



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:05 PM UTC

PDB ID : 4V85 / pdb_00004v85
Title : Crystal Structure of Release Factor RF3 Trapped in the GTP State on a Rotated Conformation of the Ribosome.
Authors : Zhou, J.; Lancaster, L.; Trakhanov, S.; Noller, H.F.
Deposited on : 2011-06-13
Resolution : 3.20 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

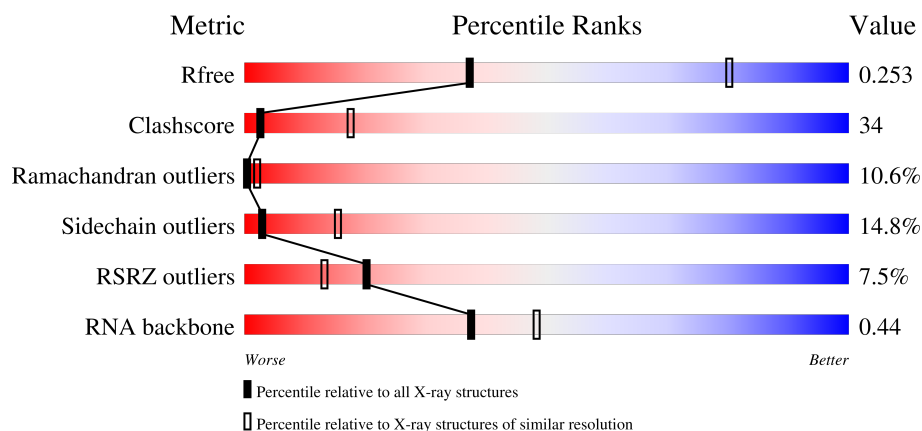
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1533	4% 28% 56% 16%
2	AB	241	10% 24% 47% 17% 10%
3	AC	233	6% 29% 44% 14% 12%
4	AD	206	17% 25% 58% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	AE	167	
6	AF	131	
7	AG	156	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	27	
23	AW	529	
24	AY	6	
25	B0	85	
26	B1	78	
27	B2	63	
28	B3	59	
29	B4	57	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	B5	55	
31	B6	46	
32	B7	65	
33	B8	38	
34	BA	2903	
35	BB	118	
36	BC	273	
37	BD	209	
38	BE	201	
39	BF	179	
40	BG	177	
41	BH	165	
42	BI	142	
43	BJ	121	
43	BK	121	
43	BL	121	
43	BM	121	
44	BN	142	
45	BO	123	
46	BP	144	
47	BQ	136	
48	BR	127	
49	BS	117	
50	BT	115	
51	BU	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	BV	103	
53	BW	116	
54	BX	100	
55	BY	104	
56	BZ	94	

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
24	KBE	AY	1	-	-	X	-
24	UAL	AY	5	-	-	X	-
24	5OH	AY	6	-	-	X	-
57	MG	BA	3349	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 147221 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	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- 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
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- 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
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- 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
			1022	634	206	179	3			

- 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
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 15 is a protein called 30S ribosomal protein S15 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AY	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	50	Total	C	N	O	S	0	0	0
			409	263	75	71				

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 33 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	2853	Total	C	N	O	P	0	0	0
			61252	27324	11274	19801	2853			

- Molecule 35 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 38 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 39 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 41 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	163	Total	C	N	O	S	0	0	0
			1230	775	219	229	7			

- Molecule 42 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 43 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BK	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BL	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BM	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 44 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BN	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 45 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BO	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 46 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BP	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BP	77	ILE	VAL	SEE REMARK 999	UNP C3SR37

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BQ	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 48 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BR	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 49 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BS	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

- Molecule 50 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 51 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BU	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 52 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BV	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 53 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BW	110	Total	C	N	O	S	0	0	0
			856	532	166	155	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	111	HIS	-	expression tag	UNP C3SQW7
BW	112	HIS	-	expression tag	UNP C3SQW7
BW	113	HIS	-	expression tag	UNP C3SQW7
BW	114	HIS	-	expression tag	UNP C3SQW7
BW	115	HIS	-	expression tag	UNP C3SQW7
BW	116	HIS	-	expression tag	UNP C3SQW7

- Molecule 54 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BX	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 55 is a protein called 50S ribosomal protein L24 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BY	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 56 is a protein called 50S ribosomal protein L25 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BZ	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

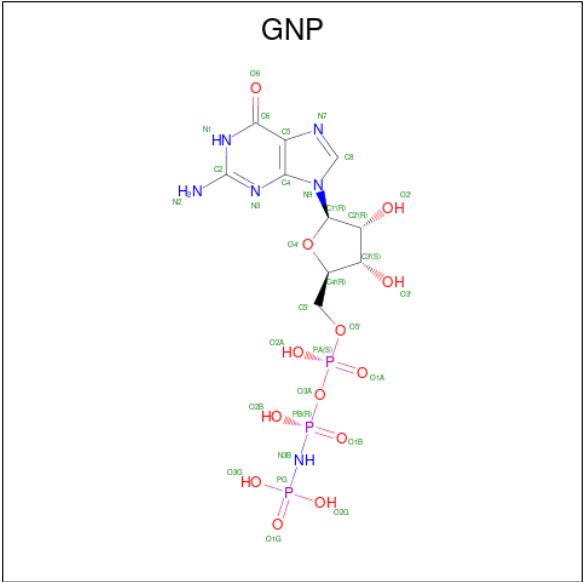
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	102	Total	Mg	0	0
			102	102		
57	AF	1	Total	Mg	0	0
			1	1		
57	AH	1	Total	Mg	0	0
			1	1		
57	AL	2	Total	Mg	0	0
			2	2		
57	AM	1	Total	Mg	0	0
			1	1		
57	AW	1	Total	Mg	0	0
			1	1		
57	B0	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B2	1	Total 1	Mg 1	0	0
57	B4	1	Total 1	Mg 1	0	0
57	BA	357	Total 357	Mg 357	0	0
57	BB	9	Total 9	Mg 9	0	0
57	BC	1	Total 1	Mg 1	0	0
57	BD	5	Total 5	Mg 5	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BQ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	BT	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AW	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

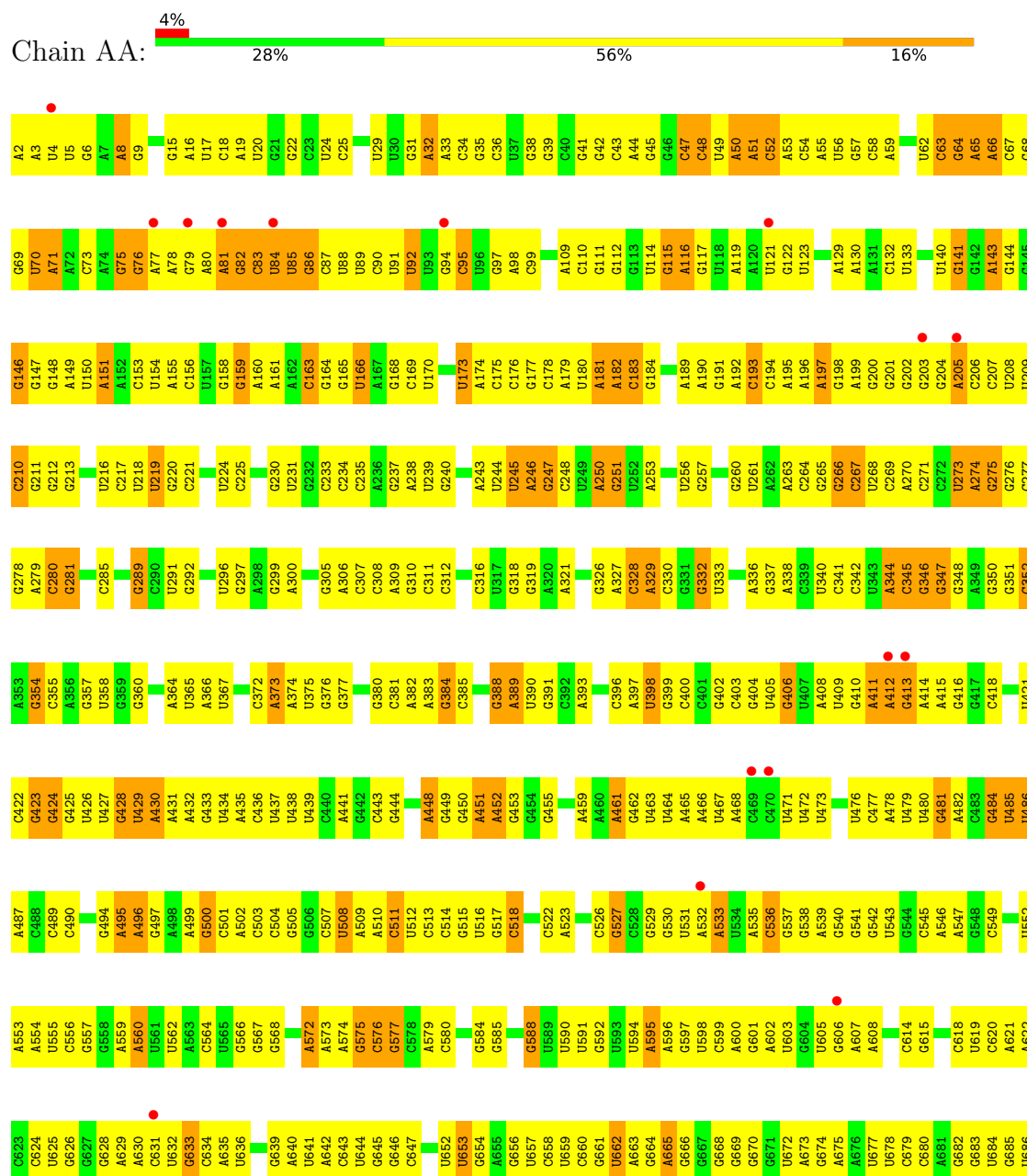
- Molecule 59 is water.

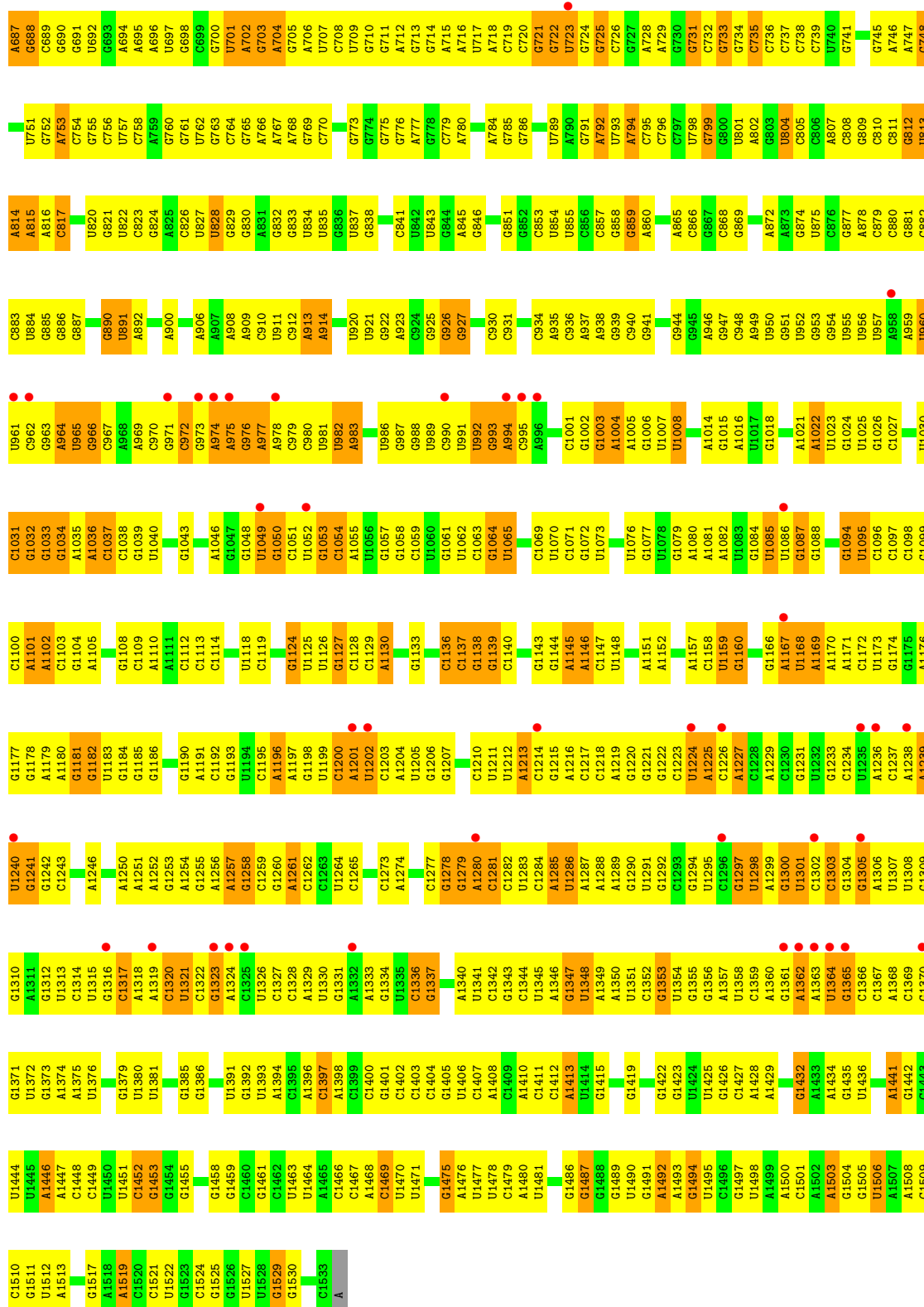
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AW	2	Total	O	0	0
			2	2		
59	B8	1	Total	O	0	0
			1	1		
59	BA	8	Total	O	0	0
			8	8		
59	BC	2	Total	O	0	0
			2	2		
59	BD	1	Total	O	0	0
			1	1		
59	BF	1	Total	O	0	0
			1	1		
59	BG	1	Total	O	0	0
			1	1		
59	BW	1	Total	O	0	0
			1	1		

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.

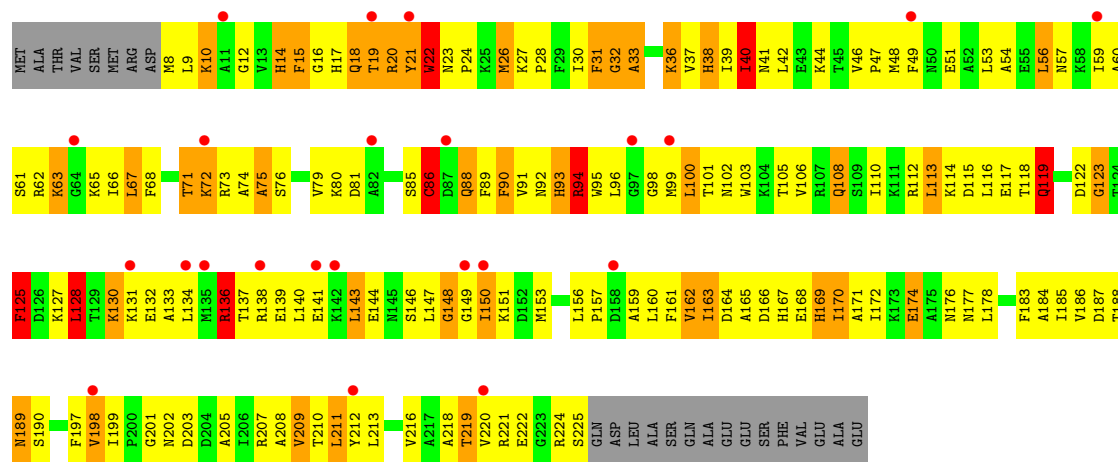
• Molecule 1: 16S rRNA



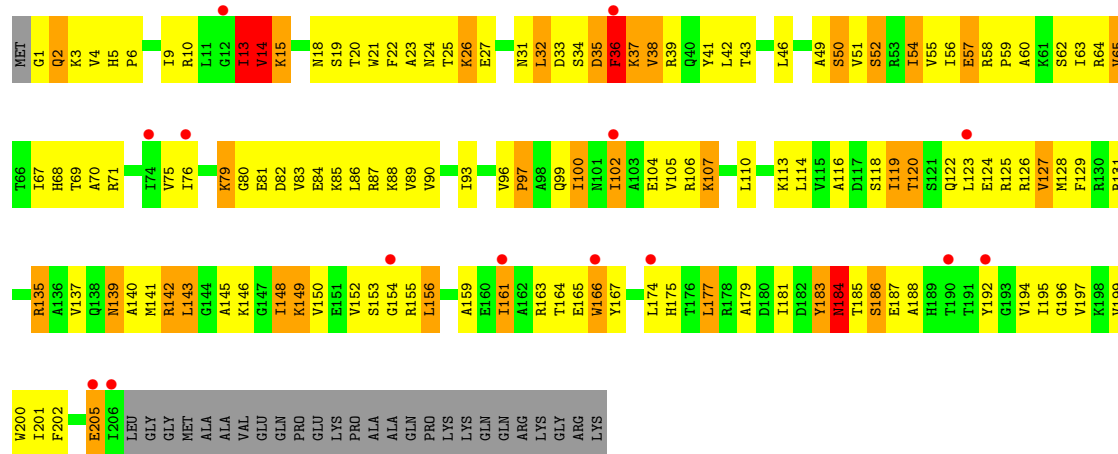


• Molecule 2: 30S ribosomal protein S2

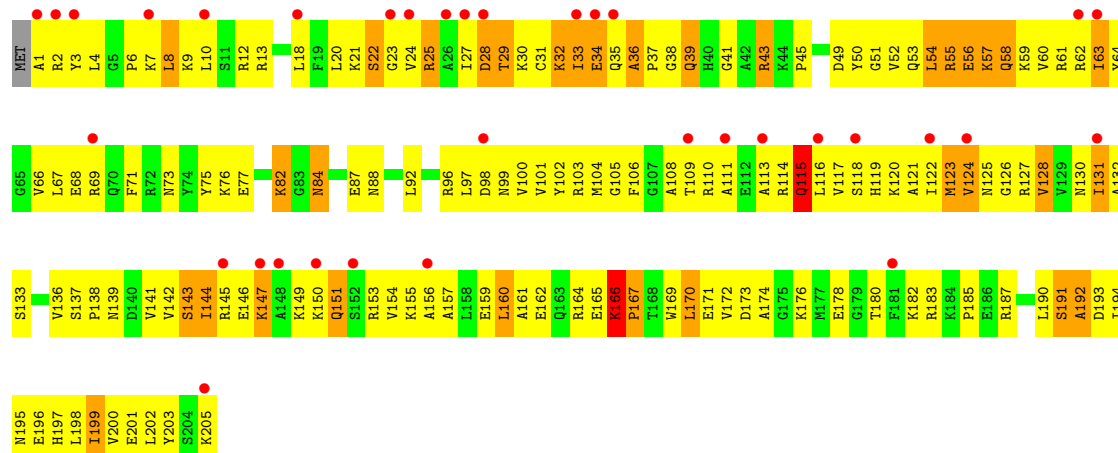




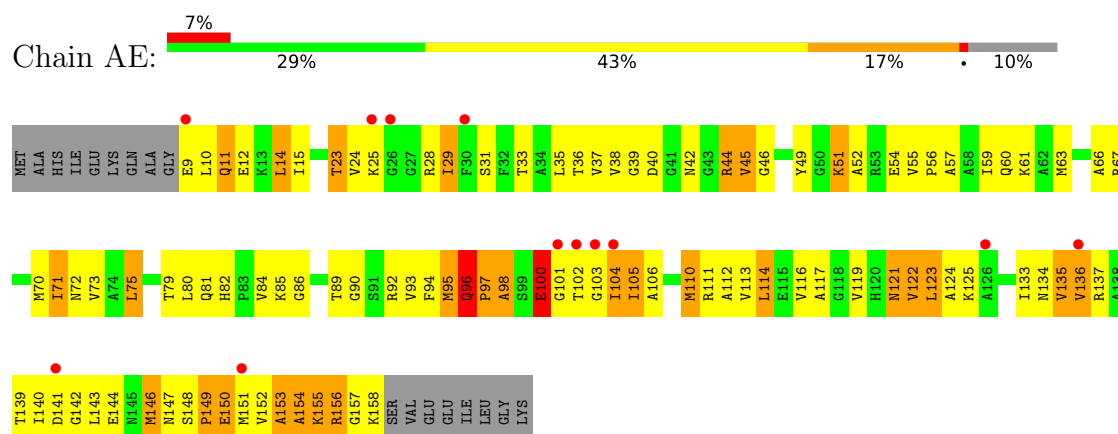
• Molecule 3: 30S ribosomal protein S3



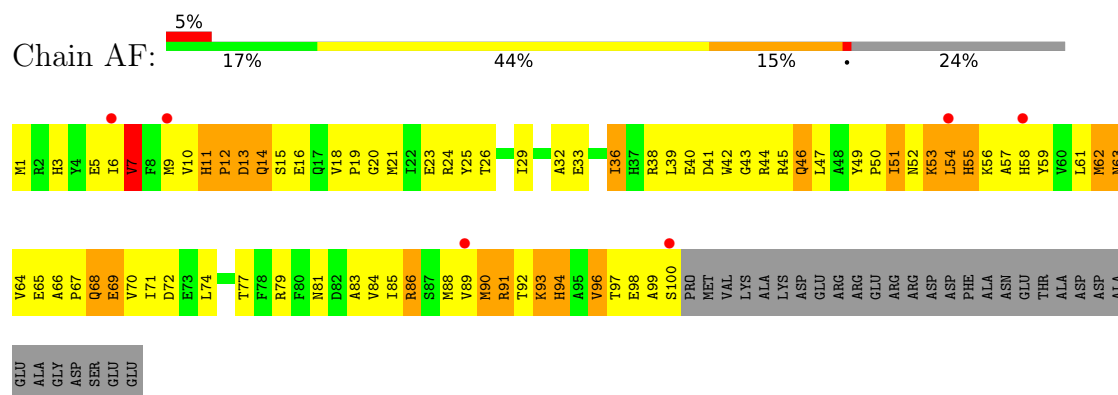
• Molecule 4: 30S ribosomal protein S4



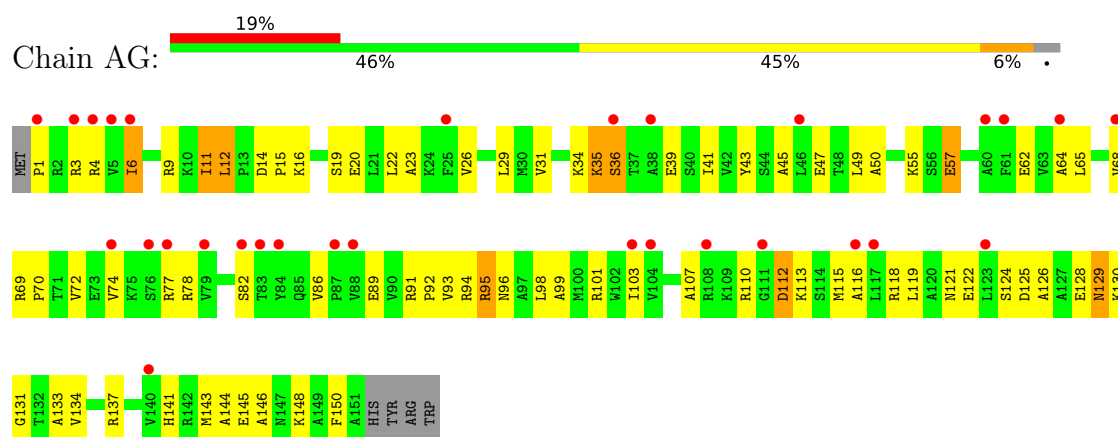
- Molecule 5: 30S ribosomal protein S5



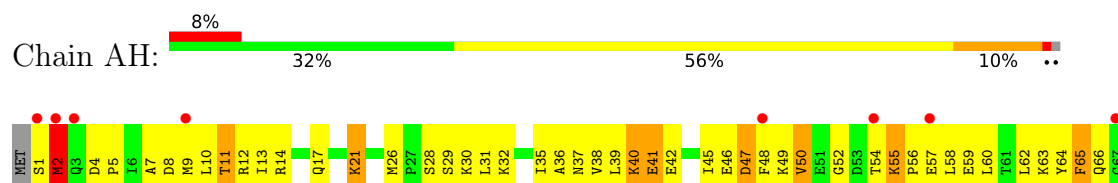
- Molecule 6: 30S ribosomal protein S6 1

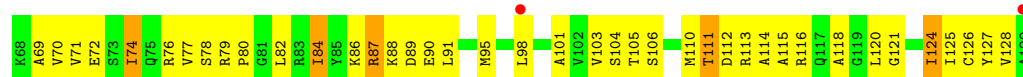


- Molecule 7: 30S ribosomal protein S7

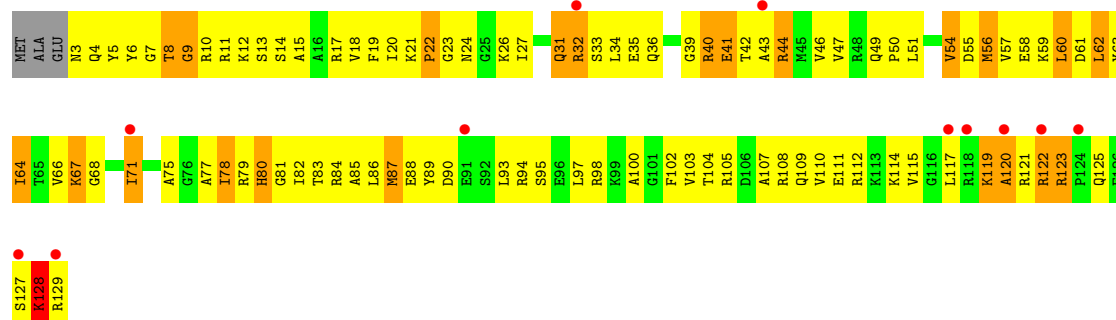


- Molecule 8: 30S ribosomal protein S8

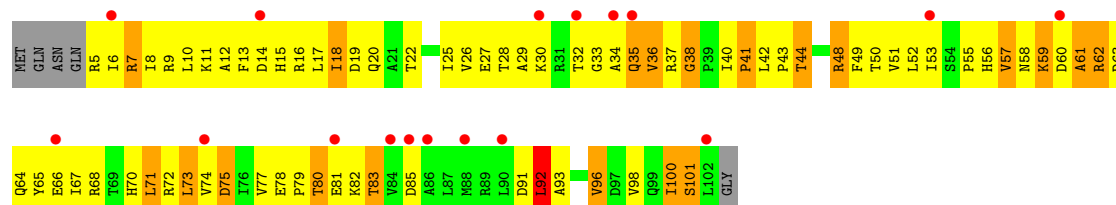




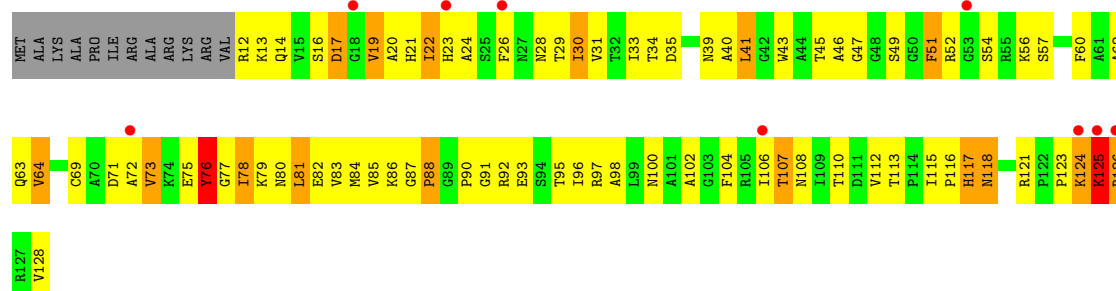
• Molecule 9: 30S ribosomal protein S9



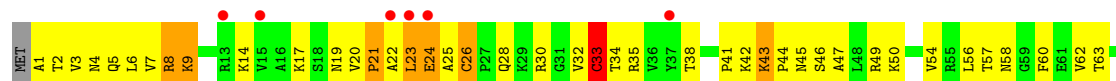
• Molecule 10: 30S ribosomal protein S10

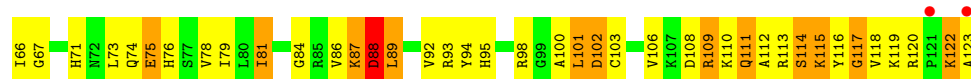


• Molecule 11: 30S ribosomal protein S11

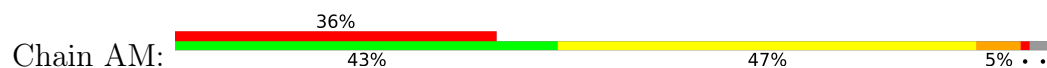


• Molecule 12: 30S ribosomal protein S12 1

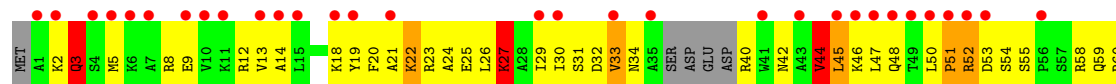




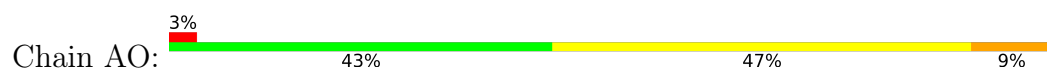
• Molecule 13: 30S ribosomal protein S13



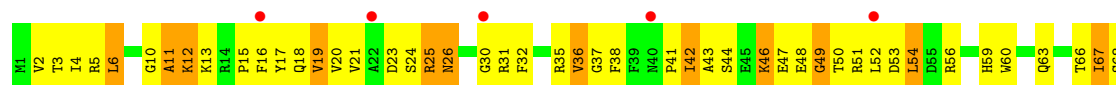
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15 1

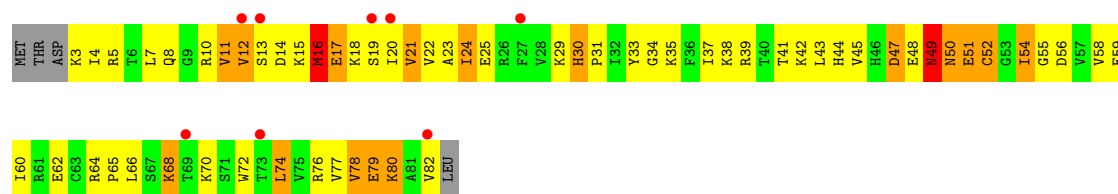


• Molecule 16: 30S ribosomal protein S16

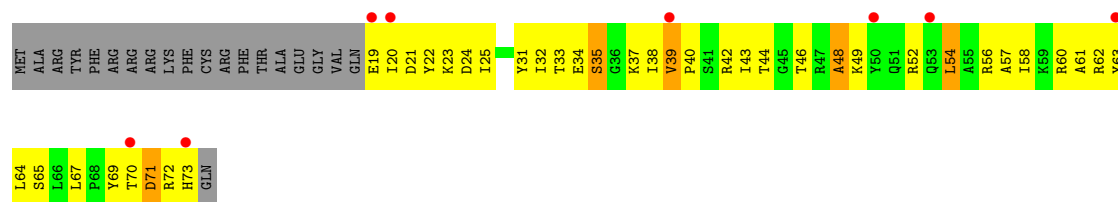
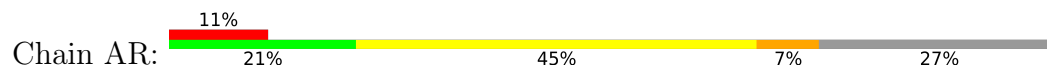


• Molecule 17: 30S ribosomal protein S17

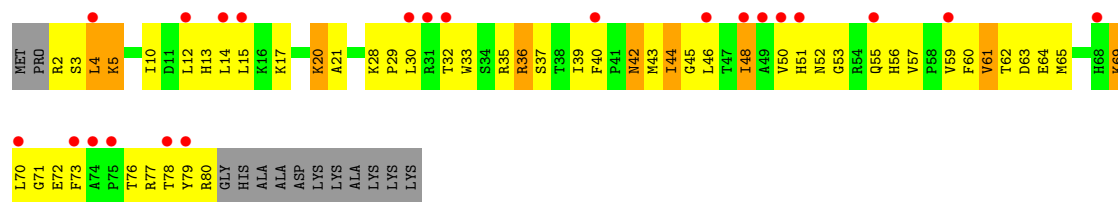
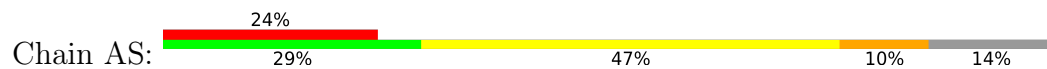




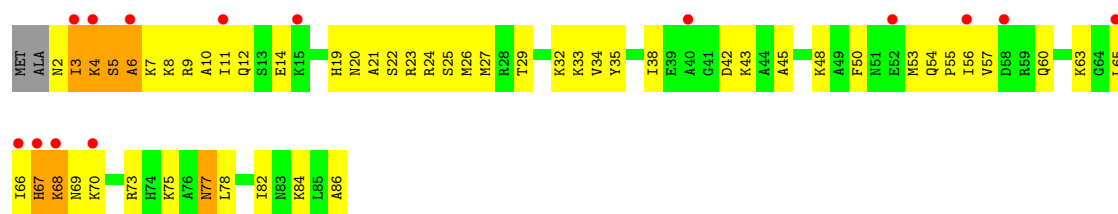
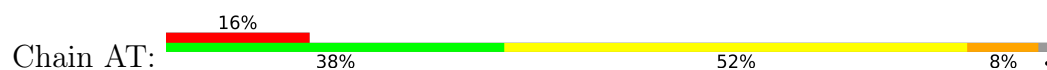
• Molecule 18: 30S ribosomal protein S18



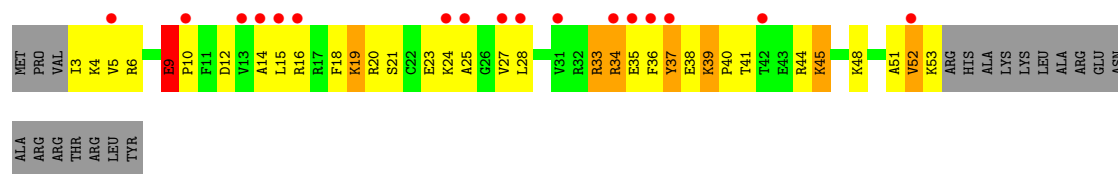
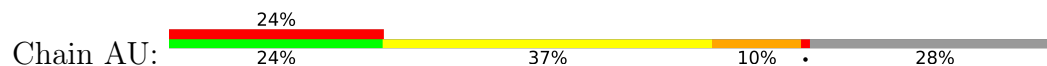
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



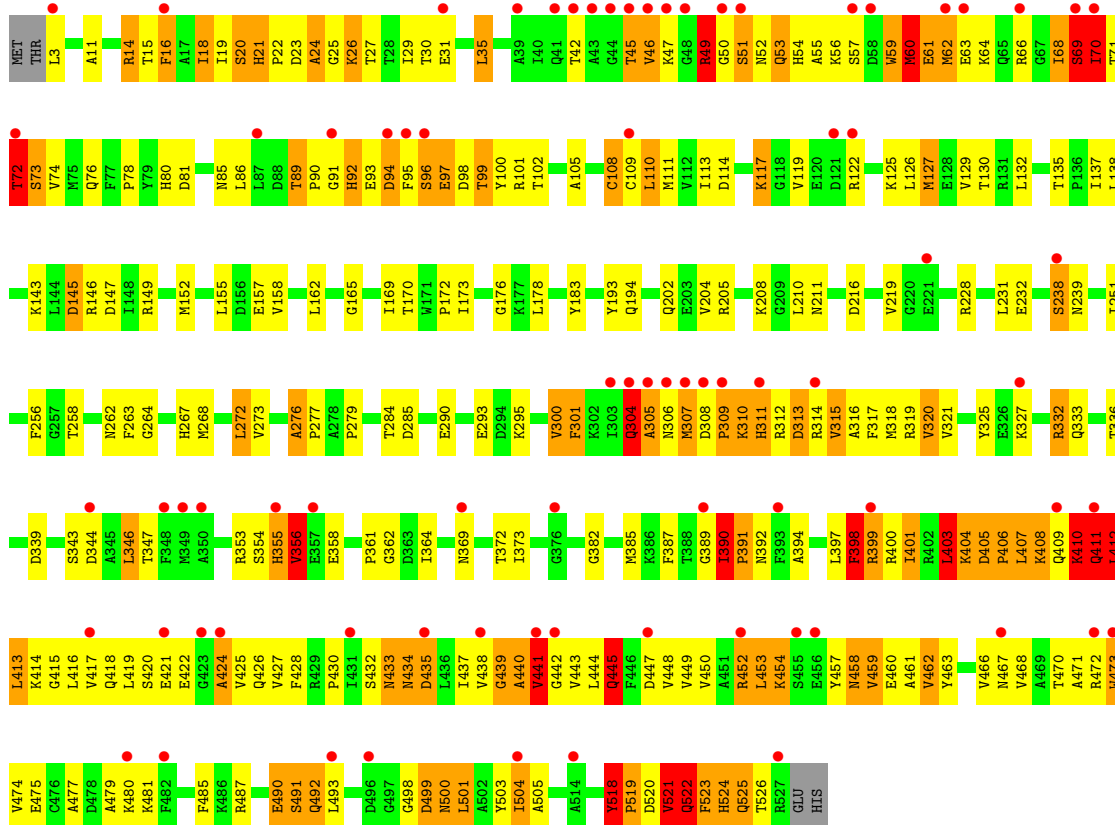
• Molecule 21: 30S ribosomal protein S21



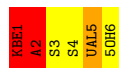
• Molecule 22: messenger RNA



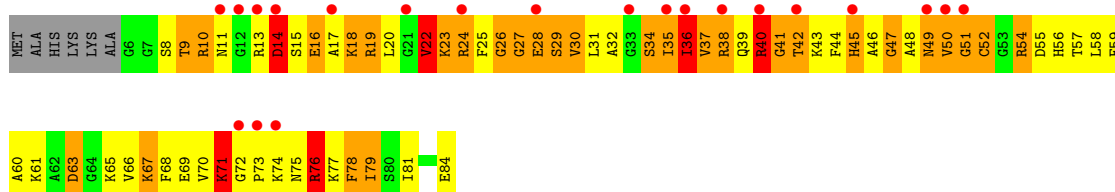
• Molecule 23: Peptide chain release factor 3



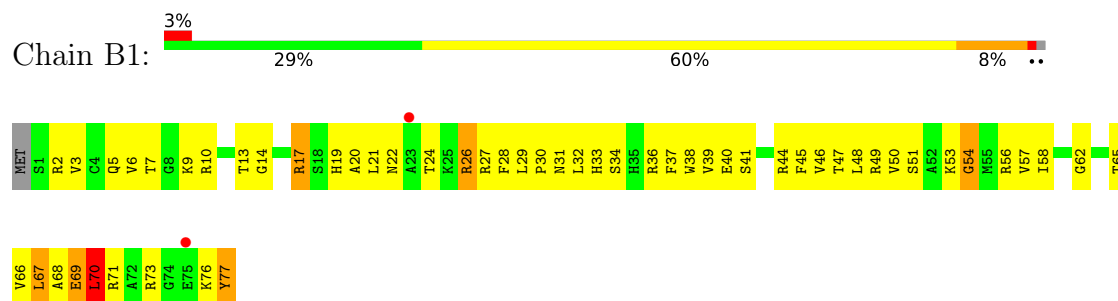
• Molecule 24: Viomycin



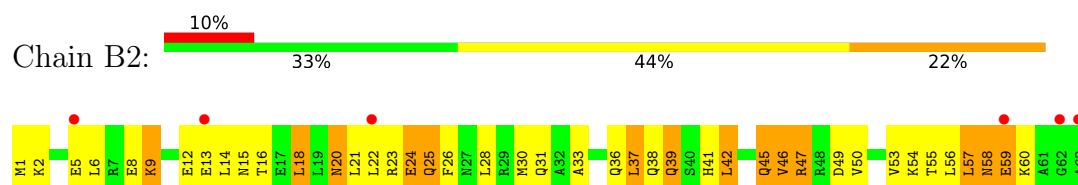
• Molecule 25: 50S ribosomal protein L27



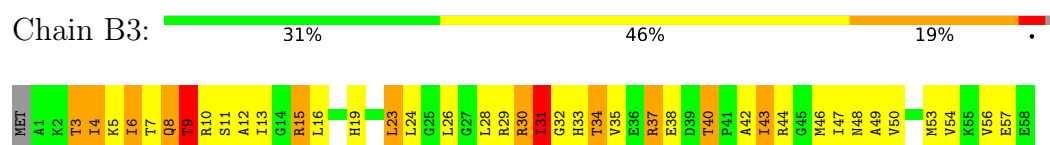
- Molecule 26: 50S ribosomal protein L28



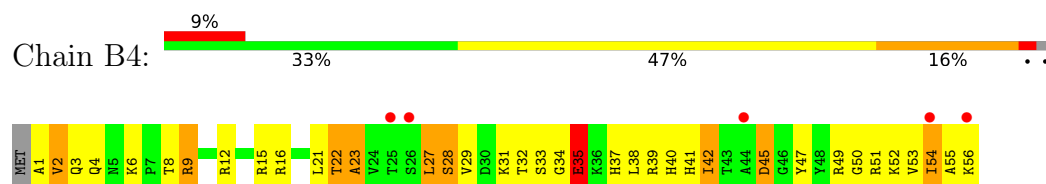
- Molecule 27: 50S ribosomal protein L29



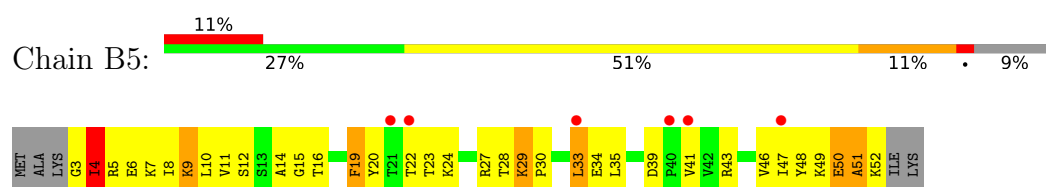
- Molecule 28: 50S ribosomal protein L30



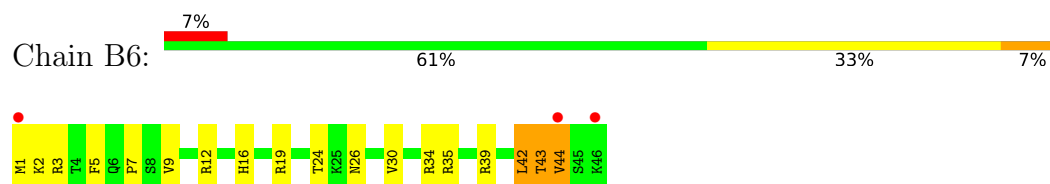
- Molecule 29: 50S ribosomal protein L32



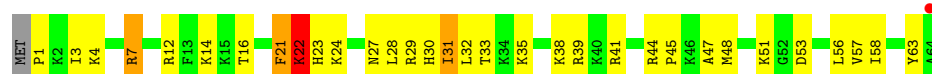
- Molecule 30: 50S ribosomal protein L33



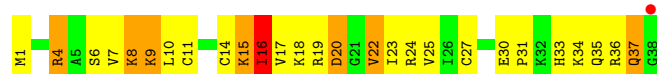
- Molecule 31: 50S ribosomal protein L34



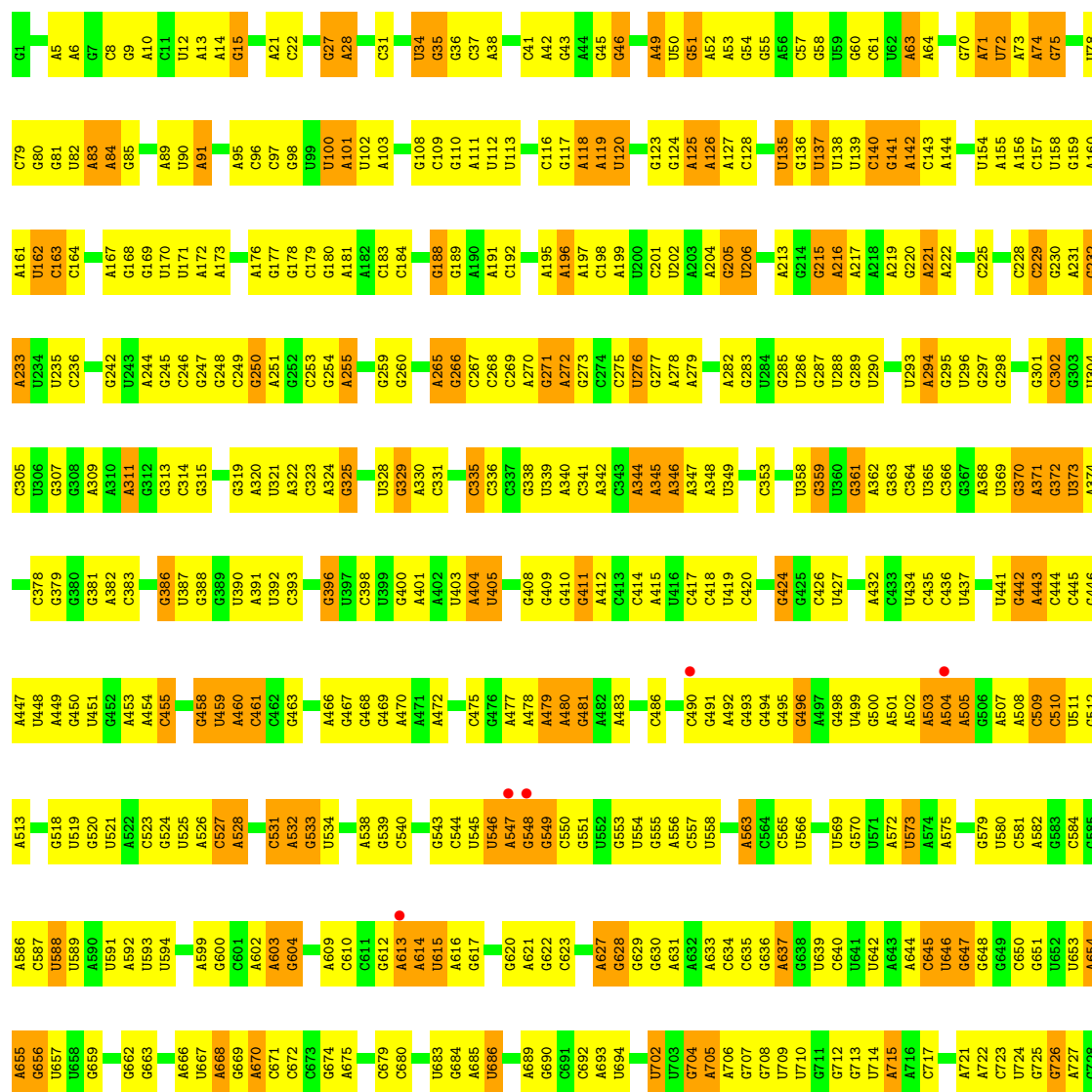
- Molecule 32: 50S ribosomal protein L35



• Molecule 33: 50S ribosomal protein L36 1

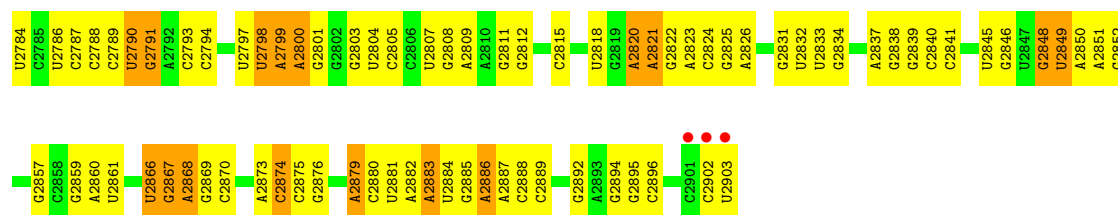


• Molecule 34: 23S rRNA

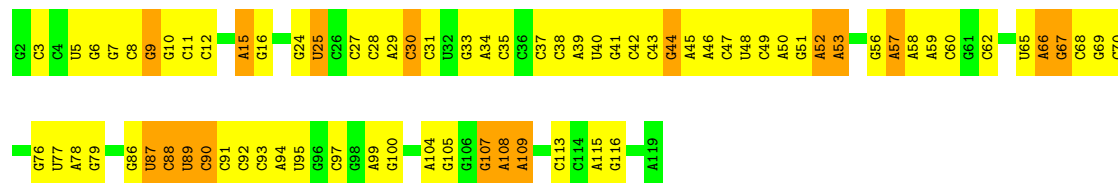


U1648	A1566	G1421	G1355	A1287	G1216	G1139	C1072	A1001	C935	U871	G805	G729
G1649	G1567	G1422	G1358	G1288	U1217	C1140	A1073	G1002	A936	U872	G809	A730
A1650	A1497		A1359	C1289	U1218	U1141	G1074	C1005	G938	C873	G812	C731
G1651	C1498	A1427	G1360	C1290	U1219	A1142	C1076		G938	C874	C814	C732
A1652	G1428	G1429	G1361	C1291		A1143	U1078	A1010	A941	C875	U813	G733
G1653	G1499	G1430	C1362	C1292	G1223	A1144	U1079	G1011	G942	C876	C815	A742
A1654	G1501	G1431	G1363	C1293	U1224	A1147	A1080	G1012	G943	A877	C816	A743
A1655	A1502	G1432	G1364		G1225	U1148	U1081	C1013	A944	A878	C817	U744
G1656	A1503	A1433	A1365	G1300	C1229	U1149	C1079	U1014	A945	C879	C818	G745
U1657	A1504	A1434	A1366	A1301	U1230	C1150	U1082	A1015	A946	C880	G819	U746
	A1505	A1435	G1368	A1302	U1231	C1151	U1083	U1016	A947	C881	A819	U747
A1665	U1506	G1436	G1371	G1303	C1232	C1152	U1084	G1017	C948	C882	A820	U748
G1666	C1507	C1437		G1304	U1233	C1153	A1085	U1018	C949	C883	A821	A749
G1667	A1508		G1374	A1304	U1234	G1154	U1086	U1019	G950	A884		
A1668	G1510	G1444	G1375	C1305	U1235	A1155	G1087	A1020	C951	C885	A752	
A1669	C1577		C1376	C1306	G1236	A1156	A1088	U1021		U	A824	A753
	U1578		G1377	A1307	A1237	G1157	A1089	A1022		C	U825	U754
G1674	A1581	G1450	A1378	A1308	G1238	G1161	A1090	U1023		C	U826	U755
G1675	G1515	C1451	U1379	G1309	U1239	G1162	C1091	G1024		G	U827	A756
A1676	G1516	G1452	G1380		U1240		G1092	G1025		A	U828	
A1677	G1517	A1453	G1381	C1313	A1244		G1093	G1026			U829	G760
G1682	G1518	C1454	G1382	C1314	G1245	A1165	U1094	A1027			G830	A761
U1683	G1519	G1455	A1383	C1315	G1246	G1166	A1095	A1028			U831	
	U1520	G1456	A1384	U1316	A1247	C1167	U1096	A1029			U832	A764
A1593	G1521	U1457	A1385	G1317	A1248	G1168	U1097	G1030			U833	
U1594	A1522	U1458	A1386	U1318	U1249	C1169	A1098	U1031			U834	
C1595	U1523	G1459	C1387	C1319	G1250	C1170	U1099	U1032			C897	G768
G1596	G1524	U1460	A1388	C1320	G1251	G1171	A1032	A1033			C898	U769
A1597	A1525	C1461	G1389	C1321	C1252	C1172	U1101	U1033			C899	G770
U1598		G1462	U1390	A1322	U1253	U1173	U1102	C968			A900	G771
G1600	G1530	C1463	U1391	C1323	A1254	U1174	A1103	U1039			C901	C772
G1601	C1531	G1464	A1392	G1324	A1254	A1175	G1104	A1040			C902	
U1602	U1532	U1465	A1393		U1255	U1176	U1105	A1041			C903	G775
A1603	C1533	G1466	A1394	A1327	U1256	G1177	G1106	C1042			G904	G776
	A1535	U1467	U1395	A1328	C1257	C1178	G1107	C1043				G777
A1608	G1536	U1468	U1396	U1329	U1258	G1179	U1108	G1044			A844	G778
A1609	G1537	A1469	U1397		G1259	U1180	C1109	A1045			U845	U779
A1610	U1538	A1470	C1398	G1332	A1260	U1181	G1110	A1046			U846	G780
G1613	U1539		C1399	G1333	C1261	U1182	U1111	G1047			U847	A781
A1614	G1540	G1474	U1400	C1334	A1262	U1183	C1048	A1048			C948	A782
G1615	C1541	G1475	U1401	C1335	U1263	U1184	U1049	C981			A849	A783
G1616	U1542	U1476	G1401	C1336		G1185	G914	C982			U850	G784
G1617	G1543	A1477	U1402	A1337	A1265	G1186	C915	A983			C851	G785
A1618	A1544	G1478	A1403	G1338	U1266	G1187	U1065	A984			C786	
G1619	A1545		C1404	G1339	U1267	U1188	C985	C985			C787	
G1620	G1546		U1405	U1340	A1268	U1189	C986	C986			C855	
		U1481	U1406	G1341	C1270	A1189	U1919	A988			G856	
A1722	C1550	G1482	U1409	A1342	G1271	G1197	A920	A920			G857	A789
G1723	A1551	U1483	G1410	U1343	A1272	U1198	U1060	G989			U859	A793
G1724	A1552	U1484	U1411	U1344	U1273	U1199	U1061	C991			A861	C795
U1725	G1558	U1485	C1414	C1345	A1275	C1200	G1062	C992			G862	C796
C1726	U1559	G1486	G1415	G1346	A1276	U1205	G1063	C992			A863	G797
C1727	C1560	U1487	U1416	A1347	G1277	G1206	U1064	C994			G864	G798
G1728	G1561	C1488	G1417	A1348	C1278	C1211	U1065	C994			C995	G799
U1729	U1562	A1489	C1418	C1349	G1279	G1212	A1067	A996			G865	A800
C1730	C1563	G1490	G1419	C1349	G1280	G1213	U1068	C997			C866	G801
G1731	U1564	G1491	A1419	U1352	U1286	A1213	G1069	C998			U868	
C1732	C1565	A1494	A1420	A1353		G1136	A1070	C999			U869	A802
G1733				A1354	A1286	G1138	G1071	A1000			U870	A804

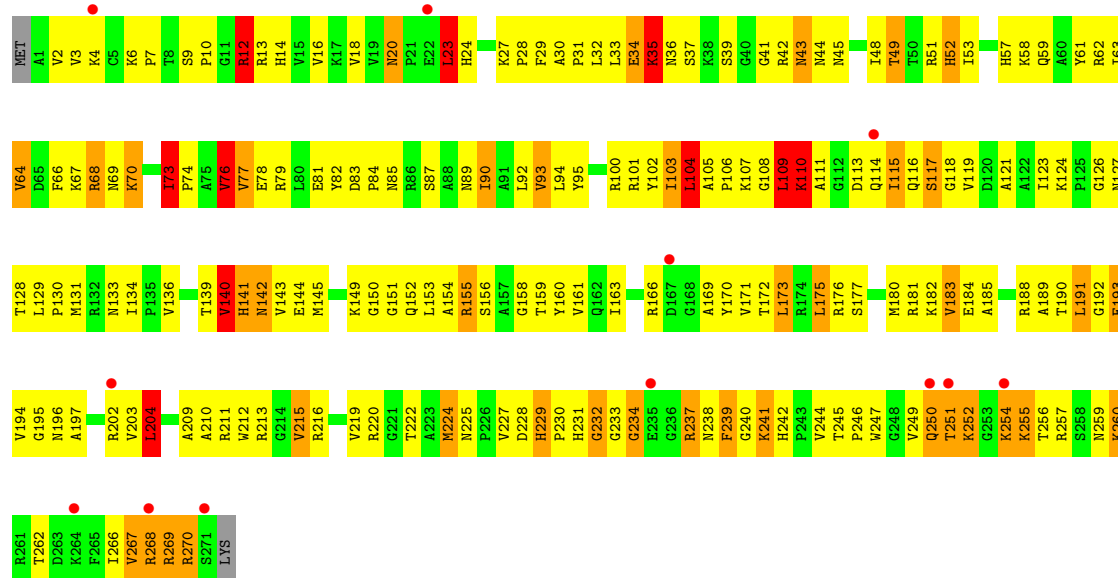
G2708	C2636	U2561	C2465	C3885	G2319	G2255	C	G	C2047	G1964	U1886	G1811	G1734
G2709	U2637	U2562	C2466	A2386	U2320	G2256	C	A	G2048	C1965	C1887	U1812	A1735
C2710	G2638	U2563	C2467	U2387	A2321	G2257	U2179	U	G1888	A1966	G1889	G1813	U1736
G2714	A2639	A2564	A2467	A2388	A2322	C2258	U2180	A	C2050	C1967	G1889	G1814	G1737
C2715	G2640	A2565	A2468	A2389	G2323	C2259	U2181	G	A2051	G1968	C1893	A1815	G1738
G2716	G2641	A2566	A2469	U2390	U2324	C2260	U2182	G	A2052	A1969	C1894	G1816	A1739
C2717	G2642	G2567	G2470	G2391	G2325	C2261	A2183	U	C	A1970	C1895	G1817	G1740
	G2643	U2568	A2471	A2392	C2326	U2262	A2184	G	C2055	G1971	C1896	U1818	C1741
U2720	G2644	G2570	U2472	U2393	A2327	U2263	U2185	G	G2056	G1972		A1819	U1742
G2722	C2645	U2571	U2473	U2186	G2264	C2265	G2187	A	G2057	C1973	A1900	U1820	G1743
A2721	G2646	A2572	U2474	U2187			U2188	G	A2058	C1974	A1901	A1821	A1744
C2723	U2647		C2475	U2188	A2268	A2269	U2189	C	A2059	G1984	C1902	G1822	A1745
G2648	G2648	C2575	A2476	U2402	G2269	A2270	U2194	U	G2061	C1985	G1903	G1823	A1746
U2725	U2650	G2576	A2477	C2403	G2271	A2272	U2195	C	A2062	C1986	C1905	G1824	
A2726	C2651	A2577	A2478	U2404	G2272	G2273	U2196	U	C2063	C1986	C1906	U1825	A1749
G2727	C2652	G2578	C2480	A2406	A2274	A2275	C2197	U	C2064	C1990	G1907	G1826	G1756
U2728	U2653	C2579	C2481	A2407	A2276	C2276	U2198	G	C2065	G1991	C1908	U1827	U1757
G2729	A2654			A2411	G2277	G2278	U2199	G	C2066	G1992	C1909	A1829	U1758
C2730	G2655	G2583	C2486	A2412	G2279	A2280	C2200			U1993	G1910	G1830	A1759
G2731	U2656	U2584	U2489	A2413	G2280	G2281	G2201		G2069	C1996	U1911	G1831	C1760
U2732	A2657	U2585	G2490	A2414	A2282	G2283	G2202		A2070	C1997	A1912	C1832	C1761
A2733	C2657	U2586	G2491	A2415	G2284	C2284	U2203		A2071	C1998	A1913	C1833	
G2734	G2661	A2587	U2492	C2420	G2285	G2286	G2204		C2072	A1998	C1914	C1833	
C2735	G2662		U2493	G2421	G2287	G2288	U2210		C2073	U1915	U1915	G1838	C1764
	G2663		G2494	A2422	G2288	G2289	A2211		U2074	C2006	A1916	G1839	A1773
A2740	G2664	G2590	C2495	U2423	G2289	G2290	A2212		U2075		A1917	G1840	C1774
G2741	C2667	C2592	G2496	G2424	G2291	G2292	U2213		A2013	A2013	A1918	U1841	U1775
U2743		U2593	A2497	A2425	U2293	G2294	U2214		A2014	A2014	A1919	G1842	U1776
	G2674	A2598	C2498	C2426	G2295	G2296	G2217		A2015	A2015	G1920	C1843	U1777
U2746	A2675	G2599	G2499	G2427	G2296	G2297	G2218		U2016	U2016	G1921	U1778	U1779
G2747	G2676	A2600	G2502	C2428	G2298	G2299	G2219		U2017	U2017	G1922	G1846	U1780
A2748	G2677	C2601	U2503	A2429	G2299	G2300	U2220		U2018	A2019	C1925	A1781	U1782
	C2678	A2602	U2504	G2430	U2299	G2301	G2221		A2019	A2019	C1925	G1849	U1782
U2753	A2679	G2603	G2505	U2431	U2300	G2302	C2222		A2020	A2020	U1926	G1850	A1783
G2754	C2680		U2506	A2432	G2301	G2303	G2223		C2021	C2021	A1927	U1851	A1784
C2755	G2681	G2607	C2507	G2433	G2302	G2304	G2224		U2022	U2022	A1928	U1852	A1785
U2756	A2682	G2608	U2511	A2434	G2303	G2305	A2225		C2023	C2023	G1929	A1853	A1786
A2757	C2683	U2609	G2512	A2435	G2304	G2306	A2226		G2024	G2024	U1930	A1854	C1787
G2758			U2513	U2441	G2305	G2307	A2227		C2025	C2025	U1931	U1855	C1788
U2759	G2688	U2613	A2516	G2442	G2306	G2308	G2228		U2026	U2026	G1935	U1856	A1789
C2762	U2689	A2614	C2517	C2443	G2307	G2309	G2229		G2027	G2027	A1936	G1857	C1790
G2763	U2690	U2615	A2518	G2444	G2308	G2310	U2230		A1937	A1937	A1937	U1858	G1792
A2765	C2691	G2616	U2519	G2445	G2309	G2311	U2231		A1938	A1938	C1793	G1860	C1793
G2766		U2617	C2520		G2310	G2312	U2232				U1943	U1863	C1794
U2769	G2694	G2618	G2529	A2448	G2311	G2313	G2233				U1944	U1864	C1795
	U2695	C2619	G2530	U2449	G2312	G2314	G2234				G1945	U1869	U1798
U2773	G2696	C2620	A2542	A2451	G2313	G2315	G2235				U1946	U1799	U1799
C2774	U2697	G2623	G2547	C2452	G2314	G2316	G2236				C1947	G1870	C1800
G2775	C2699	G2624	U2548	A2453	G2315	G2317	G2237				U1955	A1871	C1801
A2778	A2700	U2627	U2549	G2454	G2316	G2318	U2243				U1956	A1872	C1802
G2779	U2701	C2628	G2554	U2455	G2317	G2319	U2244				C1957	G1873	C1803
U2781	G2702	U2629	U2555	C2456	G2318	G2320	U2245				U1957	G1874	C1804
C2780	C2703	A2632	U2556	U2457	A2381	G2321	U2246				U1958	G1875	C1805
G2781	C2704	G2633	C2557	G2458	G2382	G2322	C2248				U1959	G1884	A1808
U2782	A2705	A2634	U2558	U2459	G2383	G2323	U2249				U1960	A1809	A1809
U2783	G2707	A2635		A2461	U2384	G2324	G2250				C1961	C1962	A1810



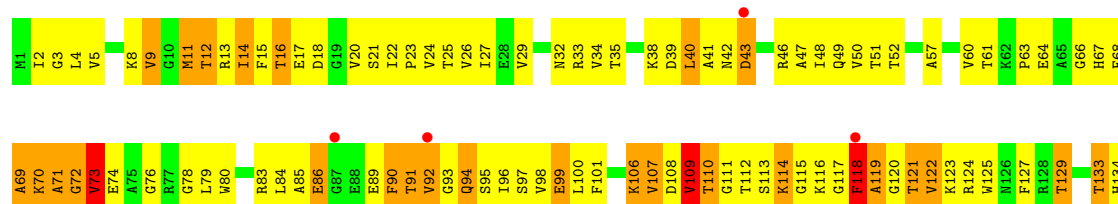
• Molecule 35: 5S ribosomal RNA

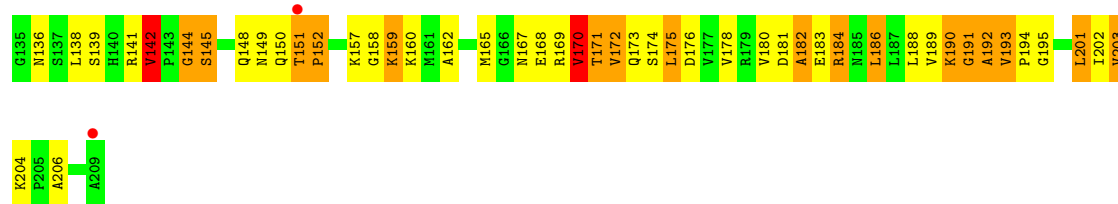


• Molecule 36: 50S ribosomal protein L2

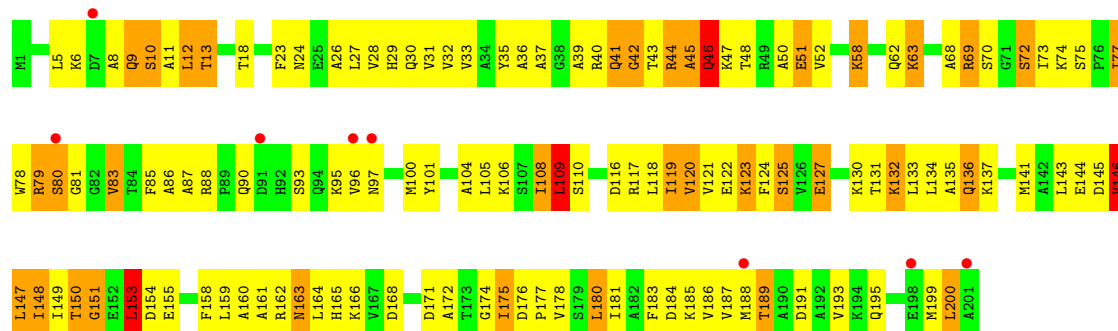


• Molecule 37: 50S ribosomal protein L3

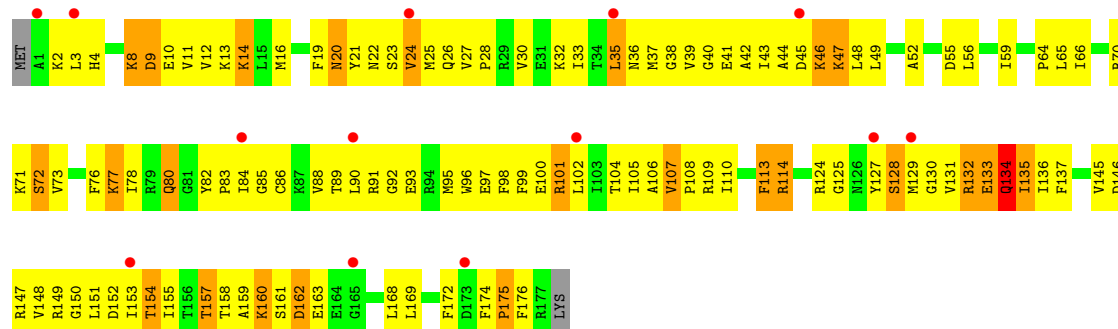




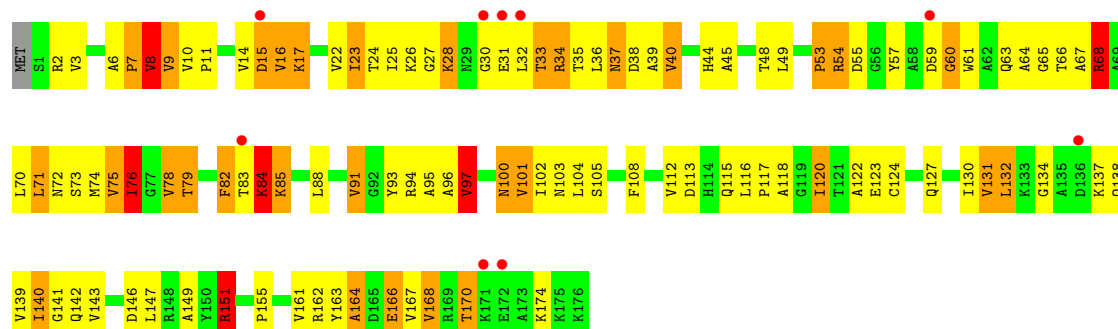
• Molecule 38: 50S ribosomal protein L4

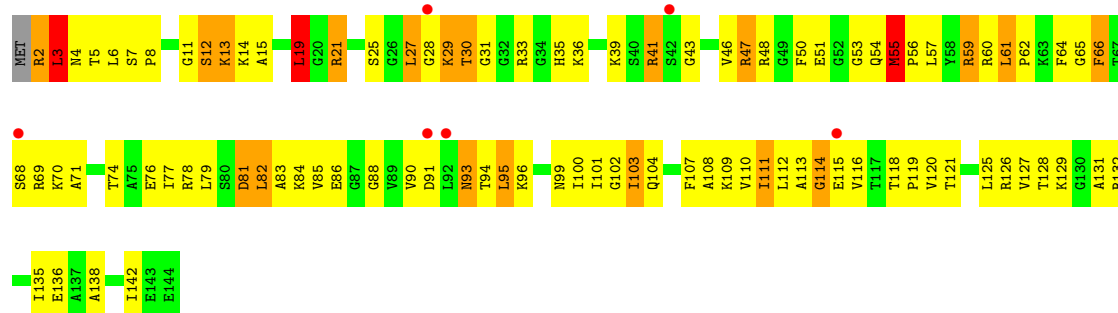


• Molecule 39: 50S ribosomal protein L5

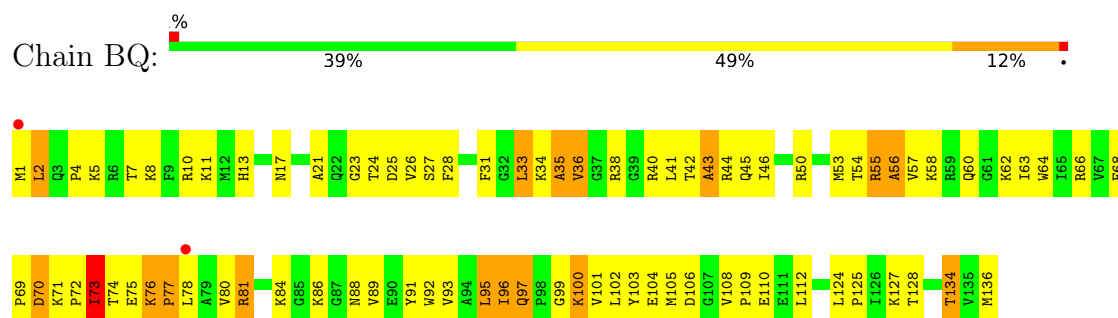


• Molecule 40: 50S ribosomal protein L6

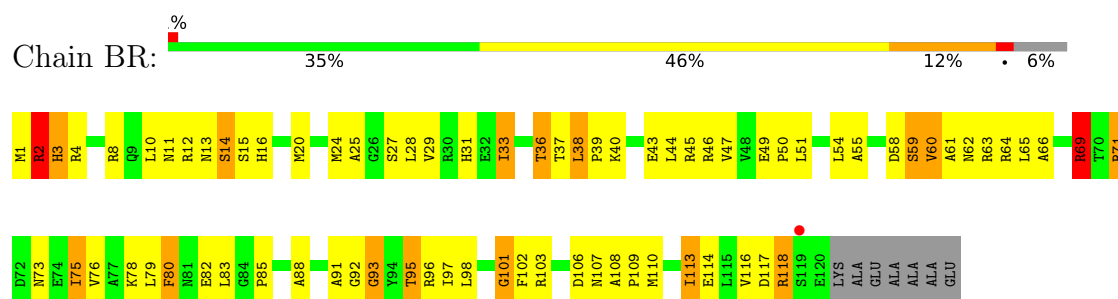




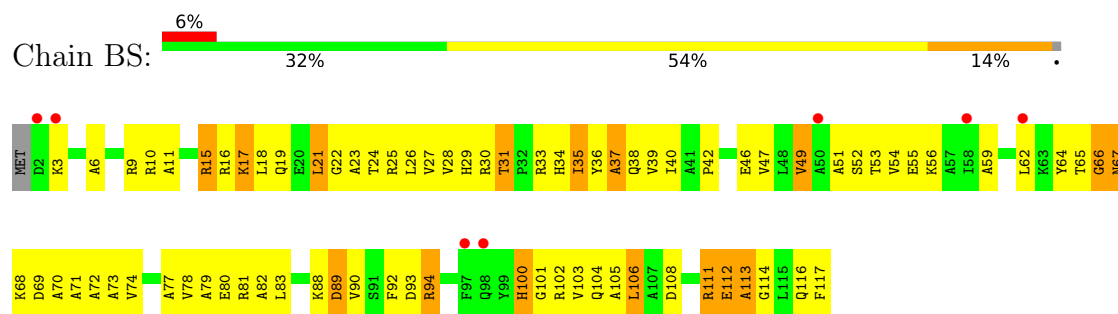
• Molecule 47: 50S ribosomal protein L16



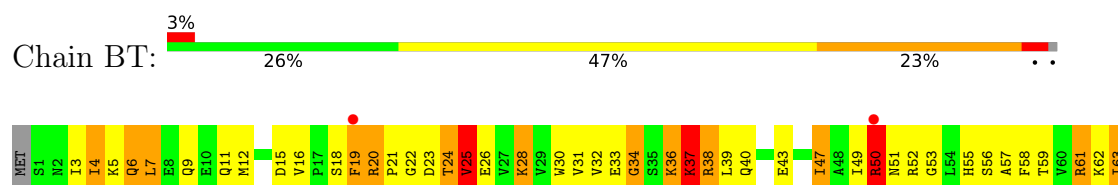
• Molecule 48: 50S ribosomal protein L17



• Molecule 49: 50S ribosomal protein L18



• Molecule 50: 50S ribosomal protein L19

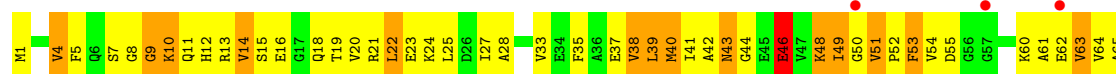




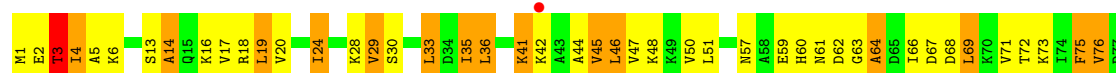
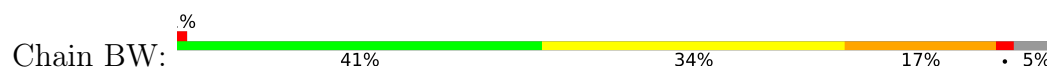
- Molecule 51: 50S ribosomal protein L20



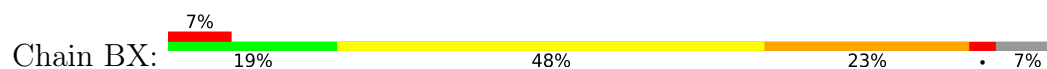
- Molecule 52: 50S ribosomal protein L21



- Molecule 53: 50S ribosomal protein L22

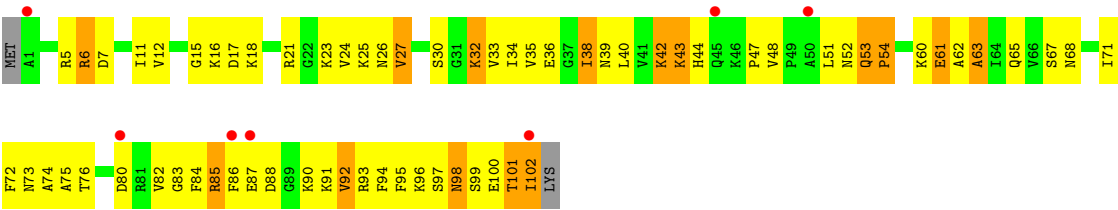


- Molecule 54: 50S ribosomal protein L23

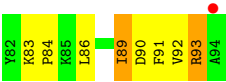
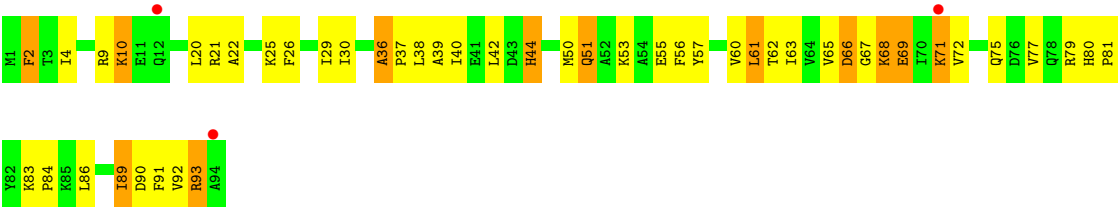


- Molecule 55: 50S ribosomal protein L24 1





● Molecule 56: 50S ribosomal protein L25 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 99.9 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX, CNS 1.2	Depositor
R, R_{free}	0.210 , 0.250 0.227 , 0.253	Depositor DCC
R_{free} test set	26311 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 90.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	147221	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: GNP, DPP, MG, 5OH, UAL, KBE

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	0.27	0/36809	0.40	0/57423
2	AB	0.37	0/1735	0.77	0/2338
3	AC	0.38	0/1651	0.82	2/2225 (0.1%)
4	AD	0.36	0/1665	0.81	4/2227 (0.2%)
5	AE	0.45	0/1118	0.93	2/1504 (0.1%)
6	AF	0.36	0/835	0.81	2/1128 (0.2%)
7	AG	0.31	0/1195	0.76	0/1602
8	AH	0.39	0/989	0.86	2/1326 (0.2%)
9	AI	0.31	0/1034	0.77	2/1375 (0.1%)
10	AJ	0.41	0/796	0.86	1/1077 (0.1%)
11	AK	0.38	0/893	0.83	0/1205
12	AL	0.52	0/969	0.98	2/1300 (0.2%)
13	AM	0.31	0/892	0.76	0/1193
14	AN	0.35	0/785	0.76	0/1043
15	AO	0.36	0/722	0.77	0/964
16	AP	0.40	0/659	0.74	0/884
17	AQ	0.36	0/657	0.89	2/881 (0.2%)
18	AR	0.40	0/462	0.93	2/621 (0.3%)
19	AS	0.30	0/652	0.74	0/877
20	AT	0.41	0/671	0.83	0/888
21	AU	0.37	0/430	0.84	0/570
22	AV	0.32	0/144	0.46	0/222
23	AW	0.62	7/4221 (0.2%)	1.10	29/5702 (0.5%)
24	AY	0.86	0/11	0.67	0/13
25	B0	0.56	0/603	0.95	1/797 (0.1%)
26	B1	0.45	0/635	0.94	1/848 (0.1%)
27	B2	0.40	0/510	0.86	2/677 (0.3%)
28	B3	0.52	0/453	0.95	0/605
29	B4	0.56	0/450	0.98	4/599 (0.7%)
30	B5	0.36	0/416	0.77	0/554
31	B6	0.52	0/380	0.89	0/498
32	B7	0.46	0/513	0.85	1/676 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.53	0/303	1.00	2/397 (0.5%)
34	BA	0.36	4/68601 (0.0%)	0.44	10/107017 (0.0%)
35	BB	0.25	0/2828	0.39	0/4410
36	BC	0.53	0/2121	1.07	11/2852 (0.4%)
37	BD	0.59	0/1586	1.13	10/2134 (0.5%)
38	BE	0.47	0/1571	0.87	4/2113 (0.2%)
39	BF	0.32	0/1434	0.77	1/1926 (0.1%)
40	BG	0.47	0/1343	0.88	1/1816 (0.1%)
41	BH	0.38	0/1244	0.84	1/1675 (0.1%)
42	BI	0.32	0/1046	0.79	0/1410
43	BJ	0.39	0/227	0.86	0/304
43	BK	0.32	0/227	0.75	0/304
43	BL	0.37	0/227	0.77	0/304
43	BM	0.33	0/227	0.70	0/304
44	BN	0.55	0/1152	0.97	1/1551 (0.1%)
45	BO	0.61	0/947	1.05	7/1268 (0.6%)
46	BP	0.47	0/1054	0.97	3/1403 (0.2%)
47	BQ	0.50	0/1093	1.01	2/1460 (0.1%)
48	BR	0.58	0/973	0.95	1/1301 (0.1%)
49	BS	0.43	0/902	0.82	0/1209
50	BT	0.56	0/929	0.95	3/1242 (0.2%)
51	BU	0.53	0/960	0.88	0/1278
52	BV	0.45	0/829	0.95	6/1107 (0.5%)
53	BW	0.66	0/863	0.91	1/1156 (0.1%)
54	BX	0.52	0/744	0.96	1/994 (0.1%)
55	BY	0.48	0/787	0.88	1/1051 (0.1%)
56	BZ	0.39	0/766	0.83	3/1025 (0.3%)
All	All	0.38	11/158939 (0.0%)	0.60	128/236853 (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
12	AL	0	1
23	AW	0	2
24	AY	0	2
All	All	0	5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	2106	U	O3'-P	16.62	1.86	1.61
34	BA	2183	A	O3'-P	12.55	1.79	1.61
34	BA	974	G	O3'-P	-12.31	1.42	1.61
34	BA	973	A	O3'-P	-10.96	1.44	1.61
23	AW	25	GLY	C-N	9.66	1.45	1.33

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	2183	A	O3'-P-O5'	-15.64	80.55	104.00
37	BD	151	THR	CA-C-N	-10.86	107.00	119.05
37	BD	151	THR	C-N-CA	-10.86	107.00	119.05
37	BD	172	VAL	N-CA-C	10.33	121.19	111.48
36	BC	73	ILE	CA-C-N	9.04	129.72	120.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AL	22	ALA	Peptide
23	AW	410	LYS	Peptide
23	AW	411	GLN	Peptide
24	AY	1	KBE	Mainchain
24	AY	2	DPP	Mainchain

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	32873	0	16542	1457	0
2	AB	1704	0	1732	197	0
3	AC	1624	0	1699	170	7
4	AD	1643	0	1710	209	0
5	AE	1105	0	1148	139	0
6	AF	817	0	808	113	0
7	AG	1181	0	1240	76	0
8	AH	979	0	1034	101	0
9	AI	1022	0	1070	131	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	786	0	828	99	0
11	AK	877	0	887	109	0
12	AL	955	0	1019	125	0
13	AM	883	0	944	97	0
14	AN	774	0	827	99	0
15	AO	714	0	737	47	0
16	AP	649	0	666	65	0
17	AQ	648	0	691	68	0
18	AR	455	0	478	44	0
19	AS	637	0	665	72	0
20	AT	665	0	714	64	0
21	AU	425	0	449	71	0
22	AV	129	0	65	9	0
23	AW	4144	0	4127	291	0
24	AY	48	0	40	31	0
25	B0	596	0	610	170	0
26	B1	625	0	655	57	0
27	B2	509	0	543	41	0
28	B3	449	0	491	54	0
29	B4	444	0	461	36	0
30	B5	409	0	440	39	0
31	B6	377	0	418	21	0
32	B7	504	0	574	52	0
33	B8	302	0	340	41	0
34	BA	61252	0	30808	2059	7
35	BB	2529	0	1281	94	0
36	BC	2082	0	2157	234	0
37	BD	1565	0	1616	210	0
38	BE	1552	0	1619	160	0
39	BF	1410	0	1447	151	0
40	BG	1323	0	1374	143	0
41	BH	1230	0	1282	265	0
42	BI	1032	0	1088	89	0
43	BJ	227	0	237	51	0
43	BK	227	0	237	25	0
43	BL	227	0	237	37	0
43	BM	227	0	237	46	0
44	BN	1129	0	1162	152	0
45	BO	938	0	1012	122	0
46	BP	1045	0	1117	114	0
47	BQ	1074	0	1157	84	0
48	BR	960	0	1000	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	BS	892	0	923	77	0
50	BT	917	0	965	127	0
51	BU	947	0	1022	113	0
52	BV	816	0	839	102	0
53	BW	856	0	922	61	0
54	BX	738	0	807	117	0
55	BY	779	0	834	78	0
56	BZ	753	0	780	57	0
57	AA	102	0	0	0	0
57	AF	1	0	0	0	0
57	AH	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	1	0	0	0	0
57	AW	1	0	0	0	0
57	B0	3	0	0	0	0
57	B2	1	0	0	0	0
57	B4	1	0	0	0	0
57	BA	357	0	0	0	0
57	BB	9	0	0	0	0
57	BC	1	0	0	0	0
57	BD	5	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	BR	2	0	0	0	0
57	BT	1	0	0	0	0
57	BX	1	0	0	0	0
58	AW	32	0	13	6	0
59	AW	2	0	0	2	0
59	B8	1	0	0	0	0
59	BA	8	0	0	0	0
59	BC	2	0	0	0	0
59	BD	1	0	0	0	0
59	BF	1	0	0	0	0
59	BG	1	0	0	0	0
59	BW	1	0	0	1	0
All	All	147221	0	100825	8378	7

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 34.

The worst 5 of 8378 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)
1:AA:1495:U:O4	24:AY:1:KBE:CE	1.84	1.26
1:AA:1494:G:N7	24:AY:1:KBE:HGA	1.52	1.24
1:AA:1494:G:O6	24:AY:1:KBE:HG	1.35	1.22
1:AA:1495:U:C4	24:AY:1:KBE:HE	1.75	1.20
51:BU:63:ARG:NH1	51:BU:96:ASP:HA	1.58	1.18

The worst 5 of 7 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)
3:AC:131:ARG:NH2	34:BA:2157:G:P[4_445]	1.17	1.03
3:AC:131:ARG:CZ	34:BA:2157:G:OP1[4_445]	1.23	0.97
3:AC:131:ARG:NH2	34:BA:2157:G:OP1[4_445]	1.40	0.80
3:AC:131:ARG:NH2	34:BA:2157:G:O5'[4_445]	1.48	0.72
3:AC:131:ARG:NE	34:BA:2157:G:OP1[4_445]	1.68	0.52

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	216/241 (90%)	130 (60%)	52 (24%)	34 (16%)	0	0
3	AC	204/233 (88%)	156 (76%)	32 (16%)	16 (8%)	1	5
4	AD	203/206 (98%)	134 (66%)	45 (22%)	24 (12%)	0	1
5	AE	148/167 (89%)	97 (66%)	31 (21%)	20 (14%)	0	1
6	AF	98/131 (75%)	66 (67%)	19 (19%)	13 (13%)	0	1
7	AG	149/156 (96%)	112 (75%)	28 (19%)	9 (6%)	1	10
8	AH	127/130 (98%)	96 (76%)	27 (21%)	4 (3%)	3	22
9	AI	125/130 (96%)	83 (66%)	25 (20%)	17 (14%)	0	1
10	AJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	0	2
11	AK	115/129 (89%)	82 (71%)	25 (22%)	8 (7%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	121/124 (98%)	89 (74%)	22 (18%)	10 (8%)	0	4
13	AM	112/118 (95%)	78 (70%)	27 (24%)	7 (6%)	1	8
14	AN	92/101 (91%)	55 (60%)	24 (26%)	13 (14%)	0	1
15	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	3	20
16	AP	80/82 (98%)	57 (71%)	16 (20%)	7 (9%)	0	3
17	AQ	78/84 (93%)	57 (73%)	10 (13%)	11 (14%)	0	1
18	AR	53/75 (71%)	38 (72%)	12 (23%)	3 (6%)	1	11
19	AS	77/92 (84%)	60 (78%)	14 (18%)	3 (4%)	2	18
20	AT	83/87 (95%)	59 (71%)	20 (24%)	4 (5%)	2	14
21	AU	49/71 (69%)	24 (49%)	19 (39%)	6 (12%)	0	1
23	AW	523/529 (99%)	381 (73%)	82 (16%)	60 (12%)	0	1
24	AY	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	B0	77/85 (91%)	35 (46%)	18 (23%)	24 (31%)	0	0
26	B1	75/78 (96%)	56 (75%)	16 (21%)	3 (4%)	2	17
27	B2	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	0	4
28	B3	56/59 (95%)	46 (82%)	5 (9%)	5 (9%)	0	3
29	B4	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	6
30	B5	48/55 (87%)	41 (85%)	3 (6%)	4 (8%)	0	4
31	B6	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	2	15
32	B7	62/65 (95%)	53 (86%)	6 (10%)	3 (5%)	2	14
33	B8	36/38 (95%)	27 (75%)	5 (14%)	4 (11%)	0	2
36	BC	269/273 (98%)	212 (79%)	31 (12%)	26 (10%)	0	3
37	BD	207/209 (99%)	157 (76%)	23 (11%)	27 (13%)	0	1
38	BE	199/201 (99%)	143 (72%)	33 (17%)	23 (12%)	0	1
39	BF	175/179 (98%)	117 (67%)	41 (23%)	17 (10%)	0	3
40	BG	174/177 (98%)	104 (60%)	44 (25%)	26 (15%)	0	1
41	BH	161/165 (98%)	98 (61%)	38 (24%)	25 (16%)	0	0
42	BI	139/142 (98%)	83 (60%)	38 (27%)	18 (13%)	0	1
43	BJ	28/121 (23%)	17 (61%)	6 (21%)	5 (18%)	0	0
43	BK	28/121 (23%)	21 (75%)	5 (18%)	2 (7%)	1	6
43	BL	28/121 (23%)	22 (79%)	4 (14%)	2 (7%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BM	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	6
44	BN	140/142 (99%)	101 (72%)	24 (17%)	15 (11%)	0	2
45	BO	120/123 (98%)	88 (73%)	19 (16%)	13 (11%)	0	2
46	BP	141/144 (98%)	88 (62%)	34 (24%)	19 (14%)	0	1
47	BQ	134/136 (98%)	104 (78%)	18 (13%)	12 (9%)	0	3
48	BR	118/127 (93%)	86 (73%)	20 (17%)	12 (10%)	0	2
49	BS	114/117 (97%)	90 (79%)	14 (12%)	10 (9%)	0	3
50	BT	112/115 (97%)	74 (66%)	21 (19%)	17 (15%)	0	0
51	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	9
52	BV	101/103 (98%)	75 (74%)	18 (18%)	8 (8%)	1	5
53	BW	108/116 (93%)	89 (82%)	15 (14%)	4 (4%)	2	18
54	BX	91/100 (91%)	49 (54%)	23 (25%)	19 (21%)	0	0
55	BY	100/104 (96%)	65 (65%)	22 (22%)	13 (13%)	0	1
56	BZ	92/94 (98%)	72 (78%)	14 (15%)	6 (6%)	1	8
All	All	6272/6999 (90%)	4427 (71%)	1181 (19%)	664 (11%)	0	2

5 of 664 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	22	TRP
2	AB	33	ALA
2	AB	40	ILE
2	AB	75	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	180/199 (90%)	149 (83%)	31 (17%)	2	10
3	AC	170/190 (90%)	142 (84%)	28 (16%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	149 (87%)	23 (13%)	4	19
5	AE	113/126 (90%)	93 (82%)	20 (18%)	2	10
6	AF	87/112 (78%)	76 (87%)	11 (13%)	4	21
7	AG	124/129 (96%)	120 (97%)	4 (3%)	34	65
8	AH	104/105 (99%)	92 (88%)	12 (12%)	5	24
9	AI	105/107 (98%)	94 (90%)	11 (10%)	6	28
10	AJ	86/90 (96%)	69 (80%)	17 (20%)	1	8
11	AK	90/99 (91%)	73 (81%)	17 (19%)	1	9
12	AL	103/104 (99%)	87 (84%)	16 (16%)	2	14
13	AM	92/96 (96%)	90 (98%)	2 (2%)	45	71
14	AN	79/84 (94%)	70 (89%)	9 (11%)	5	24
15	AO	76/77 (99%)	66 (87%)	10 (13%)	4	19
16	AP	65/65 (100%)	54 (83%)	11 (17%)	2	11
17	AQ	74/78 (95%)	63 (85%)	11 (15%)	3	15
18	AR	48/65 (74%)	43 (90%)	5 (10%)	7	28
19	AS	70/79 (89%)	62 (89%)	8 (11%)	5	24
20	AT	65/66 (98%)	57 (88%)	8 (12%)	4	22
21	AU	44/61 (72%)	38 (86%)	6 (14%)	3	18
23	AW	447/453 (99%)	372 (83%)	75 (17%)	2	11
24	AY	2/2 (100%)	2 (100%)	0	100	100
25	B0	59/63 (94%)	42 (71%)	17 (29%)	0	1
26	B1	67/68 (98%)	57 (85%)	10 (15%)	3	15
27	B2	55/55 (100%)	46 (84%)	9 (16%)	2	12
28	B3	48/49 (98%)	37 (77%)	11 (23%)	1	5
29	B4	47/48 (98%)	39 (83%)	8 (17%)	2	11
30	B5	45/49 (92%)	39 (87%)	6 (13%)	4	19
31	B6	38/38 (100%)	35 (92%)	3 (8%)	11	40
32	B7	51/52 (98%)	49 (96%)	2 (4%)	28	62
33	B8	34/34 (100%)	31 (91%)	3 (9%)	9	35
36	BC	216/218 (99%)	174 (81%)	42 (19%)	1	8
37	BD	164/164 (100%)	138 (84%)	26 (16%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BE	165/165 (100%)	137 (83%)	28 (17%)	2	11
39	BF	148/150 (99%)	136 (92%)	12 (8%)	11	39
40	BG	137/138 (99%)	112 (82%)	25 (18%)	2	9
41	BH	123/123 (100%)	109 (89%)	14 (11%)	5	24
42	BI	109/110 (99%)	103 (94%)	6 (6%)	19	52
43	BJ	26/85 (31%)	22 (85%)	4 (15%)	2	14
43	BK	26/85 (31%)	26 (100%)	0	100	100
43	BL	26/85 (31%)	25 (96%)	1 (4%)	29	62
43	BM	26/85 (31%)	24 (92%)	2 (8%)	12	41
44	BN	116/116 (100%)	92 (79%)	24 (21%)	1	7
45	BO	103/104 (99%)	75 (73%)	28 (27%)	0	2
46	BP	102/103 (99%)	84 (82%)	18 (18%)	2	10
47	BQ	109/109 (100%)	91 (84%)	18 (16%)	2	12
48	BR	100/103 (97%)	89 (89%)	11 (11%)	6	26
49	BS	86/87 (99%)	74 (86%)	12 (14%)	3	17
50	BT	99/100 (99%)	80 (81%)	19 (19%)	1	8
51	BU	89/90 (99%)	71 (80%)	18 (20%)	1	7
52	BV	84/84 (100%)	72 (86%)	12 (14%)	3	16
53	BW	93/99 (94%)	69 (74%)	24 (26%)	0	3
54	BX	80/84 (95%)	66 (82%)	14 (18%)	2	10
55	BY	83/85 (98%)	74 (89%)	9 (11%)	6	27
56	BZ	78/78 (100%)	73 (94%)	5 (6%)	16	48
All	All	5228/5666 (92%)	4452 (85%)	776 (15%)	3	15

5 of 776 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BD	138	LEU
44	BN	55	ILE
38	BE	51	GLU
37	BD	133	THR
40	BG	68	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 205 such sidechains are listed below:

Mol	Chain	Res	Type
36	BC	24	HIS
39	BF	22	ASN
56	BZ	24	ASN
36	BC	85	ASN
37	BD	126	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1531/1533 (99%)	300 (19%)	45 (2%)
22	AV	5/27 (18%)	3 (60%)	0
34	BA	2849/2903 (98%)	577 (20%)	95 (3%)
35	BB	117/118 (99%)	22 (18%)	3 (2%)
All	All	4502/4581 (98%)	902 (20%)	143 (3%)

5 of 902 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	19	A
1	AA	22	G
1	AA	31	G

5 of 143 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1930	G
34	BA	2033	A
34	BA	2638	G
34	BA	60	G
34	BA	51	G

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

4 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	UAL	AY	5	24	6,8,9	2.53	2 (33%)	4,9,11	1.30	1 (25%)
24	5OH	AY	6	24	7,12,13	0.53	0	4,16,18	0.72	0
24	KBE	AY	1	24	8,8,9	0.57	0	6,8,10	1.30	1 (16%)
24	DPP	AY	2	24	4,5,6	1.10	1 (25%)	1,5,7	0.18	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	UAL	AY	5	24	-	0/3/7/9	-
24	5OH	AY	6	24	-	0/2/18/20	0/1/1/1
24	KBE	AY	1	24	-	1/7/7/8	-
24	DPP	AY	2	24	-	0/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	5	UAL	C-CA	4.89	1.53	1.45
24	AY	5	UAL	C1-N1	-3.17	1.35	1.40
24	AY	2	DPP	O-C	2.15	1.28	1.20

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	1	KBE	CB-CA-C	2.61	116.38	112.17
24	AY	5	UAL	O-C-CA	-2.37	122.42	125.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	1	KBE	C-CA-CB-N

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	5	UAL	4	0
24	AY	6	5OH	7	0
24	AY	1	KBE	17	0
24	AY	2	DPP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 494 ligands modelled in this entry, 493 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	$\# Z > 2$
58	GNP	AW	602	57	34,34,34	1.48	5 (14%)	47,54,54	1.37	8 (17%)

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
58	GNP	AW	602	57	-	7/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AW	602	GNP	PG-O1G	5.02	1.53	1.46
58	AW	602	GNP	PA-O3A	-4.25	1.54	1.59
58	AW	602	GNP	PB-O3A	-2.48	1.56	1.59
58	AW	602	GNP	PA-O2A	-2.15	1.45	1.55
58	AW	602	GNP	PB-O2B	-2.02	1.51	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AW	602	GNP	O2B-PB-O1B	3.44	117.24	109.87
58	AW	602	GNP	O2G-PG-O3G	3.31	116.48	107.59
58	AW	602	GNP	O3G-PG-O1G	-2.98	105.98	113.45
58	AW	602	GNP	O1B-PB-N3B	2.83	115.94	111.77
58	AW	602	GNP	C5'-C4'-C3'	-2.31	106.90	115.21

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

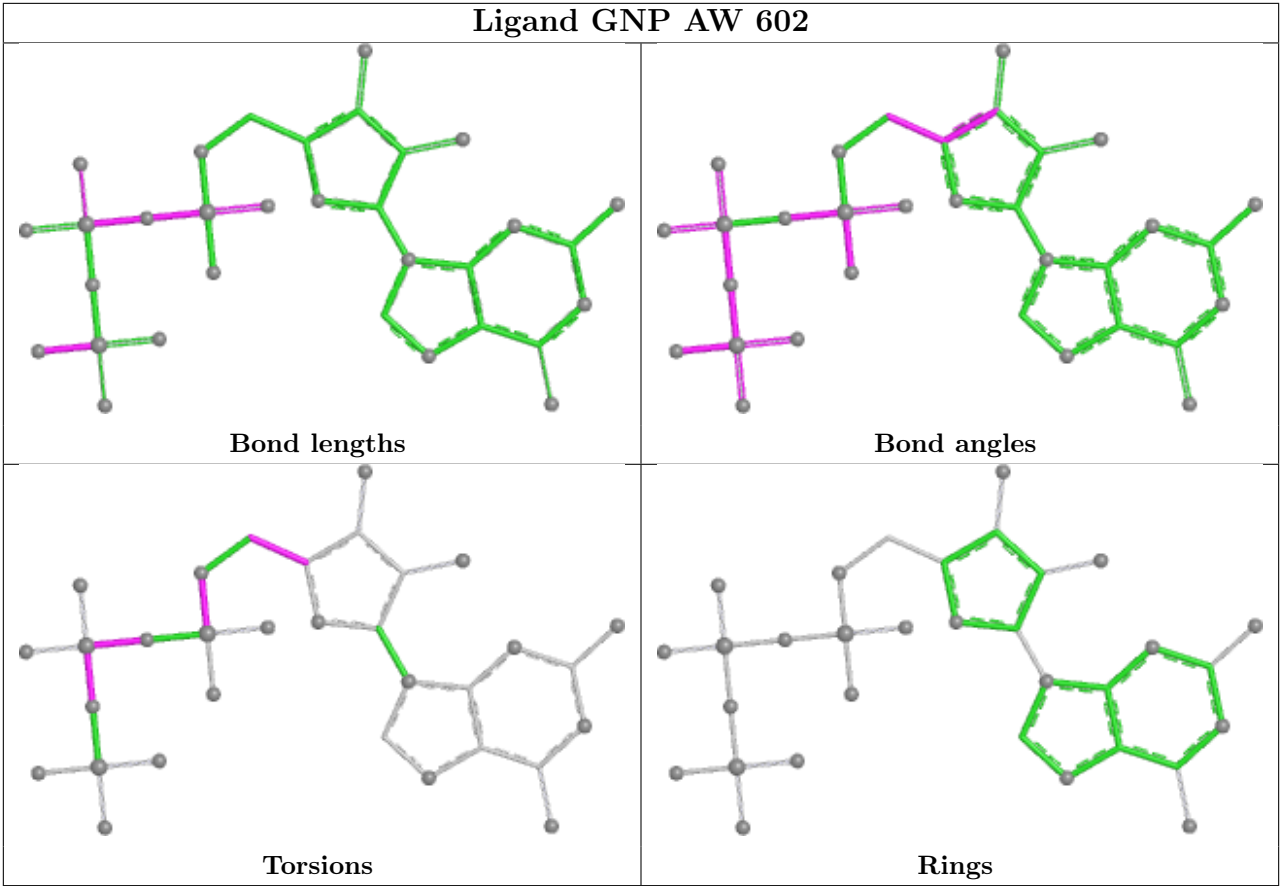
Mol	Chain	Res	Type	Atoms
58	AW	602	GNP	PG-N3B-PB-O1B
58	AW	602	GNP	PG-N3B-PB-O3A
58	AW	602	GNP	PA-O3A-PB-O2B
58	AW	602	GNP	C5'-O5'-PA-O3A
58	AW	602	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AW	602	GNP	6	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2106:U	O3'	2107:G	P	1.86
1	BA	2183:A	O3'	2184:A	P	1.80

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	1532/1533 (99%)	0.36	58 (3%) 44 27	51, 102, 197, 245	0
2	AB	218/241 (90%)	0.88	23 (10%) 11 8	91, 120, 142, 158	0
3	AC	206/233 (88%)	0.61	14 (6%) 23 15	75, 114, 132, 139	0
4	AD	205/206 (99%)	1.12	34 (16%) 4 3	86, 110, 132, 147	0
5	AE	150/167 (89%)	0.74	12 (8%) 18 12	73, 94, 129, 143	0
6	AF	100/131 (76%)	0.62	6 (6%) 27 17	98, 122, 135, 145	0
7	AG	151/156 (96%)	1.30	30 (19%) 3 2	107, 144, 159, 163	0
8	AH	129/130 (99%)	0.65	10 (7%) 19 12	77, 97, 121, 139	0
9	AI	127/130 (97%)	0.97	11 (8%) 16 11	77, 122, 148, 159	0
10	AJ	98/103 (95%)	1.32	17 (17%) 4 3	89, 106, 143, 156	0
11	AK	117/129 (90%)	0.85	9 (7%) 19 13	73, 105, 133, 150	0
12	AL	123/124 (99%)	0.58	8 (6%) 25 16	55, 74, 111, 142	0
13	AM	114/118 (96%)	1.67	43 (37%) 1 1	137, 149, 163, 165	0
14	AN	96/101 (95%)	1.69	36 (37%) 1 1	79, 128, 152, 160	0
15	AO	88/89 (98%)	0.49	3 (3%) 48 30	79, 101, 131, 142	0
16	AP	82/82 (100%)	0.78	6 (7%) 21 13	72, 95, 131, 147	0
17	AQ	80/84 (95%)	1.21	8 (10%) 12 8	78, 111, 136, 147	0
18	AR	55/75 (73%)	0.99	8 (14%) 6 5	77, 100, 126, 165	0
19	AS	79/92 (85%)	1.57	22 (27%) 1 1	131, 153, 159, 164	0
20	AT	85/87 (97%)	1.12	14 (16%) 4 3	80, 105, 126, 142	0
21	AU	51/71 (71%)	1.60	17 (33%) 1 1	106, 132, 153, 157	0
22	AV	6/27 (22%)	2.34	3 (50%) 0 1	181, 198, 202, 206	0
23	AW	525/529 (99%)	0.94	78 (14%) 5 4	47, 99, 188, 267	0
24	AY	2/6 (33%)	1.41	0 100 100	85, 85, 85, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	79/85 (92%)	1.38	21 (26%) 1 1	62, 87, 115, 129	0
26	B1	77/78 (98%)	0.37	2 (2%) 57 37	55, 71, 124, 126	0
27	B2	63/63 (100%)	0.69	6 (9%) 14 9	69, 101, 126, 140	0
28	B3	58/59 (98%)	0.28	0 100 100	63, 75, 121, 129	0
29	B4	56/57 (98%)	0.26	5 (8%) 15 10	42, 63, 97, 125	0
30	B5	50/55 (90%)	1.21	6 (12%) 9 6	114, 128, 137, 151	0
31	B6	46/46 (100%)	0.28	3 (6%) 25 16	43, 56, 77, 114	0
32	B7	64/65 (98%)	0.36	1 (1%) 70 51	57, 68, 83, 90	0
33	B8	38/38 (100%)	0.69	1 (2%) 57 37	61, 78, 90, 105	0
34	BA	2853/2903 (98%)	-0.22	46 (1%) 70 51	35, 67, 195, 445	0
35	BB	118/118 (100%)	0.10	0 100 100	61, 106, 152, 188	0
36	BC	271/273 (99%)	0.25	12 (4%) 39 24	36, 66, 83, 108	0
37	BD	209/209 (100%)	0.05	6 (2%) 53 35	37, 57, 89, 99	0
38	BE	201/201 (100%)	0.28	8 (3%) 42 26	37, 76, 109, 131	0
39	BF	177/179 (98%)	0.94	13 (7%) 21 13	106, 128, 152, 165	0
40	BG	176/177 (99%)	0.42	9 (5%) 33 21	54, 80, 116, 131	0
41	BH	163/165 (98%)	1.94	60 (36%) 1 1	55, 145, 163, 185	1 (0%)
42	BI	141/142 (99%)	1.82	54 (38%) 1 1	135, 157, 169, 176	0
43	BJ	30/121 (24%)	1.27	6 (20%) 3 2	126, 137, 143, 145	0
43	BK	30/121 (24%)	1.38	6 (20%) 3 2	133, 146, 152, 156	0
43	BL	30/121 (24%)	2.16	14 (46%) 0 1	132, 148, 158, 163	0
43	BM	30/121 (24%)	1.20	5 (16%) 4 3	128, 142, 149, 151	0
44	BN	142/142 (100%)	0.29	10 (7%) 22 14	45, 65, 91, 117	0
45	BO	122/123 (99%)	0.18	4 (3%) 49 30	41, 61, 84, 104	0
46	BP	143/144 (99%)	0.58	6 (4%) 40 25	41, 84, 112, 132	0
47	BQ	136/136 (100%)	0.11	2 (1%) 72 52	47, 70, 100, 126	0
48	BR	120/127 (94%)	-0.09	1 (0%) 82 67	40, 56, 72, 138	0
49	BS	116/117 (99%)	0.68	7 (6%) 27 17	81, 100, 121, 128	0
50	BT	114/115 (99%)	0.27	3 (2%) 57 37	48, 71, 112, 121	0
51	BU	117/118 (99%)	0.16	4 (3%) 48 30	37, 59, 94, 108	0
52	BV	103/103 (100%)	0.43	3 (2%) 53 35	43, 86, 111, 119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
53	BW	110/116 (94%)	-0.11	1 (0%) 81 64	41, 54, 82, 127	0
54	BX	93/100 (93%)	0.55	7 (7%) 20 13	50, 81, 134, 144	0
55	BY	102/104 (98%)	0.66	7 (6%) 23 14	63, 84, 126, 141	0
56	BZ	94/94 (100%)	0.31	3 (3%) 50 31	68, 94, 113, 126	0
All	All	10891/11580 (94%)	0.43	812 (7%) 20 13	35, 89, 165, 445	1 (0%)

The worst 5 of 812 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BL	22	LEU	9.7
11	AK	125	LYS	9.6
23	AW	424	ALA	7.3
4	AD	24	VAL	6.9
2	AB	150	ILE	6.8

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	UAL	AY	5	9/10	0.66	0.16	81,82,83,84	0
24	KBE	AY	1	9/10	0.69	0.25	78,79,82,82	0
24	5OH	AY	6	12/13	0.75	0.20	84,89,92,94	0
24	DPP	AY	2	6/7	0.85	0.18	79,82,82,84	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
57	MG	BA	3350	1/1	0.59	0.22	80,80,80,80	0
57	MG	BA	3242	1/1	0.60	0.18	72,72,72,72	0
57	MG	BA	3141	1/1	0.61	0.25	54,54,54,54	0
57	MG	BA	3281	1/1	0.63	0.23	73,73,73,73	0
57	MG	BA	3349	1/1	0.66	0.40	79,79,79,79	0
57	MG	BA	3317	1/1	0.66	0.34	88,88,88,88	0
57	MG	BA	3306	1/1	0.67	0.19	67,67,67,67	0
57	MG	BA	3330	1/1	0.70	0.17	83,83,83,83	0
57	MG	BA	3333	1/1	0.70	0.29	77,77,77,77	0
57	MG	AA	1680	1/1	0.71	0.20	55,55,55,55	0
57	MG	AA	1687	1/1	0.72	0.20	81,81,81,81	0
57	MG	BA	3346	1/1	0.72	0.27	83,83,83,83	0
57	MG	AA	1701	1/1	0.73	0.18	79,79,79,79	0
57	MG	BA	3343	1/1	0.74	0.16	71,71,71,71	0
57	MG	BA	3357	1/1	0.74	0.19	81,81,81,81	0
57	MG	BA	3305	1/1	0.76	0.23	71,71,71,71	0
57	MG	B0	103	1/1	0.77	0.13	54,54,54,54	0
57	MG	BA	3065	1/1	0.77	0.28	46,46,46,46	0
57	MG	AA	1700	1/1	0.77	0.29	65,65,65,65	0
57	MG	BA	3214	1/1	0.77	0.13	43,43,43,43	0
57	MG	AA	1686	1/1	0.78	0.17	93,93,93,93	0
57	MG	BA	3284	1/1	0.78	0.21	73,73,73,73	0
57	MG	BA	3298	1/1	0.78	0.22	76,76,76,76	0
57	MG	BA	3205	1/1	0.78	0.15	50,50,50,50	0
57	MG	BA	3355	1/1	0.78	0.21	69,69,69,69	0
57	MG	BA	3334	1/1	0.78	0.15	56,56,56,56	0
57	MG	BA	3311	1/1	0.79	0.14	48,48,48,48	0
57	MG	BA	3312	1/1	0.79	0.14	56,56,56,56	0
57	MG	AA	1679	1/1	0.79	0.22	62,62,62,62	0
57	MG	AA	1659	1/1	0.79	0.08	55,55,55,55	0
57	MG	BA	3352	1/1	0.79	0.16	61,61,61,61	0
57	MG	BA	3270	1/1	0.79	0.24	59,59,59,59	0
57	MG	AA	1696	1/1	0.79	0.20	89,89,89,89	0
57	MG	AA	1621	1/1	0.80	0.25	57,57,57,57	0
57	MG	BA	3104	1/1	0.80	0.18	45,45,45,45	0
57	MG	AW	601	1/1	0.80	0.10	36,36,36,36	0
57	MG	AA	1662	1/1	0.80	0.24	57,57,57,57	0
57	MG	BA	3348	1/1	0.80	0.09	67,67,67,67	0
57	MG	BB	203	1/1	0.80	0.10	51,51,51,51	0
57	MG	BA	3152	1/1	0.81	0.09	41,41,41,41	0
57	MG	BA	3177	1/1	0.81	0.27	59,59,59,59	0
57	MG	AM	201	1/1	0.81	0.10	80,80,80,80	0
57	MG	BA	3211	1/1	0.81	0.18	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1668	1/1	0.81	0.10	51,51,51,51	0
57	MG	AA	1633	1/1	0.81	0.24	53,53,53,53	0
57	MG	BA	3243	1/1	0.81	0.16	62,62,62,62	0
57	MG	BO	201	1/1	0.81	0.14	41,41,41,41	0
57	MG	BA	3244	1/1	0.82	0.26	76,76,76,76	0
57	MG	BA	3262	1/1	0.82	0.47	85,85,85,85	0
57	MG	BA	3075	1/1	0.82	0.09	43,43,43,43	0
57	MG	AA	1649	1/1	0.82	0.25	49,49,49,49	0
57	MG	AA	1689	1/1	0.82	0.37	69,69,69,69	0
57	MG	BA	3216	1/1	0.82	0.22	63,63,63,63	0
57	MG	BA	3001	1/1	0.82	0.33	42,42,42,42	0
57	MG	BB	205	1/1	0.82	0.33	79,79,79,79	0
57	MG	BD	303	1/1	0.82	0.07	57,57,57,57	0
57	MG	AA	1651	1/1	0.82	0.12	51,51,51,51	0
57	MG	BA	3184	1/1	0.83	0.09	37,37,37,37	0
57	MG	BA	3299	1/1	0.83	0.19	64,64,64,64	0
57	MG	BA	3105	1/1	0.83	0.25	49,49,49,49	0
57	MG	BA	3335	1/1	0.83	0.13	58,58,58,58	0
57	MG	AA	1667	1/1	0.83	0.11	87,87,87,87	0
57	MG	AA	1646	1/1	0.83	0.16	50,50,50,50	0
57	MG	BA	3174	1/1	0.83	0.14	49,49,49,49	0
57	MG	AA	1669	1/1	0.83	0.07	71,71,71,71	0
57	MG	BA	3148	1/1	0.84	0.16	50,50,50,50	0
57	MG	AA	1672	1/1	0.84	0.07	52,52,52,52	0
57	MG	BA	3160	1/1	0.84	0.19	49,49,49,49	0
57	MG	BA	3170	1/1	0.84	0.15	52,52,52,52	0
57	MG	BA	3172	1/1	0.84	0.14	53,53,53,53	0
57	MG	AA	1638	1/1	0.84	0.11	55,55,55,55	0
57	MG	AA	1639	1/1	0.84	0.13	49,49,49,49	0
57	MG	BA	3287	1/1	0.84	0.14	83,83,83,83	0
57	MG	AA	1645	1/1	0.84	0.16	62,62,62,62	0
57	MG	BA	3197	1/1	0.84	0.08	38,38,38,38	0
57	MG	AA	1656	1/1	0.84	0.21	73,73,73,73	0
57	MG	BA	3117	1/1	0.84	0.19	46,46,46,46	0
57	MG	BA	3125	1/1	0.84	0.31	53,53,53,53	0
57	MG	AA	1657	1/1	0.84	0.10	83,83,83,83	0
57	MG	BA	3316	1/1	0.84	0.17	61,61,61,61	0
57	MG	BA	3232	1/1	0.84	0.19	54,54,54,54	0
57	MG	AA	1694	1/1	0.85	0.13	75,75,75,75	0
57	MG	AA	1658	1/1	0.85	0.26	61,61,61,61	0
57	MG	BA	3321	1/1	0.85	0.13	73,73,73,73	0
57	MG	AA	1683	1/1	0.85	0.08	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3354	1/1	0.85	0.08	62,62,62,62	0
57	MG	BA	3332	1/1	0.85	0.15	96,96,96,96	0
57	MG	AA	1647	1/1	0.85	0.13	60,60,60,60	0
57	MG	BA	3261	1/1	0.85	0.17	63,63,63,63	0
57	MG	AA	1635	1/1	0.85	0.19	58,58,58,58	0
57	MG	AA	1688	1/1	0.85	0.15	77,77,77,77	0
57	MG	BE	301	1/1	0.85	0.12	67,67,67,67	0
57	MG	AA	1650	1/1	0.85	0.19	67,67,67,67	0
57	MG	AA	1603	1/1	0.86	0.34	42,42,42,42	0
57	MG	BA	3136	1/1	0.86	0.28	53,53,53,53	0
57	MG	BA	3223	1/1	0.86	0.39	75,75,75,75	0
57	MG	BA	3225	1/1	0.86	0.29	60,60,60,60	0
57	MG	AA	1671	1/1	0.86	0.12	53,53,53,53	0
57	MG	BA	3303	1/1	0.86	0.08	56,56,56,56	0
57	MG	AA	1685	1/1	0.86	0.08	64,64,64,64	0
57	MG	BA	3016	1/1	0.86	0.30	39,39,39,39	0
57	MG	BA	3157	1/1	0.86	0.26	46,46,46,46	0
57	MG	BA	3247	1/1	0.86	0.19	61,61,61,61	0
57	MG	BA	3313	1/1	0.86	0.22	67,67,67,67	0
57	MG	BA	3356	1/1	0.86	0.16	61,61,61,61	0
57	MG	BA	3253	1/1	0.86	0.17	65,65,65,65	0
57	MG	BA	3255	1/1	0.86	0.09	66,66,66,66	0
57	MG	BA	3201	1/1	0.86	0.19	47,47,47,47	0
57	MG	BB	208	1/1	0.86	0.11	59,59,59,59	0
57	MG	BC	301	1/1	0.86	0.14	53,53,53,53	0
57	MG	BA	3032	1/1	0.86	0.31	38,38,38,38	0
57	MG	BA	3331	1/1	0.86	0.15	64,64,64,64	0
57	MG	BA	3169	1/1	0.86	0.16	39,39,39,39	0
57	MG	BA	3215	1/1	0.87	0.09	53,53,53,53	0
57	MG	AA	1675	1/1	0.87	0.11	57,57,57,57	0
57	MG	BA	3219	1/1	0.87	0.28	69,69,69,69	0
57	MG	BA	3294	1/1	0.87	0.11	43,43,43,43	0
57	MG	BA	3295	1/1	0.87	0.18	57,57,57,57	0
57	MG	BA	3296	1/1	0.87	0.16	60,60,60,60	0
57	MG	AA	1677	1/1	0.87	0.16	57,57,57,57	0
57	MG	AA	1648	1/1	0.87	0.06	54,54,54,54	0
57	MG	BA	3227	1/1	0.87	0.17	63,63,63,63	0
57	MG	BA	3231	1/1	0.87	0.14	56,56,56,56	0
57	MG	AA	1632	1/1	0.87	0.20	40,40,40,40	0
57	MG	AA	1610	1/1	0.87	0.17	45,45,45,45	0
57	MG	AA	1634	1/1	0.87	0.18	55,55,55,55	0
57	MG	BA	3144	1/1	0.87	0.12	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3198	1/1	0.87	0.16	60,60,60,60	0
57	MG	BA	3048	1/1	0.87	0.27	40,40,40,40	0
57	MG	AA	1652	1/1	0.87	0.17	60,60,60,60	0
57	MG	BA	3207	1/1	0.87	0.29	54,54,54,54	0
57	MG	AF	201	1/1	0.87	0.17	65,65,65,65	0
57	MG	BA	3096	1/1	0.87	0.17	44,44,44,44	0
57	MG	AA	1606	1/1	0.88	0.25	45,45,45,45	0
57	MG	AA	1673	1/1	0.88	0.16	84,84,84,84	0
57	MG	BA	3288	1/1	0.88	0.15	95,95,95,95	0
57	MG	BA	3353	1/1	0.88	0.26	73,73,73,73	0
57	MG	AA	1674	1/1	0.88	0.15	55,55,55,55	0
57	MG	AA	1666	1/1	0.88	0.16	62,62,62,62	0
57	MG	AA	1670	1/1	0.88	0.12	62,62,62,62	0
57	MG	BA	3154	1/1	0.88	0.35	43,43,43,43	0
57	MG	AA	1636	1/1	0.88	0.08	36,36,36,36	0
57	MG	AL	201	1/1	0.88	0.26	54,54,54,54	0
57	MG	BA	3161	1/1	0.88	0.12	42,42,42,42	0
57	MG	BA	3268	1/1	0.88	0.08	52,52,52,52	0
57	MG	BA	3345	1/1	0.88	0.23	67,67,67,67	0
57	MG	BA	3202	1/1	0.88	0.18	57,57,57,57	0
57	MG	BA	3204	1/1	0.88	0.20	72,72,72,72	0
57	MG	BA	3109	1/1	0.89	0.15	38,38,38,38	0
57	MG	BA	3115	1/1	0.89	0.15	37,37,37,37	0
57	MG	BA	3274	1/1	0.89	0.24	52,52,52,52	0
57	MG	AA	1699	1/1	0.89	0.36	49,49,49,49	0
57	MG	BA	3124	1/1	0.89	0.23	42,42,42,42	0
57	MG	BA	3222	1/1	0.89	0.09	50,50,50,50	0
57	MG	BA	3338	1/1	0.89	0.08	61,61,61,61	0
57	MG	BA	3037	1/1	0.89	0.24	36,36,36,36	0
57	MG	BA	3131	1/1	0.89	0.14	40,40,40,40	0
57	MG	BA	3179	1/1	0.89	0.16	46,46,46,46	0
57	MG	BA	3347	1/1	0.89	0.15	76,76,76,76	0
57	MG	BA	3134	1/1	0.89	0.24	49,49,49,49	0
57	MG	BA	3187	1/1	0.89	0.23	56,56,56,56	0
57	MG	BA	3235	1/1	0.89	0.14	64,64,64,64	0
57	MG	BA	3301	1/1	0.89	0.27	64,64,64,64	0
57	MG	AA	1625	1/1	0.89	0.09	40,40,40,40	0
57	MG	BA	3304	1/1	0.89	0.19	50,50,50,50	0
57	MG	B0	102	1/1	0.89	0.14	33,33,33,33	0
57	MG	AA	1613	1/1	0.89	0.24	58,58,58,58	0
57	MG	BA	3079	1/1	0.89	0.24	44,44,44,44	0
57	MG	BA	3248	1/1	0.89	0.21	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3095	1/1	0.89	0.21	42,42,42,42	0
57	MG	AA	1663	1/1	0.89	0.15	74,74,74,74	0
57	MG	AA	1654	1/1	0.89	0.22	58,58,58,58	0
57	MG	BD	302	1/1	0.89	0.27	53,53,53,53	0
57	MG	BA	3318	1/1	0.89	0.27	57,57,57,57	0
57	MG	BA	3023	1/1	0.89	0.29	39,39,39,39	0
57	MG	BA	3323	1/1	0.89	0.08	64,64,64,64	0
57	MG	BA	3237	1/1	0.90	0.10	51,51,51,51	0
57	MG	BA	3286	1/1	0.90	0.11	48,48,48,48	0
57	MG	BA	3238	1/1	0.90	0.12	50,50,50,50	0
57	MG	BA	3046	1/1	0.90	0.28	27,27,27,27	0
57	MG	BA	3351	1/1	0.90	0.16	58,58,58,58	0
57	MG	AA	1631	1/1	0.90	0.13	60,60,60,60	0
57	MG	BA	3322	1/1	0.90	0.12	62,62,62,62	0
57	MG	AA	1692	1/1	0.90	0.14	67,67,67,67	0
57	MG	BA	3327	1/1	0.90	0.11	64,64,64,64	0
57	MG	BA	3153	1/1	0.90	0.17	59,59,59,59	0
57	MG	AA	1608	1/1	0.90	0.21	59,59,59,59	0
57	MG	BB	201	1/1	0.90	0.27	54,54,54,54	0
57	MG	BA	3189	1/1	0.90	0.12	51,51,51,51	0
57	MG	AA	1624	1/1	0.90	0.20	51,51,51,51	0
57	MG	BA	3029	1/1	0.90	0.19	28,28,28,28	0
57	MG	BA	3030	1/1	0.90	0.24	38,38,38,38	0
57	MG	AA	1615	1/1	0.90	0.13	40,40,40,40	0
57	MG	BA	3203	1/1	0.90	0.17	50,50,50,50	0
57	MG	BA	3138	1/1	0.90	0.25	58,58,58,58	0
57	MG	AA	1682	1/1	0.90	0.05	76,76,76,76	0
58	GNP	AW	602	32/32	0.90	0.10	58,71,81,83	0
57	MG	BA	3256	1/1	0.91	0.11	56,56,56,56	0
57	MG	BA	3258	1/1	0.91	0.09	50,50,50,50	0
57	MG	BA	3064	1/1	0.91	0.14	24,24,24,24	0
57	MG	BA	3326	1/1	0.91	0.09	42,42,42,42	0
57	MG	AA	1641	1/1	0.91	0.09	67,67,67,67	0
57	MG	BA	3264	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3068	1/1	0.91	0.25	28,28,28,28	0
57	MG	BA	3070	1/1	0.91	0.16	44,44,44,44	0
57	MG	AA	1678	1/1	0.91	0.17	65,65,65,65	0
57	MG	BA	3276	1/1	0.91	0.24	58,58,58,58	0
57	MG	BA	3279	1/1	0.91	0.13	50,50,50,50	0
57	MG	BA	3280	1/1	0.91	0.22	73,73,73,73	0
57	MG	BA	3339	1/1	0.91	0.17	76,76,76,76	0
57	MG	BA	3218	1/1	0.91	0.16	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3344	1/1	0.91	0.10	71,71,71,71	0
57	MG	BA	3076	1/1	0.91	0.19	36,36,36,36	0
57	MG	BA	3078	1/1	0.91	0.23	32,32,32,32	0
57	MG	BA	3039	1/1	0.91	0.23	31,31,31,31	0
57	MG	BA	3181	1/1	0.91	0.11	44,44,44,44	0
57	MG	BA	3291	1/1	0.91	0.20	58,58,58,58	0
57	MG	BA	3140	1/1	0.91	0.23	46,46,46,46	0
57	MG	BA	3186	1/1	0.91	0.12	47,47,47,47	0
57	MG	BA	3045	1/1	0.91	0.28	35,35,35,35	0
57	MG	BA	3297	1/1	0.91	0.11	49,49,49,49	0
57	MG	BA	3143	1/1	0.91	0.07	32,32,32,32	0
57	MG	BA	3195	1/1	0.91	0.06	47,47,47,47	0
57	MG	AA	1605	1/1	0.91	0.18	38,38,38,38	0
57	MG	BA	3145	1/1	0.91	0.24	55,55,55,55	0
57	MG	BA	3097	1/1	0.91	0.20	48,48,48,48	0
57	MG	BA	3102	1/1	0.91	0.20	36,36,36,36	0
57	MG	BA	3246	1/1	0.91	0.08	48,48,48,48	0
57	MG	BB	207	1/1	0.91	0.07	47,47,47,47	0
57	MG	BA	3307	1/1	0.91	0.07	52,52,52,52	0
57	MG	BA	3012	1/1	0.91	0.22	18,18,18,18	0
57	MG	BA	3051	1/1	0.91	0.15	33,33,33,33	0
57	MG	BA	3250	1/1	0.91	0.34	66,66,66,66	0
57	MG	BA	3061	1/1	0.91	0.28	48,48,48,48	0
57	MG	BA	3254	1/1	0.91	0.15	59,59,59,59	0
57	MG	BA	3206	1/1	0.91	0.09	52,52,52,52	0
57	MG	AA	1661	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3171	1/1	0.92	0.11	57,57,57,57	0
57	MG	BA	3251	1/1	0.92	0.15	49,49,49,49	0
57	MG	BA	3137	1/1	0.92	0.19	42,42,42,42	0
57	MG	BA	3098	1/1	0.92	0.12	47,47,47,47	0
57	MG	BA	3175	1/1	0.92	0.11	44,44,44,44	0
57	MG	BA	3066	1/1	0.92	0.24	41,41,41,41	0
57	MG	AA	1616	1/1	0.92	0.14	37,37,37,37	0
57	MG	B4	101	1/1	0.92	0.24	40,40,40,40	0
57	MG	BA	3107	1/1	0.92	0.16	36,36,36,36	0
57	MG	BA	3185	1/1	0.92	0.18	52,52,52,52	0
57	MG	BA	3308	1/1	0.92	0.12	82,82,82,82	0
57	MG	AA	1612	1/1	0.92	0.18	29,29,29,29	0
57	MG	BA	3112	1/1	0.92	0.08	41,41,41,41	0
57	MG	BA	3229	1/1	0.92	0.10	46,46,46,46	0
57	MG	BA	3314	1/1	0.92	0.13	56,56,56,56	0
57	MG	BA	3315	1/1	0.92	0.20	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3275	1/1	0.92	0.08	59,59,59,59	0
57	MG	AA	1665	1/1	0.92	0.17	56,56,56,56	0
57	MG	BA	3278	1/1	0.92	0.20	48,48,48,48	0
57	MG	BA	3319	1/1	0.92	0.12	68,68,68,68	0
57	MG	BA	3193	1/1	0.92	0.18	61,61,61,61	0
57	MG	AA	1627	1/1	0.92	0.16	40,40,40,40	0
57	MG	AL	202	1/1	0.92	0.24	73,73,73,73	0
57	MG	BA	3089	1/1	0.92	0.17	52,52,52,52	0
57	MG	BA	3158	1/1	0.92	0.13	35,35,35,35	0
57	MG	AA	1655	1/1	0.92	0.16	60,60,60,60	0
57	MG	BA	3132	1/1	0.92	0.25	52,52,52,52	0
57	MG	BA	3164	1/1	0.92	0.10	45,45,45,45	0
57	MG	BT	201	1/1	0.92	0.12	40,40,40,40	0
57	MG	AA	1660	1/1	0.92	0.09	46,46,46,46	0
57	MG	BA	3329	1/1	0.93	0.12	58,58,58,58	0
57	MG	AA	1629	1/1	0.93	0.17	41,41,41,41	0
57	MG	BA	3116	1/1	0.93	0.18	41,41,41,41	0
57	MG	BA	3044	1/1	0.93	0.26	37,37,37,37	0
57	MG	BA	3292	1/1	0.93	0.12	54,54,54,54	0
57	MG	BA	3077	1/1	0.93	0.18	41,41,41,41	0
57	MG	AA	1676	1/1	0.93	0.12	52,52,52,52	0
57	MG	BA	3336	1/1	0.93	0.07	86,86,86,86	0
57	MG	BA	3337	1/1	0.93	0.09	55,55,55,55	0
57	MG	BA	3129	1/1	0.93	0.14	43,43,43,43	0
57	MG	BA	3130	1/1	0.93	0.15	41,41,41,41	0
57	MG	BA	3210	1/1	0.93	0.23	73,73,73,73	0
57	MG	AA	1618	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3300	1/1	0.93	0.21	69,69,69,69	0
57	MG	AA	1637	1/1	0.93	0.07	54,54,54,54	0
57	MG	BA	3094	1/1	0.93	0.18	47,47,47,47	0
57	MG	BA	3257	1/1	0.93	0.07	48,48,48,48	0
57	MG	AA	1622	1/1	0.93	0.16	42,42,42,42	0
57	MG	BA	3260	1/1	0.93	0.17	50,50,50,50	0
57	MG	BA	3052	1/1	0.93	0.37	39,39,39,39	0
57	MG	BA	3027	1/1	0.93	0.29	40,40,40,40	0
57	MG	BA	3310	1/1	0.93	0.10	75,75,75,75	0
57	MG	AA	1623	1/1	0.93	0.10	42,42,42,42	0
57	MG	AA	1628	1/1	0.93	0.14	44,44,44,44	0
57	MG	BA	3269	1/1	0.93	0.11	51,51,51,51	0
57	MG	BA	3103	1/1	0.93	0.16	28,28,28,28	0
57	MG	AA	1643	1/1	0.93	0.14	56,56,56,56	0
57	MG	BA	3034	1/1	0.93	0.23	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3069	1/1	0.93	0.19	39,39,39,39	0
57	MG	BA	3150	1/1	0.93	0.16	53,53,53,53	0
57	MG	AA	1684	1/1	0.93	0.23	60,60,60,60	0
57	MG	BA	3111	1/1	0.93	0.12	29,29,29,29	0
57	MG	BD	301	1/1	0.93	0.11	49,49,49,49	0
57	MG	BA	3073	1/1	0.93	0.25	42,42,42,42	0
57	MG	BA	3239	1/1	0.93	0.07	71,71,71,71	0
57	MG	BA	3325	1/1	0.93	0.20	59,59,59,59	0
57	MG	BA	3285	1/1	0.93	0.25	75,75,75,75	0
57	MG	BQ	201	1/1	0.93	0.07	44,44,44,44	0
57	MG	BA	3199	1/1	0.93	0.18	42,42,42,42	0
57	MG	BX	201	1/1	0.93	0.07	47,47,47,47	0
57	MG	BA	3328	1/1	0.93	0.10	71,71,71,71	0
57	MG	AA	1630	1/1	0.94	0.24	48,48,48,48	0
57	MG	BA	3226	1/1	0.94	0.16	51,51,51,51	0
57	MG	BA	3062	1/1	0.94	0.13	42,42,42,42	0
57	MG	BA	3178	1/1	0.94	0.22	49,49,49,49	0
57	MG	AA	1619	1/1	0.94	0.11	40,40,40,40	0
57	MG	BA	3100	1/1	0.94	0.25	36,36,36,36	0
57	MG	BA	3233	1/1	0.94	0.13	46,46,46,46	0
57	MG	AA	1690	1/1	0.94	0.09	83,83,83,83	0
57	MG	BA	3036	1/1	0.94	0.16	43,43,43,43	0
57	MG	BA	3142	1/1	0.94	0.19	50,50,50,50	0
57	MG	AA	1702	1/1	0.94	0.18	58,58,58,58	0
57	MG	BA	3188	1/1	0.94	0.26	51,51,51,51	0
57	MG	BA	3038	1/1	0.94	0.10	21,21,21,21	0
57	MG	BA	3192	1/1	0.94	0.25	59,59,59,59	0
57	MG	BA	3245	1/1	0.94	0.11	46,46,46,46	0
57	MG	AA	1691	1/1	0.94	0.07	63,63,63,63	0
57	MG	BA	3015	1/1	0.94	0.27	38,38,38,38	0
57	MG	BA	3149	1/1	0.94	0.22	42,42,42,42	0
57	MG	BA	3302	1/1	0.94	0.17	68,68,68,68	0
57	MG	BA	3249	1/1	0.94	0.07	49,49,49,49	0
57	MG	BA	3110	1/1	0.94	0.10	38,38,38,38	0
57	MG	BA	3151	1/1	0.94	0.19	47,47,47,47	0
57	MG	AA	1617	1/1	0.94	0.13	47,47,47,47	0
57	MG	BA	3017	1/1	0.94	0.15	30,30,30,30	0
57	MG	AA	1693	1/1	0.94	0.12	56,56,56,56	0
57	MG	BA	3155	1/1	0.94	0.21	51,51,51,51	0
57	MG	BA	3156	1/1	0.94	0.12	41,41,41,41	0
57	MG	AA	1602	1/1	0.94	0.22	37,37,37,37	0
57	MG	AA	1644	1/1	0.94	0.05	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3208	1/1	0.94	0.16	62,62,62,62	0
57	MG	BB	206	1/1	0.94	0.08	65,65,65,65	0
57	MG	BA	3121	1/1	0.94	0.22	39,39,39,39	0
57	MG	BA	3122	1/1	0.94	0.11	38,38,38,38	0
57	MG	BB	209	1/1	0.94	0.25	36,36,36,36	0
57	MG	BA	3267	1/1	0.94	0.12	52,52,52,52	0
57	MG	BA	3081	1/1	0.94	0.20	35,35,35,35	0
57	MG	BA	3165	1/1	0.94	0.20	52,52,52,52	0
57	MG	BA	3087	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3272	1/1	0.94	0.12	55,55,55,55	0
57	MG	BN	201	1/1	0.94	0.15	51,51,51,51	0
57	MG	BA	3088	1/1	0.94	0.14	36,36,36,36	0
57	MG	BA	3324	1/1	0.94	0.11	59,59,59,59	0
57	MG	BA	3054	1/1	0.94	0.23	36,36,36,36	0
57	MG	BA	3056	1/1	0.94	0.15	26,26,26,26	0
57	MG	BA	3059	1/1	0.94	0.12	43,43,43,43	0
57	MG	BA	3176	1/1	0.95	0.13	50,50,50,50	0
57	MG	BA	3099	1/1	0.95	0.32	44,44,44,44	0
57	MG	BA	3022	1/1	0.95	0.14	28,28,28,28	0
57	MG	BA	3228	1/1	0.95	0.10	42,42,42,42	0
57	MG	AA	1695	1/1	0.95	0.08	62,62,62,62	0
57	MG	BA	3282	1/1	0.95	0.13	55,55,55,55	0
57	MG	BA	3180	1/1	0.95	0.04	45,45,45,45	0
57	MG	AA	1604	1/1	0.95	0.25	42,42,42,42	0
57	MG	BA	3047	1/1	0.95	0.22	51,51,51,51	0
57	MG	BA	3234	1/1	0.95	0.10	49,49,49,49	0
57	MG	BA	3074	1/1	0.95	0.15	44,44,44,44	0
57	MG	BA	3289	1/1	0.95	0.06	62,62,62,62	0
57	MG	BA	3106	1/1	0.95	0.18	37,37,37,37	0
57	MG	BA	3340	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3028	1/1	0.95	0.19	26,26,26,26	0
57	MG	BA	3108	1/1	0.95	0.18	42,42,42,42	0
57	MG	BA	3240	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3146	1/1	0.95	0.20	40,40,40,40	0
57	MG	BA	3147	1/1	0.95	0.13	46,46,46,46	0
57	MG	AA	1681	1/1	0.95	0.05	38,38,38,38	0
57	MG	BA	3194	1/1	0.95	0.11	49,49,49,49	0
57	MG	BA	3010	1/1	0.95	0.12	33,33,33,33	0
57	MG	BA	3196	1/1	0.95	0.23	46,46,46,46	0
57	MG	BA	3053	1/1	0.95	0.28	31,31,31,31	0
57	MG	AA	1601	1/1	0.95	0.15	22,22,22,22	0
57	MG	BA	3014	1/1	0.95	0.19	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3058	1/1	0.95	0.22	35,35,35,35	0
57	MG	AA	1620	1/1	0.95	0.14	52,52,52,52	0
57	MG	BA	3118	1/1	0.95	0.20	40,40,40,40	0
57	MG	BA	3120	1/1	0.95	0.05	31,31,31,31	0
57	MG	BB	202	1/1	0.95	0.20	43,43,43,43	0
57	MG	B0	101	1/1	0.95	0.05	23,23,23,23	0
57	MG	BB	204	1/1	0.95	0.22	53,53,53,53	0
57	MG	BA	3090	1/1	0.95	0.20	40,40,40,40	0
57	MG	BA	3123	1/1	0.95	0.12	36,36,36,36	0
57	MG	BA	3259	1/1	0.95	0.06	69,69,69,69	0
57	MG	BA	3091	1/1	0.95	0.29	42,42,42,42	0
57	MG	BA	3209	1/1	0.95	0.13	42,42,42,42	0
57	MG	BA	3092	1/1	0.95	0.30	43,43,43,43	0
57	MG	BA	3263	1/1	0.95	0.17	53,53,53,53	0
57	MG	AA	1640	1/1	0.95	0.06	41,41,41,41	0
57	MG	BA	3166	1/1	0.95	0.06	50,50,50,50	0
57	MG	BA	3320	1/1	0.95	0.12	52,52,52,52	0
57	MG	BA	3063	1/1	0.95	0.16	32,32,32,32	0
57	MG	BA	3020	1/1	0.95	0.24	29,29,29,29	0
57	MG	BA	3041	1/1	0.95	0.10	27,27,27,27	0
57	MG	BR	202	1/1	0.95	0.10	51,51,51,51	0
57	MG	BA	3133	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3042	1/1	0.95	0.12	27,27,27,27	0
57	MG	BA	3135	1/1	0.95	0.14	45,45,45,45	0
57	MG	BA	3341	1/1	0.96	0.11	57,57,57,57	0
57	MG	BA	3342	1/1	0.96	0.09	54,54,54,54	0
57	MG	AA	1698	1/1	0.96	0.05	51,51,51,51	0
57	MG	BA	3080	1/1	0.96	0.25	43,43,43,43	0
57	MG	BA	3271	1/1	0.96	0.16	53,53,53,53	0
57	MG	BA	3183	1/1	0.96	0.05	48,48,48,48	0
57	MG	BA	3309	1/1	0.96	0.04	62,62,62,62	0
57	MG	BA	3273	1/1	0.96	0.13	72,72,72,72	0
57	MG	AA	1611	1/1	0.96	0.20	44,44,44,44	0
57	MG	BA	3139	1/1	0.96	0.15	43,43,43,43	0
57	MG	BA	3119	1/1	0.96	0.11	29,29,29,29	0
57	MG	BA	3277	1/1	0.96	0.08	42,42,42,42	0
57	MG	BA	3083	1/1	0.96	0.30	47,47,47,47	0
57	MG	BA	3212	1/1	0.96	0.24	45,45,45,45	0
57	MG	BA	3033	1/1	0.96	0.19	25,25,25,25	0
57	MG	AA	1614	1/1	0.96	0.18	42,42,42,42	0
57	MG	BA	3190	1/1	0.96	0.14	43,43,43,43	0
57	MG	BA	3283	1/1	0.96	0.20	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3217	1/1	0.96	0.12	56,56,56,56	0
57	MG	BA	3191	1/1	0.96	0.07	57,57,57,57	0
57	MG	BA	3071	1/1	0.96	0.24	35,35,35,35	0
57	MG	BA	3252	1/1	0.96	0.19	49,49,49,49	0
57	MG	BA	3220	1/1	0.96	0.16	56,56,56,56	0
57	MG	BA	3072	1/1	0.96	0.17	36,36,36,36	0
57	MG	BA	3290	1/1	0.96	0.05	56,56,56,56	0
57	MG	BA	3060	1/1	0.96	0.25	27,27,27,27	0
57	MG	BA	3224	1/1	0.96	0.10	41,41,41,41	0
57	MG	BA	3128	1/1	0.96	0.10	33,33,33,33	0
57	MG	BA	3024	1/1	0.96	0.25	32,32,32,32	0
57	MG	BA	3173	1/1	0.96	0.06	36,36,36,36	0
57	MG	BD	304	1/1	0.96	0.20	28,28,28,28	0
57	MG	BA	3093	1/1	0.96	0.14	42,42,42,42	0
57	MG	BA	3026	1/1	0.96	0.14	24,24,24,24	0
57	MG	BA	3200	1/1	0.96	0.10	44,44,44,44	0
57	MG	B2	101	1/1	0.96	0.04	49,49,49,49	0
57	MG	AA	1653	1/1	0.96	0.12	41,41,41,41	0
57	MG	BA	3266	1/1	0.96	0.05	56,56,56,56	0
57	MG	BA	3114	1/1	0.96	0.15	32,32,32,32	0
57	MG	AA	1697	1/1	0.96	0.04	64,64,64,64	0
57	MG	BA	3002	1/1	0.97	0.13	13,13,13,13	0
57	MG	BA	3221	1/1	0.97	0.23	43,43,43,43	0
57	MG	BA	3004	1/1	0.97	0.18	21,21,21,21	0
57	MG	BA	3167	1/1	0.97	0.27	48,48,48,48	0
57	MG	BA	3168	1/1	0.97	0.03	32,32,32,32	0
57	MG	BA	3049	1/1	0.97	0.14	31,31,31,31	0
57	MG	BA	3050	1/1	0.97	0.20	33,33,33,33	0
57	MG	BA	3005	1/1	0.97	0.11	20,20,20,20	0
57	MG	BA	3019	1/1	0.97	0.15	15,15,15,15	0
57	MG	BA	3293	1/1	0.97	0.08	53,53,53,53	0
57	MG	BA	3035	1/1	0.97	0.19	26,26,26,26	0
57	MG	BA	3230	1/1	0.97	0.09	46,46,46,46	0
57	MG	BA	3006	1/1	0.97	0.18	22,22,22,22	0
57	MG	BA	3021	1/1	0.97	0.13	18,18,18,18	0
57	MG	BA	3007	1/1	0.97	0.18	17,17,17,17	0
57	MG	BA	3101	1/1	0.97	0.10	43,43,43,43	0
57	MG	BA	3008	1/1	0.97	0.14	22,22,22,22	0
57	MG	BA	3236	1/1	0.97	0.06	46,46,46,46	0
57	MG	BA	3040	1/1	0.97	0.24	43,43,43,43	0
57	MG	BA	3009	1/1	0.97	0.18	14,14,14,14	0
57	MG	AA	1609	1/1	0.97	0.27	40,40,40,40	0

Continued on next page...

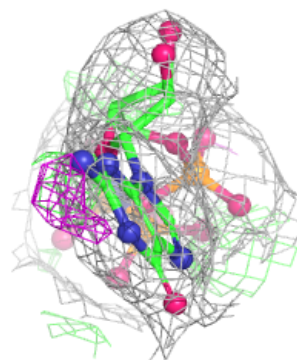
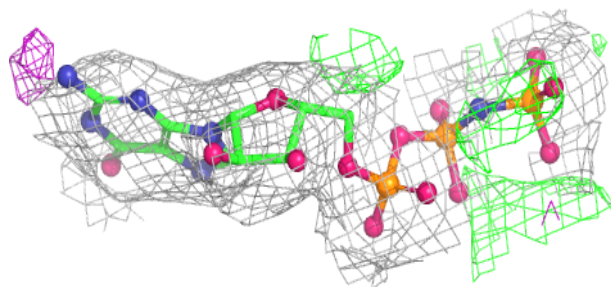
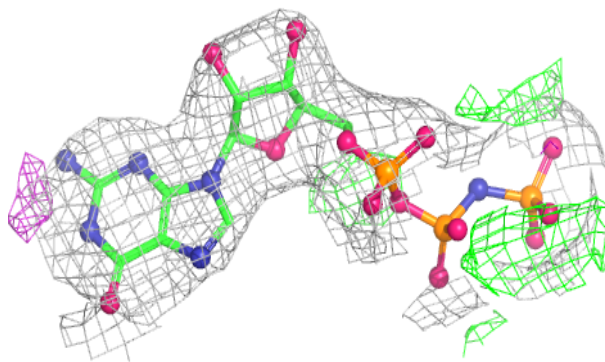
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3182	1/1	0.97	0.18	48,48,48,48	0
57	MG	BA	3043	1/1	0.97	0.23	26,26,26,26	0
57	MG	BA	3084	1/1	0.97	0.20	21,21,21,21	0
57	MG	BD	305	1/1	0.97	0.09	16,16,16,16	0
57	MG	BA	3086	1/1	0.97	0.23	43,43,43,43	0
57	MG	BA	3213	1/1	0.97	0.10	46,46,46,46	0
57	MG	BA	3011	1/1	0.97	0.30	23,23,23,23	0
57	MG	AH	201	1/1	0.97	0.11	50,50,50,50	0
57	MG	BR	201	1/1	0.97	0.12	69,69,69,69	0
57	MG	AA	1664	1/1	0.97	0.04	41,41,41,41	0
57	MG	BA	3067	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3162	1/1	0.97	0.07	56,56,56,56	0
57	MG	BA	3113	1/1	0.97	0.16	34,34,34,34	0
57	MG	BA	3013	1/1	0.98	0.18	20,20,20,20	0
57	MG	BA	3085	1/1	0.98	0.15	40,40,40,40	0
57	MG	BA	3265	1/1	0.98	0.21	45,45,45,45	0
57	MG	BA	3057	1/1	0.98	0.22	33,33,33,33	0
57	MG	BA	3159	1/1	0.98	0.17	49,49,49,49	0
57	MG	AA	1642	1/1	0.98	0.08	53,53,53,53	0
57	MG	AA	1626	1/1	0.98	0.23	45,45,45,45	0
57	MG	BA	3003	1/1	0.98	0.24	18,18,18,18	0
57	MG	BA	3163	1/1	0.98	0.14	49,49,49,49	0
57	MG	AA	1607	1/1	0.98	0.20	33,33,33,33	0
57	MG	BA	3018	1/1	0.98	0.16	16,16,16,16	0
57	MG	BA	3241	1/1	0.98	0.08	57,57,57,57	0
57	MG	BA	3025	1/1	0.98	0.17	32,32,32,32	0
57	MG	BA	3126	1/1	0.98	0.14	31,31,31,31	0
57	MG	BA	3127	1/1	0.98	0.14	38,38,38,38	0
57	MG	BA	3082	1/1	0.98	0.25	36,36,36,36	0
57	MG	BA	3055	1/1	0.98	0.18	24,24,24,24	0
57	MG	BA	3031	1/1	0.99	0.18	25,25,25,25	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 GNP AW 602:

$2mF_o-DF_c$ (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.