA	3291	1/1	0.90	0.21	27,27,27,27	0
59	MG	BA	3077	1/1	0.90	0.21	31,31,31,31	0
59	MG	BA	3186	1/1	0.90	0.10	50,50,50,50	0
59	MG	BA	3222	1/1	0.90	0.24	44,44,44,44	0
59	MG	AA	1683	1/1	0.90	0.17	25,25,25,25	0
59	MG	BA	3118	1/1	0.90	0.26	29,29,29,29	0
59	MG	BA	3151	1/1	0.90	0.08	33,33,33,33	0
59	MG	BA	3228	1/1	0.90	0.21	23,23,23,23	0
59	MG	AA	1710	1/1	0.90	0.08	35,35,35,35	0
59	MG	BA	3122	1/1	0.90	0.09	26,26,26,26	0
59	MG	AA	1798	1/1	0.90	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1608	1/1	0.90	0.23	48,48,48,48	0
59	MG	BA	3058	1/1	0.90	0.22	31,31,31,31	0
59	MG	BA	3305	1/1	0.90	0.20	52,52,52,52	0
59	MG	BA	3088	1/1	0.90	0.17	27,27,27,27	0
59	MG	AA	1623	1/1	0.90	0.32	33,33,33,33	0
59	MG	AA	1630	1/1	0.90	0.35	56,56,56,56	0
59	MG	AA	1725	1/1	0.90	0.16	35,35,35,35	0
59	MG	BA	3172	1/1	0.90	0.29	31,31,31,31	0
59	MG	BA	3051	1/1	0.91	0.27	31,31,31,31	0
59	MG	AA	1763	1/1	0.91	0.22	51,51,51,51	0
59	MG	BA	3098	1/1	0.91	0.17	25,25,25,25	0
59	MG	AA	1719	1/1	0.91	0.11	32,32,32,32	0
59	MG	BA	3277	1/1	0.91	0.35	57,57,57,57	0
59	MG	AA	1765	1/1	0.91	0.46	63,63,63,63	0
59	MG	AA	1748	1/1	0.91	0.33	56,56,56,56	0
59	MG	AA	1750	1/1	0.91	0.19	42,42,42,42	0
59	MG	BA	3108	1/1	0.91	0.15	34,34,34,34	0
59	MG	AA	1770	1/1	0.91	0.27	41,41,41,41	0
59	MG	AA	1732	1/1	0.91	0.12	20,20,20,20	0
59	MG	AA	1618	1/1	0.91	0.25	47,47,47,47	0
59	MG	AA	1692	1/1	0.91	0.28	48,48,48,48	0
59	MG	BA	3203	1/1	0.91	0.18	30,30,30,30	0
59	MG	AA	1796	1/1	0.91	0.19	44,44,44,44	0
59	MG	AA	1693	1/1	0.91	0.19	30,30,30,30	0
59	MG	AA	1714	1/1	0.91	0.29	44,44,44,44	0
59	MG	BA	3034	1/1	0.91	0.16	36,36,36,36	0
59	MG	BA	3211	1/1	0.91	0.40	58,58,58,58	0
59	MG	AA	1757	1/1	0.91	0.24	57,57,57,57	0
59	MG	BA	3169	1/1	0.91	0.32	43,43,43,43	0
59	MG	BA	3170	1/1	0.91	0.35	41,41,41,41	0
59	MG	AA	1657	1/1	0.91	0.07	32,32,32,32	0
59	MG	AA	1633	1/1	0.91	0.29	52,52,52,52	0
59	MG	BA	3131	1/1	0.91	0.29	33,33,33,33	0
59	MG	AA	1667	1/1	0.91	0.17	33,33,33,33	0
59	MG	BA	3042	1/1	0.91	0.32	45,45,45,45	0
59	MG	BA	3221	1/1	0.91	0.09	43,43,43,43	0
59	MG	BA	3013	1/1	0.91	0.29	37,37,37,37	0
59	MG	BA	3224	1/1	0.91	0.32	32,32,32,32	0
59	MG	BA	3313	1/1	0.91	0.20	36,36,36,36	0
59	MG	BA	3314	1/1	0.91	0.10	49,49,49,49	0
59	MG	AA	1605	1/1	0.91	0.32	40,40,40,40	0
59	MG	BA	3092	1/1	0.91	0.32	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3048	1/1	0.91	0.29	28,28,28,28	0
59	MG	AA	1701	1/1	0.92	0.10	30,30,30,30	0
59	MG	BA	3049	1/1	0.92	0.32	47,47,47,47	0
59	MG	AA	1670	1/1	0.92	0.17	57,57,57,57	0
59	MG	BA	3052	1/1	0.92	0.21	32,32,32,32	0
59	MG	BA	3135	1/1	0.92	0.24	58,58,58,58	0
59	MG	BA	3053	1/1	0.92	0.18	24,24,24,24	0
59	MG	BA	3054	1/1	0.92	0.25	31,31,31,31	0
59	MG	BA	3080	1/1	0.92	0.24	38,38,38,38	0
59	MG	BA	3243	1/1	0.92	0.14	32,32,32,32	0
59	MG	BA	3208	1/1	0.92	0.16	34,34,34,34	0
59	MG	BA	3245	1/1	0.92	0.16	25,25,25,25	0
59	MG	BA	3209	1/1	0.92	0.54	81,81,81,81	0
59	MG	AA	1653	1/1	0.92	0.17	19,19,19,19	0
59	MG	BA	3083	1/1	0.92	0.23	23,23,23,23	0
59	MG	BA	3038	1/1	0.92	0.23	40,40,40,40	0
59	MG	BA	3214	1/1	0.92	0.13	39,39,39,39	0
59	MG	BA	3143	1/1	0.92	0.31	57,57,57,57	0
59	MG	BA	3057	1/1	0.92	0.15	29,29,29,29	0
59	MG	BA	3117	1/1	0.92	0.16	26,26,26,26	0
59	MG	AA	1654	1/1	0.92	0.20	24,24,24,24	0
59	MG	BA	3120	1/1	0.92	0.29	43,43,43,43	0
59	MG	BA	3149	1/1	0.92	0.29	29,29,29,29	0
59	MG	BA	3014	1/1	0.92	0.36	53,53,53,53	0
59	MG	BA	3262	1/1	0.92	0.10	68,68,68,68	0
59	MG	BA	3015	1/1	0.92	0.41	63,63,63,63	0
59	MG	AA	1617	1/1	0.92	0.32	49,49,49,49	0
59	MG	AA	1680	1/1	0.92	0.20	37,37,37,37	0
59	MG	BA	3094	1/1	0.92	0.24	25,25,25,25	0
59	MG	BA	3309	1/1	0.92	0.18	50,50,50,50	0
59	MG	BA	3310	1/1	0.92	0.07	20,20,20,20	0
59	MG	BA	3195	1/1	0.92	0.18	32,32,32,32	0
59	MG	BA	3196	1/1	0.92	0.34	53,53,53,53	0
59	MG	BA	3162	1/1	0.92	0.32	45,45,45,45	0
59	MG	BA	3232	1/1	0.92	0.16	33,33,33,33	0
59	MG	AA	1665	1/1	0.92	0.25	28,28,28,28	0
60	ZN	AD	301	1/1	0.92	0.28	54,54,54,54	0
59	MG	BA	3273	1/1	0.92	0.56	72,72,72,72	0
59	MG	BA	3155	1/1	0.93	0.35	60,60,60,60	0
59	MG	BA	3066	1/1	0.93	0.14	27,27,27,27	0
59	MG	BA	3159	1/1	0.93	0.15	36,36,36,36	0
59	MG	BA	3250	1/1	0.93	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3067	1/1	0.93	0.28	71,71,71,71	0
59	MG	BA	3086	1/1	0.93	0.22	46,46,46,46	0
59	MG	BA	3192	1/1	0.93	0.18	51,51,51,51	0
59	MG	BA	3254	1/1	0.93	0.15	18,18,18,18	0
59	MG	AA	1795	1/1	0.93	0.07	46,46,46,46	0
59	MG	BA	3256	1/1	0.93	0.33	52,52,52,52	0
59	MG	BA	3069	1/1	0.93	0.20	18,18,18,18	0
59	MG	BA	3089	1/1	0.93	0.14	18,18,18,18	0
59	MG	AA	1751	1/1	0.93	0.09	46,46,46,46	0
59	MG	AA	1687	1/1	0.93	0.17	30,30,30,30	0
59	MG	AA	1603	1/1	0.93	0.28	38,38,38,38	0
59	MG	BA	3298	1/1	0.93	0.11	20,20,20,20	0
59	MG	AY	702	1/1	0.93	0.13	23,23,23,23	0
59	MG	AA	1749	1/1	0.93	0.08	38,38,38,38	0
59	MG	BA	3096	1/1	0.93	0.12	23,23,23,23	0
59	MG	BA	3145	1/1	0.93	0.17	32,32,32,32	0
59	MG	BA	3123	1/1	0.93	0.28	32,32,32,32	0
59	MG	BA	3235	1/1	0.93	0.19	29,29,29,29	0
59	MG	AA	1662	1/1	0.93	0.21	34,34,34,34	0
59	MG	BA	3001	1/1	0.93	0.09	35,35,35,35	0
59	MG	BA	3178	1/1	0.93	0.21	43,43,43,43	0
59	MG	BA	3101	1/1	0.93	0.27	29,29,29,29	0
59	MG	BA	3311	1/1	0.93	0.11	22,22,22,22	0
59	MG	BA	3272	1/1	0.93	0.40	52,52,52,52	0
59	MG	BA	3181	1/1	0.93	0.13	32,32,32,32	0
59	MG	BA	3210	1/1	0.93	0.23	23,23,23,23	0
59	MG	BA	3006	1/1	0.93	0.23	30,30,30,30	0
59	MG	BA	3319	1/1	0.93	0.09	35,35,35,35	0
59	MG	AA	1787	1/1	0.93	0.25	55,55,55,55	0
59	MG	BA	3153	1/1	0.93	0.18	54,54,54,54	0
59	MG	BA	3185	1/1	0.93	0.33	36,36,36,36	0
59	MG	BA	3285	1/1	0.94	0.23	40,40,40,40	0
59	MG	AA	1625	1/1	0.94	0.26	17,17,17,17	0
59	MG	AA	1746	1/1	0.94	0.27	47,47,47,47	0
59	MG	BA	3031	1/1	0.94	0.23	35,35,35,35	0
59	MG	BA	3099	1/1	0.94	0.13	19,19,19,19	0
59	MG	BA	3078	1/1	0.94	0.14	26,26,26,26	0
59	MG	AA	1619	1/1	0.94	0.27	37,37,37,37	0
59	MG	BA	3104	1/1	0.94	0.18	30,30,30,30	0
59	MG	AA	1698	1/1	0.94	0.32	58,58,58,58	0
59	MG	AA	1631	1/1	0.94	0.19	40,40,40,40	0
59	MG	BA	3037	1/1	0.94	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3017	1/1	0.94	0.23	37,37,37,37	0
59	MG	BA	3110	1/1	0.94	0.28	31,31,31,31	0
59	MG	AA	1723	1/1	0.94	0.10	10,10,10,10	0
59	MG	AA	1736	1/1	0.94	0.08	29,29,29,29	0
59	MG	AA	1700	1/1	0.94	0.22	27,27,27,27	0
59	MG	BA	3114	1/1	0.94	0.11	29,29,29,29	0
59	MG	BA	3115	1/1	0.94	0.34	52,52,52,52	0
59	MG	BA	3306	1/1	0.94	0.10	39,39,39,39	0
59	MG	BA	3065	1/1	0.94	0.15	21,21,21,21	0
59	MG	AA	1645	1/1	0.94	0.24	22,22,22,22	0
59	MG	AA	1664	1/1	0.94	0.24	29,29,29,29	0
59	MG	BA	3119	1/1	0.94	0.15	24,24,24,24	0
59	MG	AA	1610	1/1	0.94	0.45	46,46,46,46	0
59	MG	AA	1686	1/1	0.94	0.19	34,34,34,34	0
59	MG	AA	1706	1/1	0.94	0.16	43,43,43,43	0
59	MG	BA	3011	1/1	0.94	0.29	46,46,46,46	0
59	MG	BA	3316	1/1	0.94	0.25	34,34,34,34	0
59	MG	BA	3154	1/1	0.94	0.35	59,59,59,59	0
59	MG	BA	3124	1/1	0.94	0.17	15,15,15,15	0
59	MG	BA	3157	1/1	0.94	0.10	17,17,17,17	0
59	MG	BA	3125	1/1	0.94	0.27	122,122,122,122	0
59	MG	BA	3127	1/1	0.95	0.12	38,38,38,38	0
59	MG	AA	1742	1/1	0.95	0.24	45,45,45,45	0
59	MG	AA	1648	1/1	0.95	0.26	29,29,29,29	0
59	MG	AA	1734	1/1	0.95	0.11	41,41,41,41	0
59	MG	AA	1768	1/1	0.95	0.36	34,34,34,34	0
59	MG	AA	1688	1/1	0.95	0.16	30,30,30,30	0
59	MG	AA	1675	1/1	0.95	0.20	45,45,45,45	0
59	MG	AA	1747	1/1	0.95	0.07	23,23,23,23	0
59	MG	BA	3005	1/1	0.95	0.25	16,16,16,16	0
59	MG	BA	3189	1/1	0.95	0.11	26,26,26,26	0
59	MG	BA	3024	1/1	0.95	0.27	44,44,44,44	0
59	MG	AA	1649	1/1	0.95	0.24	23,23,23,23	0
59	MG	BA	3008	1/1	0.95	0.33	45,45,45,45	0
59	MG	AA	1616	1/1	0.95	0.22	30,30,30,30	0
59	MG	BA	3050	1/1	0.95	0.08	23,23,23,23	0
59	MG	BA	3141	1/1	0.95	0.17	29,29,29,29	0
59	MG	BA	3010	1/1	0.95	0.30	33,33,33,33	0
59	MG	BA	3074	1/1	0.95	0.21	3,3,3,3	0
59	MG	AA	1761	1/1	0.95	0.04	30,30,30,30	0
59	MG	AA	1739	1/1	0.95	0.26	28,28,28,28	0
59	MG	BA	3173	1/1	0.95	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1614	1/1	0.95	0.22	26,26,26,26	0
59	MG	AA	1612	1/1	0.95	0.36	47,47,47,47	0
59	MG	BA	3287	1/1	0.95	0.14	41,41,41,41	0
59	MG	BA	3317	1/1	0.95	0.21	29,29,29,29	0
59	MG	BA	3288	1/1	0.95	0.13	24,24,24,24	0
59	MG	BA	3103	1/1	0.95	0.16	35,35,35,35	0
59	MG	BU	201	1/1	0.95	0.10	28,28,28,28	0
59	MG	BA	3033	1/1	0.95	0.16	41,41,41,41	0
59	MG	BA	3150	1/1	0.95	0.07	15,15,15,15	0
59	MG	BA	3286	1/1	0.96	0.26	42,42,42,42	0
59	MG	AA	1721	1/1	0.96	0.05	17,17,17,17	0
59	MG	BA	3063	1/1	0.96	0.10	22,22,22,22	0
59	MG	BA	3100	1/1	0.96	0.08	24,24,24,24	0
59	MG	BA	3043	1/1	0.96	0.13	28,28,28,28	0
59	MG	BA	3076	1/1	0.96	0.17	18,18,18,18	0
59	MG	BA	3171	1/1	0.96	0.14	19,19,19,19	0
59	MG	BA	3045	1/1	0.96	0.37	54,54,54,54	0
59	MG	AA	1681	1/1	0.96	0.24	34,34,34,34	0
59	MG	BA	3223	1/1	0.96	0.24	32,32,32,32	0
59	MG	BA	3007	1/1	0.96	0.24	26,26,26,26	0
59	MG	AA	1769	1/1	0.96	0.26	33,33,33,33	0
59	MG	BA	3081	1/1	0.96	0.18	23,23,23,23	0
59	MG	AA	1794	1/1	0.96	0.29	53,53,53,53	0
59	MG	BA	3320	1/1	0.96	0.14	39,39,39,39	0
59	MG	BA	3002	1/1	0.96	0.14	39,39,39,39	0
59	MG	BA	3004	1/1	0.96	0.26	24,24,24,24	0
59	MG	BA	3180	1/1	0.96	0.28	47,47,47,47	0
59	MG	BA	3165	1/1	0.96	0.26	29,29,29,29	0
59	MG	AA	1783	1/1	0.97	0.07	43,43,43,43	0
59	MG	BA	3021	1/1	0.97	0.22	37,37,37,37	0
59	MG	AA	1778	1/1	0.97	0.07	6,6,6,6	0
59	MG	AA	1785	1/1	0.97	0.05	47,47,47,47	0
59	MG	AA	1629	1/1	0.97	0.25	44,44,44,44	0
59	MG	BA	3044	1/1	0.97	0.27	21,21,21,21	0
59	MG	BA	3156	1/1	0.97	0.06	25,25,25,25	0
59	MG	BA	3318	1/1	0.97	0.07	46,46,46,46	0
59	MG	AA	1694	1/1	0.97	0.09	19,19,19,19	0
59	MG	AA	1720	1/1	0.97	0.27	37,37,37,37	0
59	MG	BA	3307	1/1	0.97	0.12	40,40,40,40	0
59	MG	AA	1705	1/1	0.97	0.04	23,23,23,23	0
59	MG	BA	3003	1/1	0.97	0.22	20,20,20,20	0
59	MG	BA	3070	1/1	0.97	0.27	25,25,25,25	0

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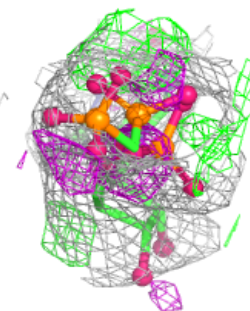
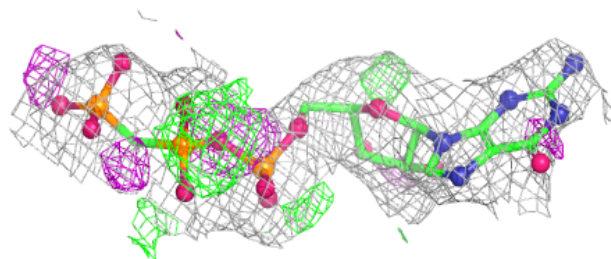
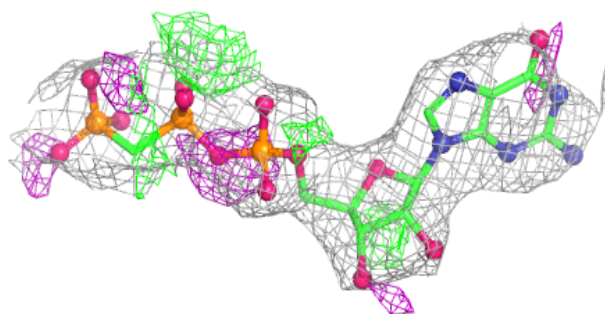
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1641	1/1	0.98	0.04	17,17,17,17	0
59	MG	BA	3109	1/1	0.98	0.22	20,20,20,20	0
59	MG	BA	3091	1/1	0.98	0.09	21,21,21,21	0
59	MG	AA	1660	1/1	0.98	0.07	19,19,19,19	0
59	MG	BA	3062	1/1	0.98	0.11	13,13,13,13	0
59	MG	AA	1602	1/1	0.98	0.27	42,42,42,42	0
59	MG	BA	3231	1/1	0.98	0.19	13,13,13,13	0
59	MG	BA	3035	1/1	0.98	0.32	31,31,31,31	0
59	MG	BA	3199	1/1	0.98	0.16	26,26,26,26	0
59	MG	BA	3249	1/1	0.99	0.17	22,22,22,22	0
59	MG	BA	3229	1/1	0.99	0.03	5,5,5,5	0
60	ZN	B9	101	1/1	1.00	0.02	49,49,49,49	0
60	ZN	AN	101	1/1	1.00	0.03	45,45,45,45	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 AY 701:

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.