



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:26 pm BST

PDB ID : 4V85
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

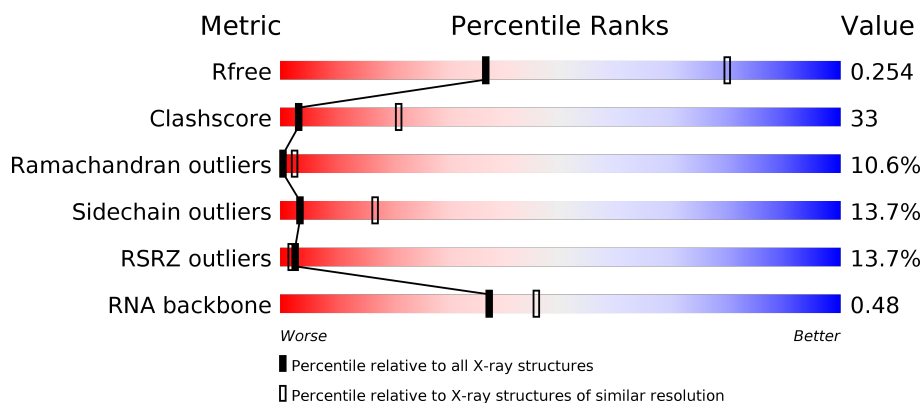
1 Overall quality at a glance ⓘ

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (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 on 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	<div> <div>8%</div> <div>28%</div> <div>56%</div> <div>16%</div> </div>
2	AB	241	<div> <div>27%</div> <div>25%</div> <div>45%</div> <div>17%</div> <div>10%</div> </div>
3	AC	233	<div> <div>9%</div> <div>30%</div> <div>44%</div> <div>13%</div> <div>12%</div> </div>
4	AD	206	<div> <div>29%</div> <div>27%</div> <div>57%</div> <div>15%</div> </div>

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	X
24	UAL	AY	5	-	-	X	-
24	5OH	AY	6	-	-	X	-
57	MG	AA	1658	-	-	-	X
57	MG	AA	1686	-	-	-	X
57	MG	AA	1687	-	-	-	X
57	MG	BA	3204	-	-	-	X
57	MG	BA	3216	-	-	-	X
57	MG	BA	3219	-	-	-	X
57	MG	BA	3233	-	-	-	X
57	MG	BA	3333	-	-	-	X
57	MG	BA	3345	-	-	-	X
57	MG	BA	3353	-	-	-	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	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	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 (three-letter code: MG) (formula: Mg).

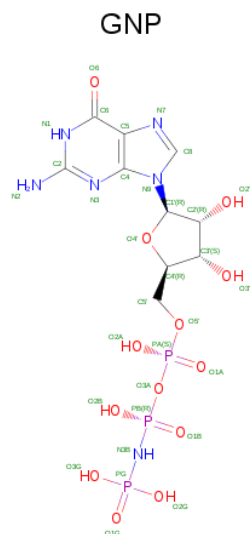
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BT	1	Total	Mg	0	0
			1	1		
57	BB	9	Total	Mg	0	0
			9	9		
57	BO	1	Total	Mg	0	0
			1	1		
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	357	Total	Mg	0	0
			357	357		
57	BN	1	Total	Mg	0	0
			1	1		
57	B2	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: 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		

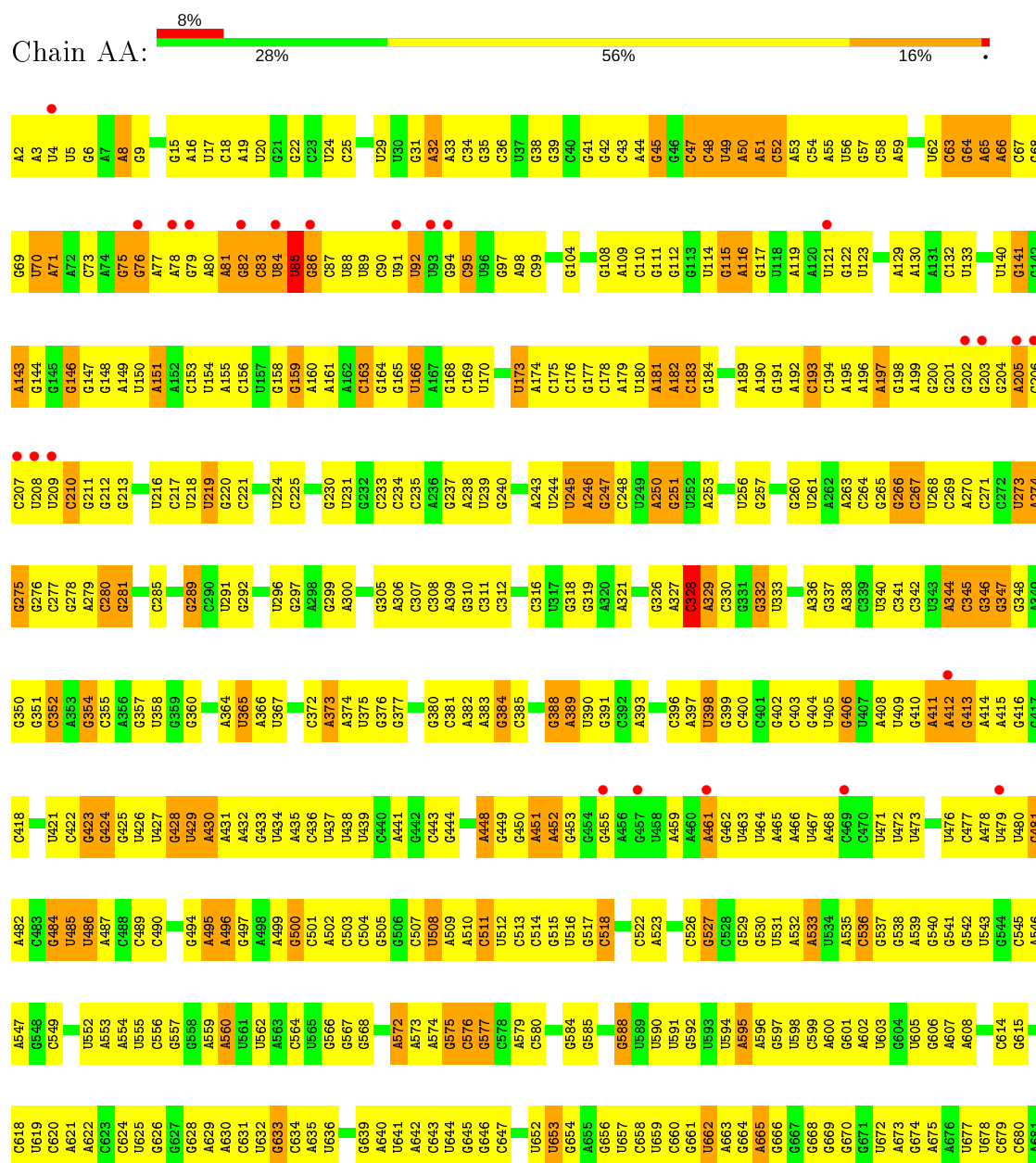
- Molecule 59 is water.

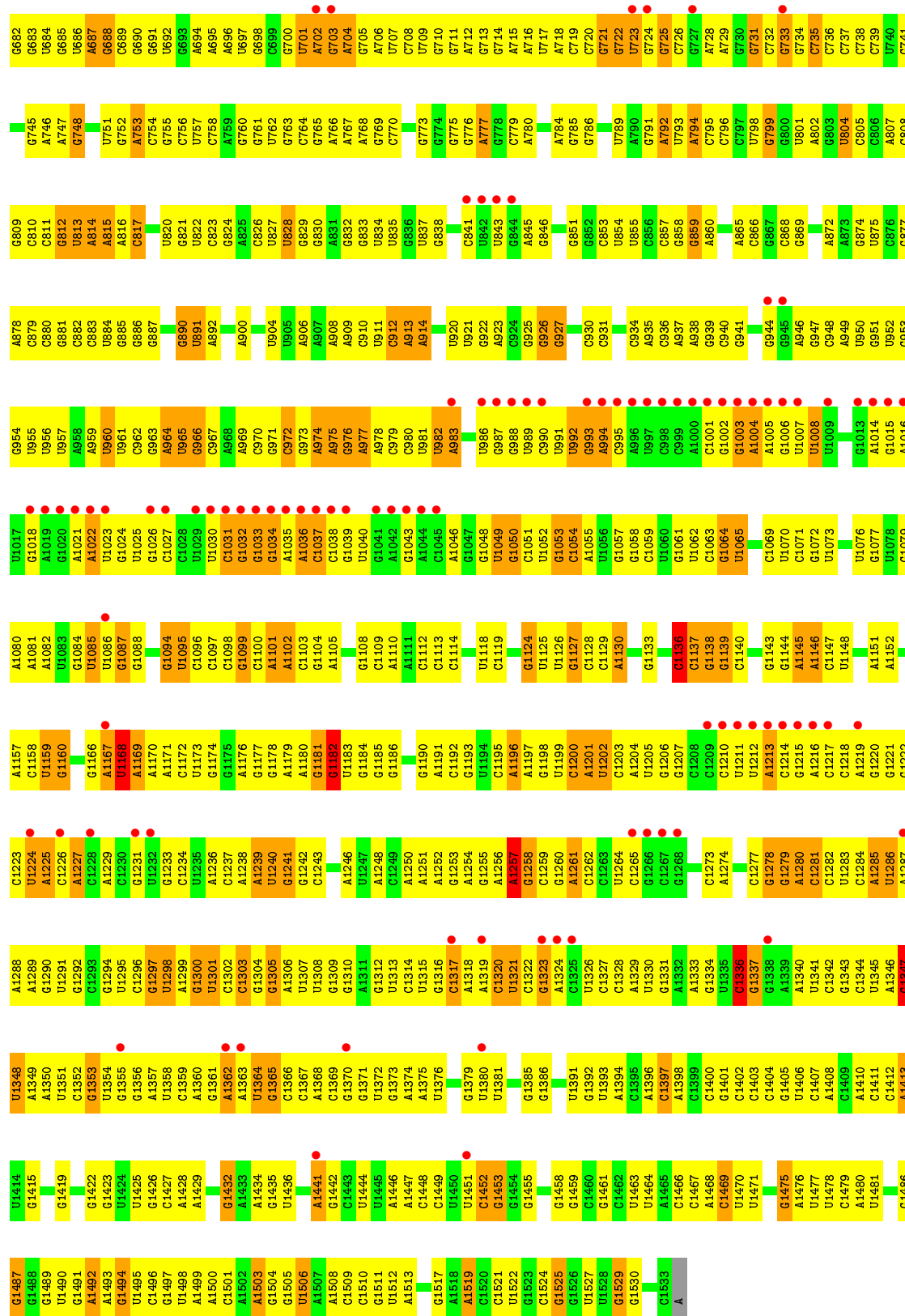
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AW	2	Total O 2 2	0	0
59	B8	1	Total O 1 1	0	0
59	BA	8	Total O 8 8	0	0
59	BC	2	Total O 2 2	0	0
59	BD	1	Total O 1 1	0	0
59	BF	1	Total O 1 1	0	0
59	BG	1	Total O 1 1	0	0
59	BW	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

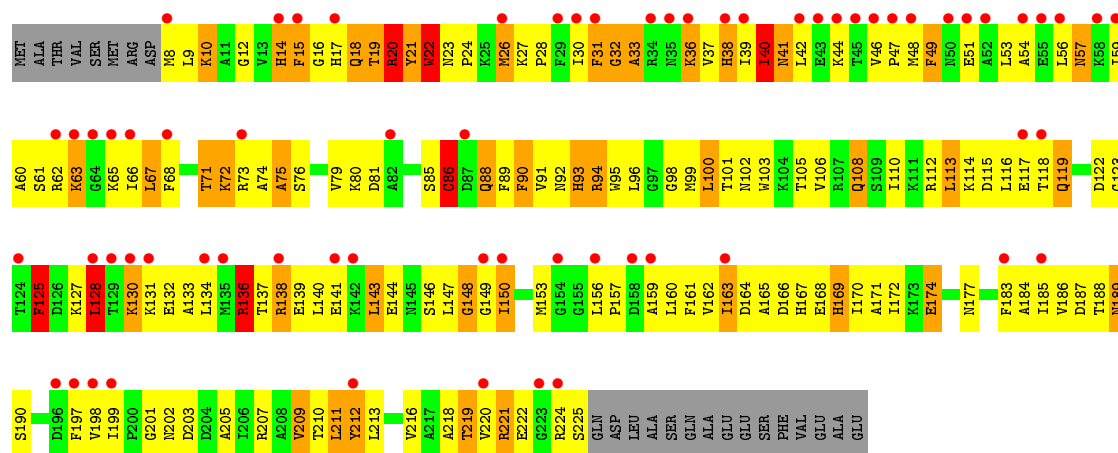
• Molecule 1: 16S rRNA



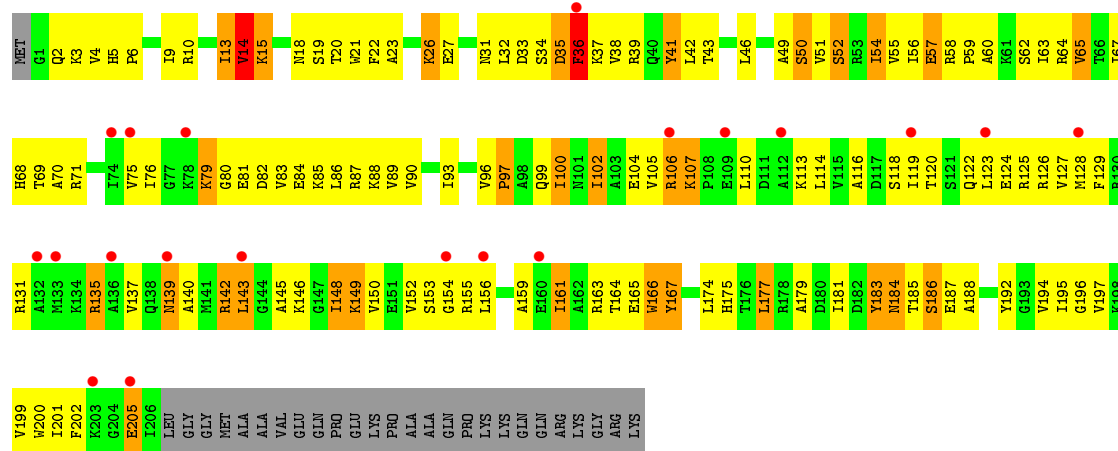


• Molecule 2: 30S ribosomal protein S2

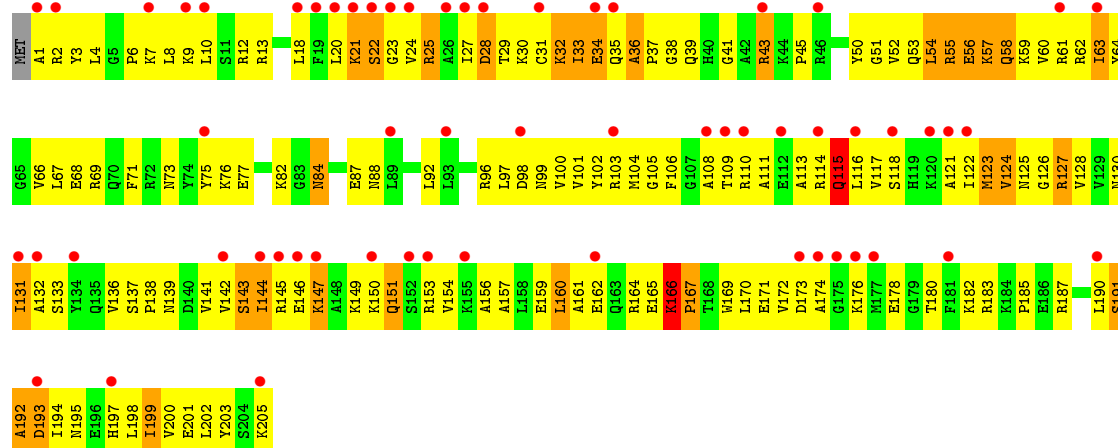




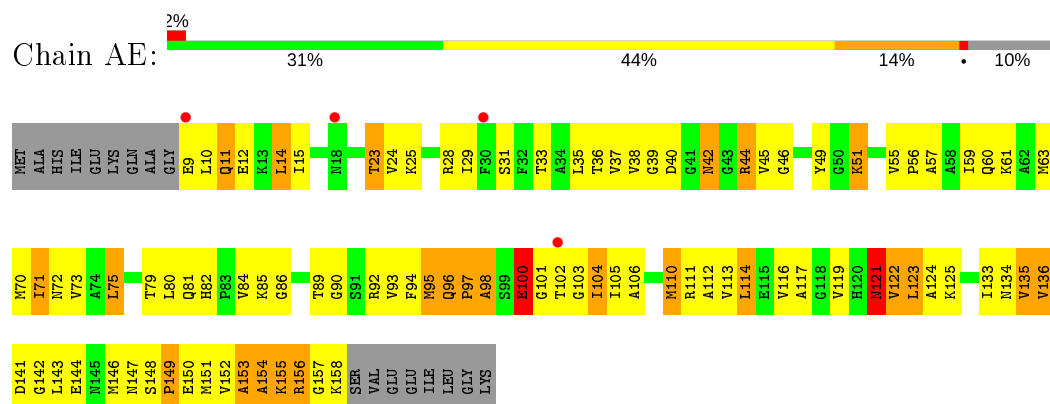
• Molecule 3: 30S ribosomal protein S3



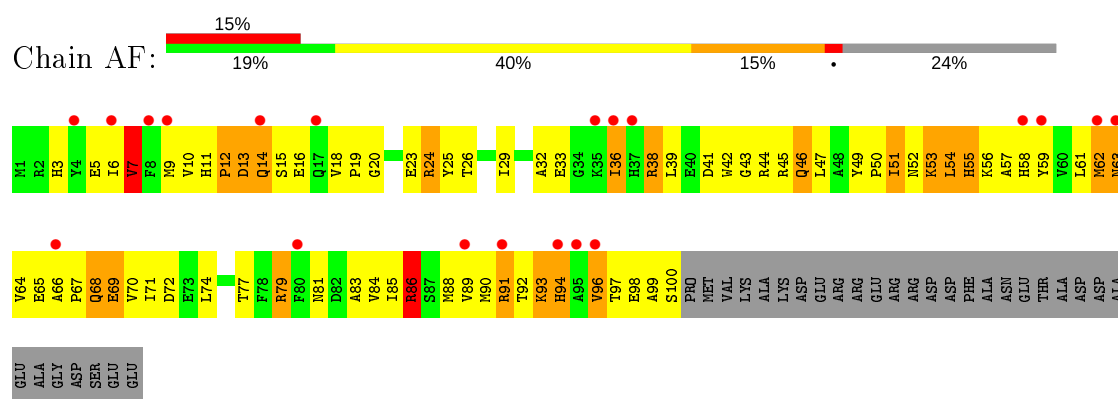
• Molecule 4: 30S ribosomal protein S4

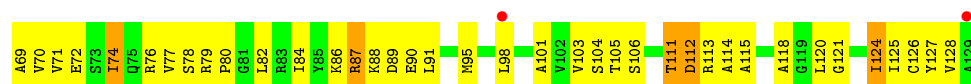


- Molecule 5: 30S ribosomal protein S5

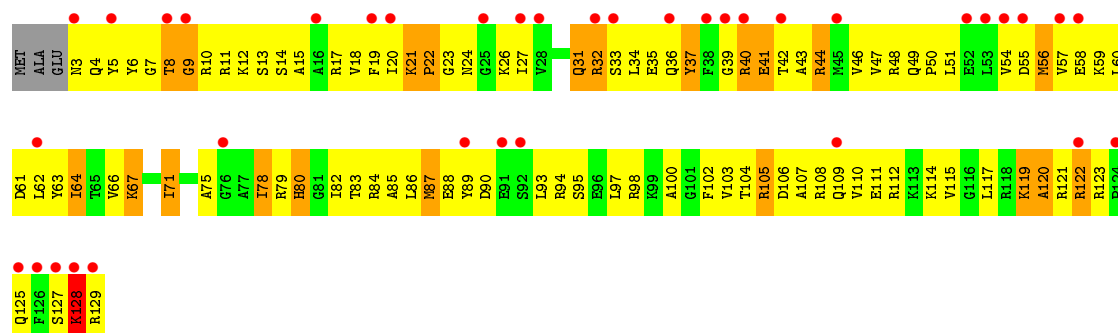


- Molecule 6: 30S ribosomal protein S6 1

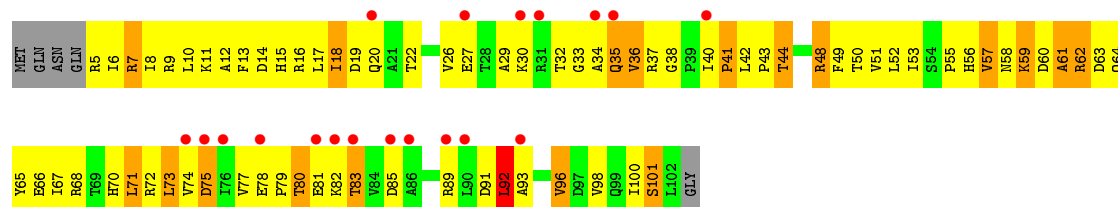




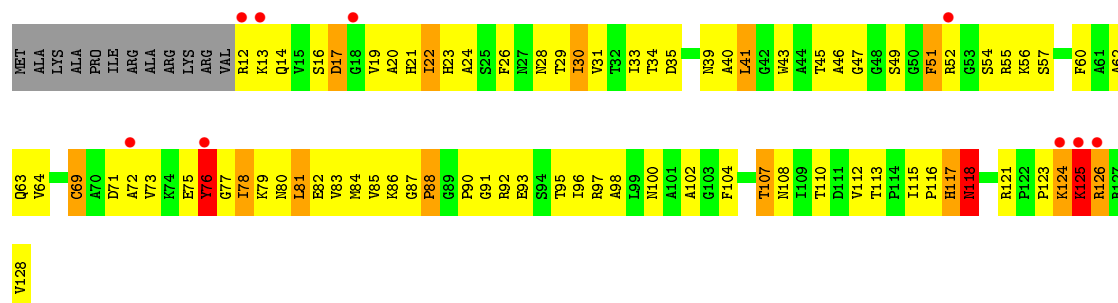
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

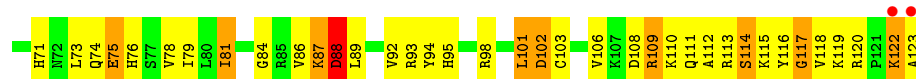


• Molecule 11: 30S ribosomal protein S11

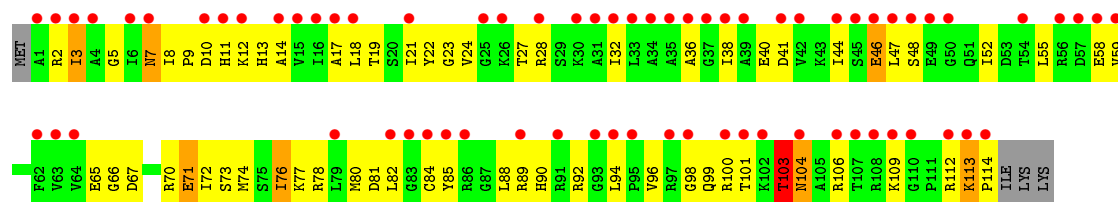


• Molecule 12: 30S ribosomal protein S12 1

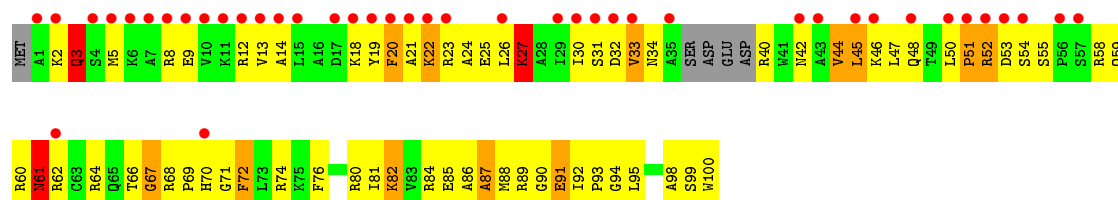




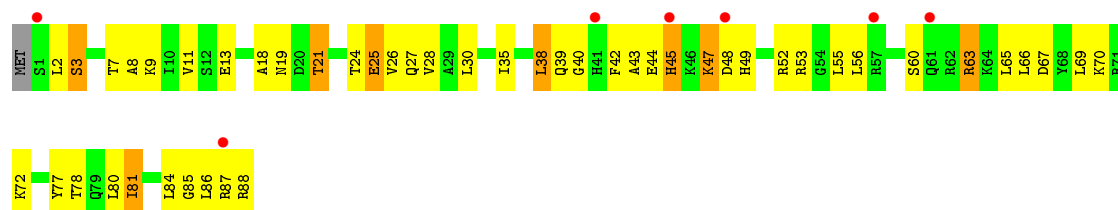
- Molecule 13: 30S ribosomal protein S13



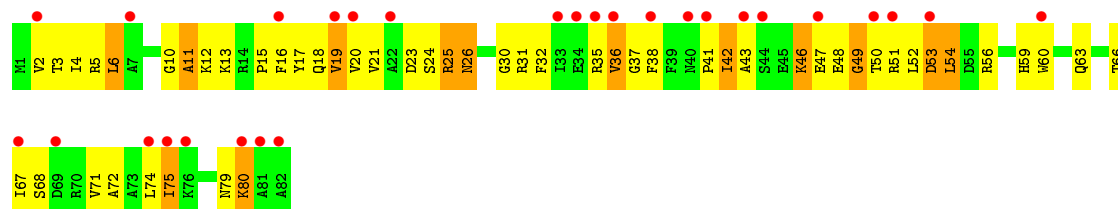
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15 1

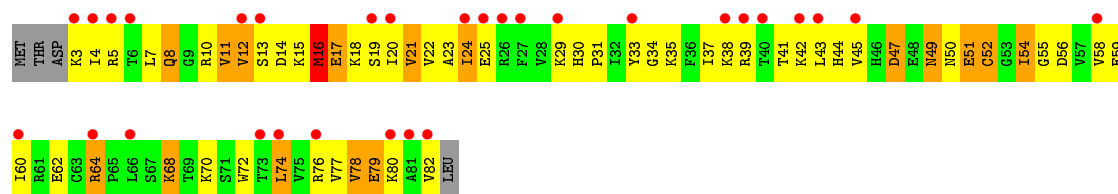


- Molecule 16: 30S ribosomal protein S16

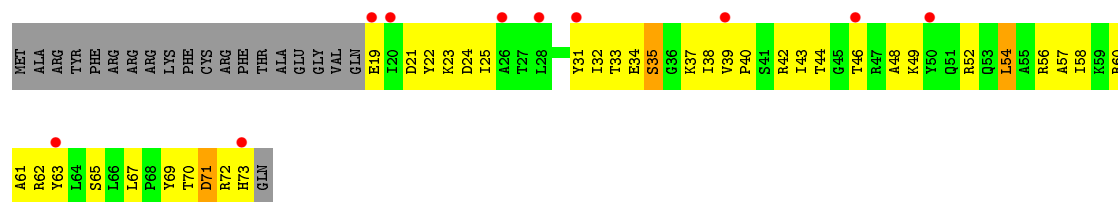


- Molecule 17: 30S ribosomal protein S17

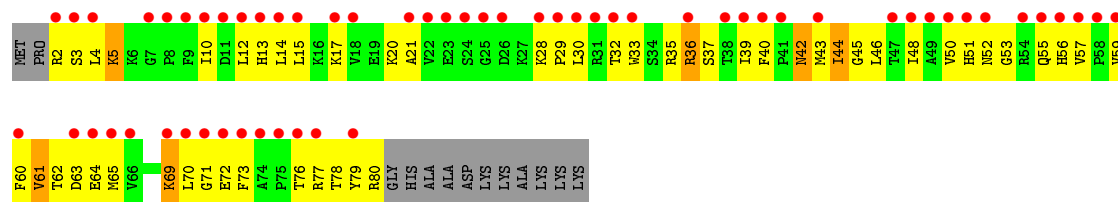




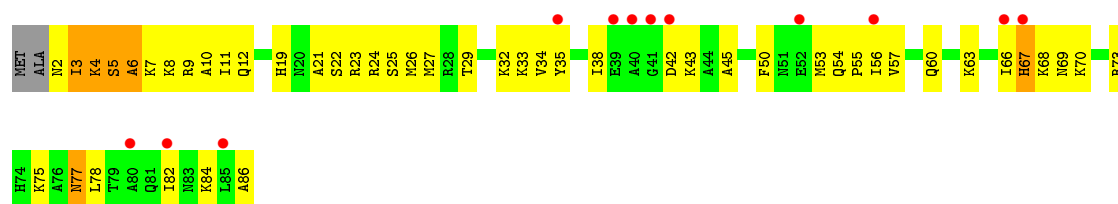
- Molecule 18: 30S ribosomal protein S18



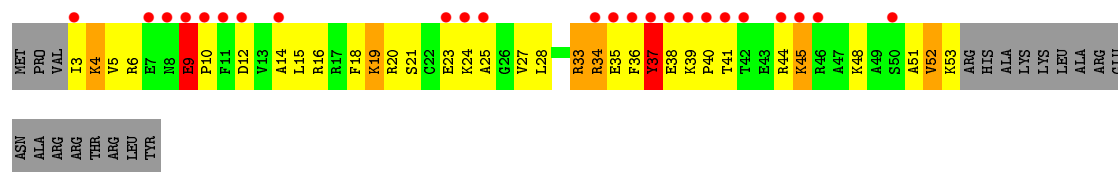
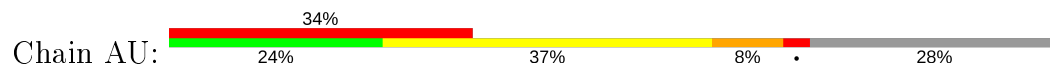
- Molecule 19: 30S ribosomal protein S19



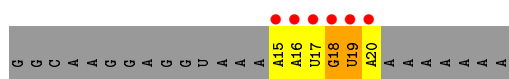
- Molecule 20: 30S ribosomal protein S20



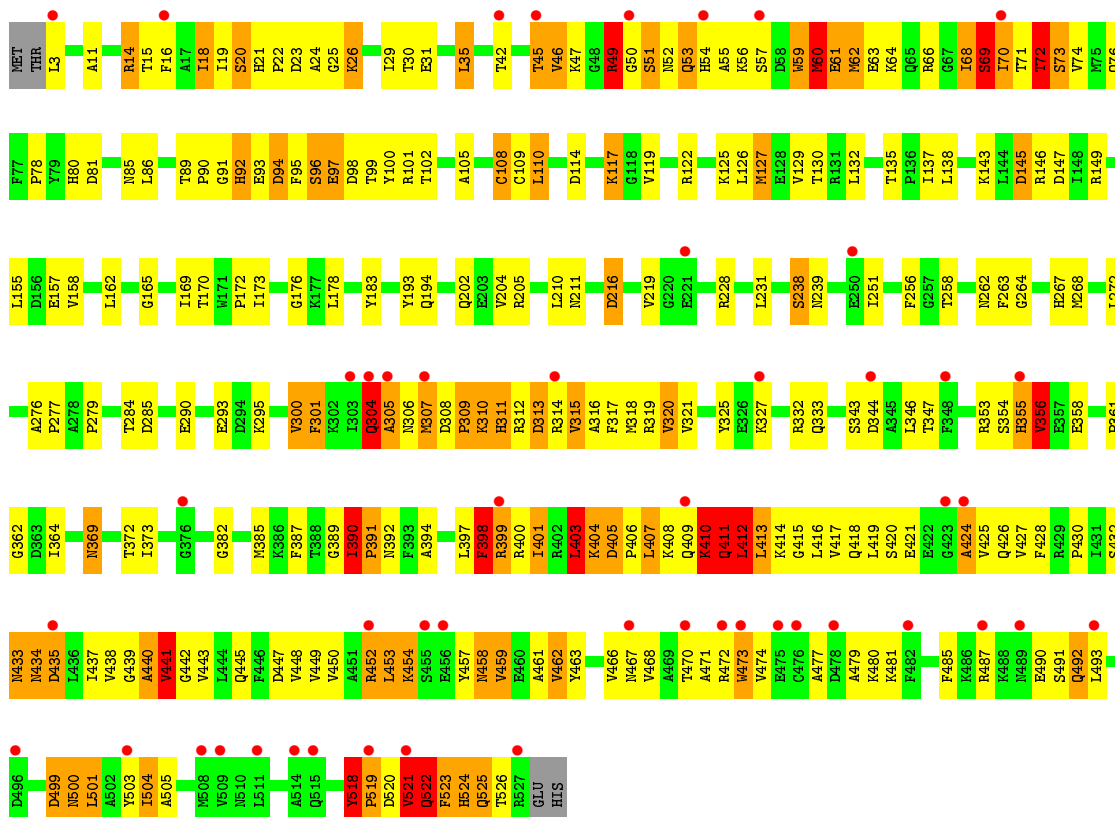
- Molecule 21: 30S ribosomal protein S21



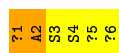
- Molecule 22: messenger RNA



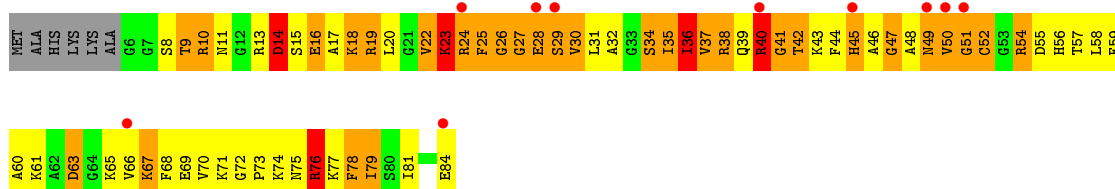
• Molecule 23: Peptide chain release factor 3



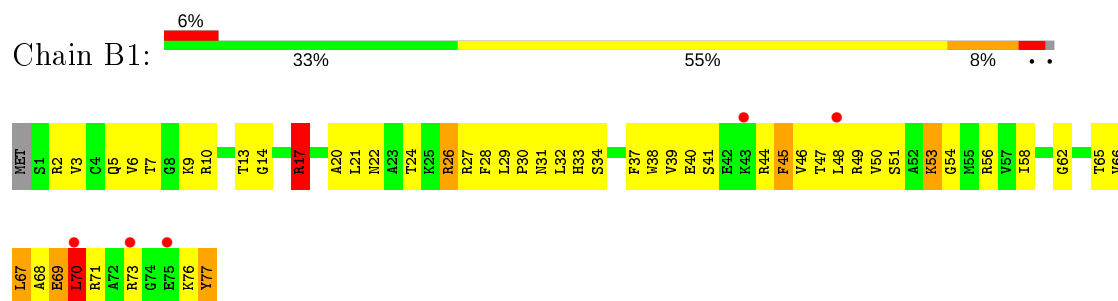
• Molecule 24: Viomycin



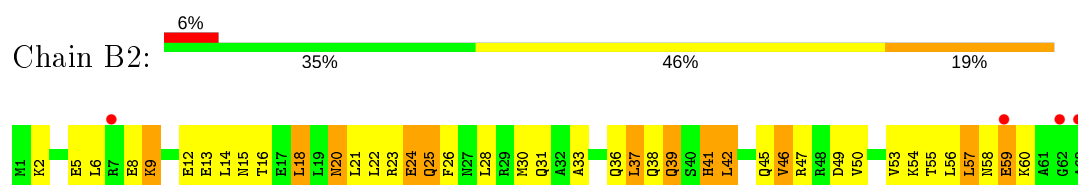
• Molecule 25: 50S ribosomal protein L27



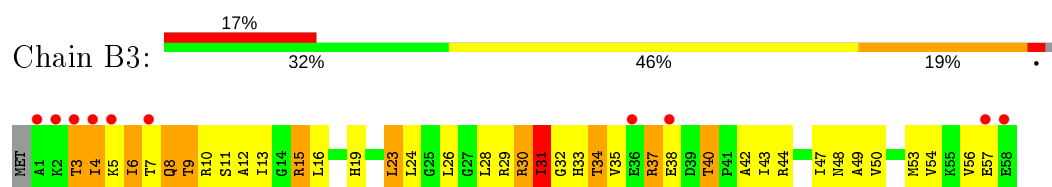
- Molecule 26: 50S ribosomal protein L28



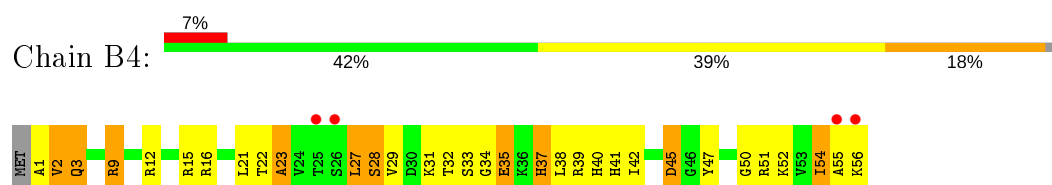
- Molecule 27: 50S ribosomal protein L29



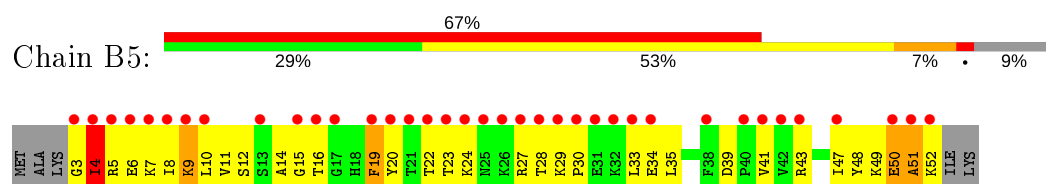
- Molecule 28: 50S ribosomal protein L30



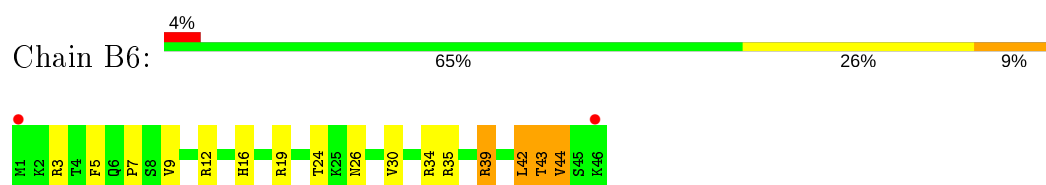
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



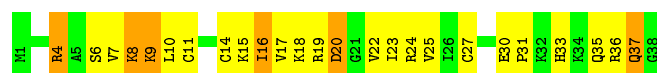
- Molecule 32: 50S ribosomal protein L35

Chain B7: 



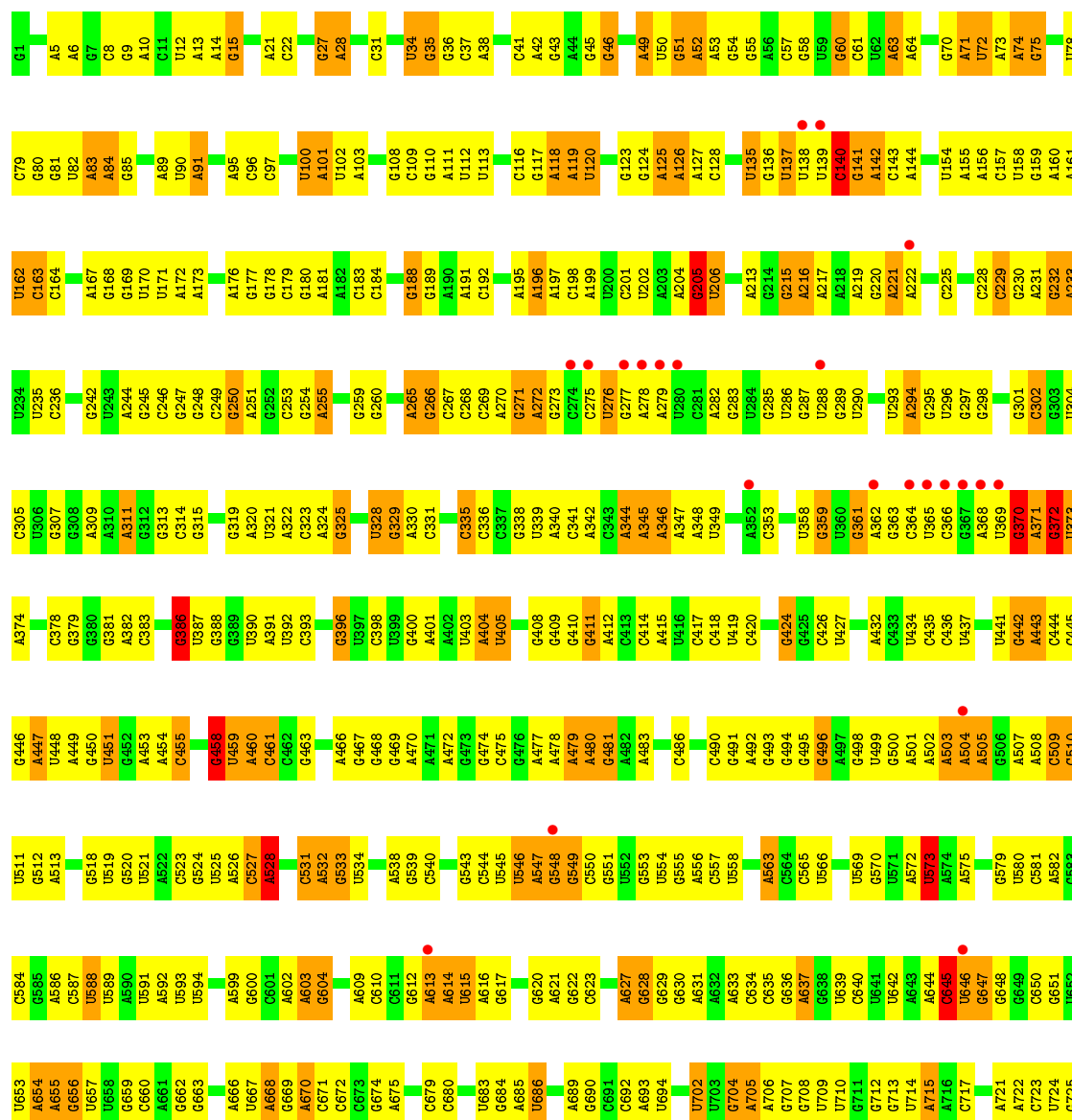
- Molecule 33: 50S ribosomal protein L36 1

Chain B8: 



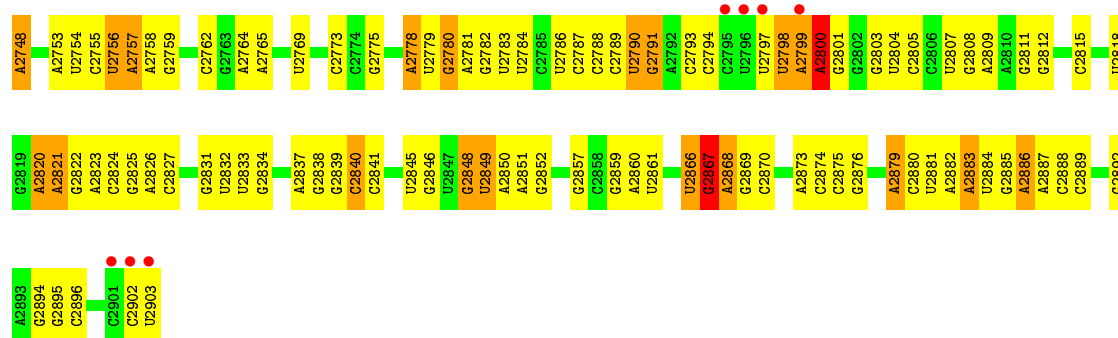
- Molecule 34: 23S rRNA

Chain BA: 



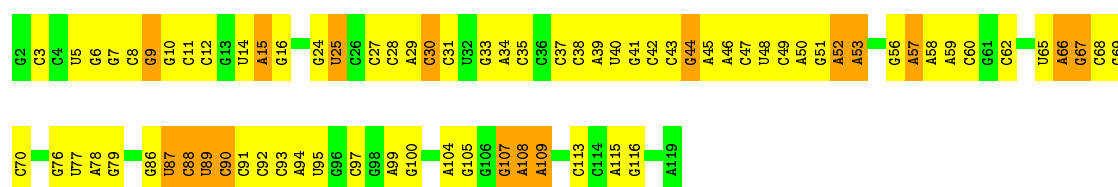
C1638	C1639	C1644	U1647	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1701	A1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726																																																																																																																																																																																																																																																																																				
U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629																																																																																																																																																																																																																																																																																									
A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	G1499	G1500	G1501	A1502	A1503	A1504	A1505	U1506	U1507	A1508	A1509	A1510	G1511	A1512	A1513	A1514	A1515	A1516	G1517	C1518	G1519	U1520	G1521	A1522	U1523	U1524	A1525	A1526	G1527	G1528	G1529	G1530	C1531	A1532	C1533	U1534	A1535	C1536	G1537	G1538	U1539	G1540	C1541	U1542	G1543	A1544	A1545	G1546	C1547	C1548	A1549	A1550	A1551	A1552	C1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560																																																																																																																																																																																																																																																																																							
C1417	G1418	A1419	A1420	G1421	G1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490																																																																																																																																																																																																																																																																																				
U1352	U1353	A1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	U1397	C1398	C1399	U1400	G1401	A1402	A1403	C1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490																																																																																																																																																																																																																			
G1279	G1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560																																																																				
G1211	G1212	A1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560
U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333																																																																																																					

C2678	C2679	C2680	C2681	C2682	C2683	G2603	A2516	C2442	C2364	C2301	G2230	C	A2097	G2029	U1946	A1871	C1800	C1727
A2679	U2680	A2518	G2608	U2609	C2683	G2607	C2517	C2443	G2365	U2302	U2331	C	G2102	A2030	C1947	A1872	C1801	C1728
C2682	A2682	C2683	U2610	U2611	U2612	G2609	U2519	G2444	A2366	G2304	G2232	G	C2103	A2031	C1952	C1873	A1805	U1729
C2683	C2684	C2685	U2613	U2614	U2615	U2616	U2449	A2448	G2368	U2306	G2237	C	U2105	A2034	U1955	G1732	A1808	G1731
C2684	C2685	C2686	U2617	U2618	U2619	U2620	U2450	A2451	A2369	G2307	U2238	U	U2106	G2035	U1956	G1733	A1809	G1733
C2685	C2686	C2687	U2621	U2622	U2623	U2624	U2452	A2452	A2370	G2308	G2239	G	U2107	G2036	U1957	G1734	A1810	G1734
C2686	C2687	C2688	U2625	U2626	U2627	U2628	U2453	A2453	A2371	G2309	G2240	A	U2108	G2037	U1958	U1735	A1811	U1735
C2687	C2688	C2689	U2629	U2630	U2631	U2632	U2454	A2454	A2372	G2310	U2241	A	U2109	U2039	C1961	U1736	A1812	U1736
C2688	C2689	C2690	U2633	U2634	U2635	U2636	U2455	A2455	A2373	G2311	U2242	A	U2110	U2040	C1962	U1737	A1813	U1737
C2689	C2690	C2691	U2637	U2638	U2639	U2640	U2456	A2456	A2374	G2312	U2243	U	U2111	U2041	C1963	U1738	A1814	U1738
C2690	C2691	C2692	U2641	U2642	U2643	U2644	U2457	A2457	A2375	G2313	U2244	U	U2112	U2042	C1964	U1739	A1815	U1739
C2691	C2692	C2693	U2645	U2646	U2647	U2648	U2458	A2458	A2376	G2314	U2245	A	U2113	U2043	C1965	G1740	A1816	G1740
C2692	C2693	C2694	U2649	U2650	U2651	U2652	U2459	A2459	A2377	G2315	U2246	C	U2114	G2046	C1966	U1741	U1817	G1741
C2693	C2694	C2695	U2653	U2654	U2655	U2656	U2460	A2460	A2378	G2316	U2247	C	U2115	G2047	C1967	U1742	U1818	U1742
C2694	C2695	C2696	U2657	U2658	U2659	U2660	U2461	A2461	U2384	G2317	U2248	A	U2116	G2048	C1968	U1743	U1819	U1743
C2695	C2696	C2697	U2661	U2662	U2663	U2664	U2462	A2462	U2385	G2318	U2249	C	U2117	G2049	C1969	U1744	U1820	U1744
C2696	C2697	C2698	U2665	U2666	U2667	U2668	U2463	A2463	U2386	G2319	U2250	C	U2118	G2050	C1970	U1745	U1821	U1745
C2697	C2698	C2699	U2669	U2670	U2671	U2672	U2464	A2464	U2387	G2320	U2251	A	U2119	G2051	C1971	U1746	U1822	U1746
C2698	C2699	C2700	U2673	U2674	U2675	U2676	U2465	A2465	U2388	G2321	U2252	A	U2120	G2052	C1972	U1747	U1823	U1747
C2699	C2700	C2701	U2677	U2678	U2679	U2680	U2466	A2466	U2389	G2322	U2253	G	U2121	G2053	C1973	U1748	U1824	U1748
C2700	C2701	C2702	U2681	U2682	U2683	U2684	U2467	A2467	U2390	G2323	U2254	U	U2122	G2054	C1974	U1749	U1825	U1749
C2701	C2702	C2703	U2685	U2686	U2687	U2688	U2468	A2468	U2391	G2324	U2255	G	U2123	G2055	C1975	U1750	U1826	U1750
C2702	C2703	C2704	U2689	U2690	U2691	U2692	U2469	A2469	U2392	G2325	U2256	G	U2124	G2056	C1976	U1751	U1827	U1751
C2703	C2704	C2705	U2693	U2694	U2695	U2696	U2470	A2470	U2393	G2326	U2257	G	U2125	G2057	C1977	U1752	U1828	U1752
C2704	C2705	C2706	U2697	U2698	U2699	U2700	U2471	A2471	U2394	G2327	U2258	U	U2126	G2058	C1978	U1753	U1829	U1753
C2705	C2706	C2707	U2701	U2702	U2703	U2704	U2472	A2472	U2395	G2328	U2259	U	U2127	G2059	C1979	U1754	U1830	U1754
C2706	C2707	C2708	U2705	U2706	U2707	U2708	U2473	A2473	U2396	G2329	U2260	U	U2128	G2060	C1980	U1755	U1831	U1755
C2707	C2708	C2709	U2709	U2710	U2711	U2712	U2474	A2474	U2397	G2330	U2261	C	U2129	G2061	C1981	U1756	U1832	U1756
C2708	C2709	C2710	U2713	U2714	U2715	U2716	U2475	A2475	U2398	G2331	U2262	U	U2130	G2062	C1982	U1757	U1833	U1757
C2709	C2710	C2711	U2717	U2718	U2719	U2720	U2476	A2476	U2399	G2332	U2263	U	U2131	G2063	C1983	U1758	U1834	U1758
C2710	C2711	C2712	U2721	U2722	U2723	U2724	U2477	A2477	U2400	G2333	U2264	U	U2132	G2064	C1984	U1759	U1835	U1759
C2711	C2712	C2713	U2725	U2726	U2727	U2728	U2478	A2478	U2401	G2334	U2265	U	U2133	G2065	C1985	U1760	U1836	U1760
C2712	C2713	C2714	U2729	U2730	U2731	U2732	U2479	A2479	U2402	G2335	U2266	U	U2134	G2066	C1986	U1761	U1837	U1761
C2713	C2714	C2715	U2733	U2734	U2735	U2736	U2480	A2480	U2403	G2336	U2267	U	U2135	G2067	C1987	U1762	U1838	U1762
C2714	C2715	C2716	U2737	U2738	U2739	U2740	U2481	A2481	U2404	G2337	U2268	U	U2136	G2068	C1988	U1763	U1839	U1763
C2715	C2716	C2717	U2741	U2742	U2743	U2744	U2482	A2482	U2405	G2338	U2269	U	U2137	G2069	C1989	U1764	U1840	U1764
C2716	C2717	C2718	U2745	U2746	U2747	U2748	U2483	A2483	U2406	G2339	U2270	U	U2138	G2070	C1990	U1765	U1841	U1765
C2717	C2718	C2719	U2749	U2750	U2751	U2752	U2484	A2484	U2407	G2340	U2271	U	U2139	G2071	C1991	U1766	U1842	U1766
C2718	C2719	C2720	U2753	U2754	U2755	U2756	U2485	A2485	U2411	G2341	U2272	U	U2140	G2072	C1992	U1767	U1843	U1767
C2719	C2720	C2721	U2757	U2758	U2759	U2760	U2486	A2486	U2412	G2342	U2273	U	U2141	G2073	C1993	U1768	U1844	U1768
C2720	C2721	C2722	U2761	U2762	U2763	U2764	U2487	A2487	U2413	G2343	U2274	U	U2142	G2074	C1994	U1769	U1845	U1769
C2721	C2722	C2723	U2765	U2766	U2767	U2768	U2488	A2488	U2414	G2344	U2275	U	U2143	G2075	C1995	U1770	U1846	U1770
C2722	C2723	C2724	U2769	U2770	U2771	U2772	U2489	A2489	U2415	G2345	U2276	U	U2144	G2076	C1996	U1771	U1847	U1771
C2723	C2724	C2725	U2773	U2774	U2775	U2776	U2490	A2490	U2416	G2346	U2277	U	U2145	G2077	C1997	U1772	U1848	U1772
C2724	C2725	C2726	U2777	U2778	U2779	U2780	U2491	A2491	U2417	G2347	U2278	U	U2146	G2078	C1998	U1773	U1849	U1773
C2725	C2726	C2727	U2781	U2782	U2783	U2784	U2492	A2492	U2418	G2348	U2279	U	U2147	G2079	C1999	U1774	U1850	U1774
C2726	C2727	C2728	U2785	U2786	U2787	U2788	U2493	A2493	U2419	G2349	U2280	U	U2148	G2080	C2000	U1775	U1851	U1775
C2727	C2728	C2729	U2789	U2790	U2791	U2792	U2494	A2494	U2420	G2350	U2281	U	U2149	G2081	C2001	U1776	U1852	U1776
C2728	C2729	C2730	U2793	U2794	U2795	U2796	U2495	A2495	U2421	G2351	U2282	U	U2150	G2082	C2002	U1777	U1853	U1777
C2729	C2730	C2731	U2797	U2798	U2799	U2800	U2496	A2496	U2422	G2352	U2283	U	U2151	G2083	C2003	U1778	U1854	U1778
C2730	C2731	C2732	U2801	U2802	U2803	U2804	U2497	A2497	U2423	G2353	U2284	U	U2152	G2084	C2004	U1779	U1855	U1779
C2731	C2732	C2733	U2805	U2806	U2807	U2808	U2498	A2498	U2424	G2354	U2285	U	U2153	G2085	C2005	U1780	U1856	U1780
C2732	C2733	C2734	U2809	U2810	U2811	U2812	U2499	A2499	U2425	G2355	U2286	U	U2154	G2086	C2006	U1781	U1857	U1781
C2733	C2734	C2735	U2813	U2814	U2815	U2816	U2500	A2500	U2426	G2356	U2287	U	U2155	G2087	C2007	U1782	U1858	U1782
C2734	C2735	C2736	U2817	U2818	U2819	U2820	U2501	A2501	U2427	G2357	U2288	U	U2156	G2088	C2008	U1783	U1859	U1783
C2735	C2736	C2737	U2821	U2822	U2823	U2824	U2502	A2502	U2428	G2358	U2289	U	U2157	G2089	C2009	U1784	U1860	U1784
C2736	C2737	C2738	U2825	U2826	U2827	U2828	U2503	A2503	U2429	G2359	U2290	U	U2158	G2090	C2010	U1785	U1861	U1785
C2737	C2738	C2739	U2829	U2830	U2831	U2832	U2504	A2504	U2430	G2360	U2291	U	U2159	G2091	C2011	U1786	U1862	U1786
C2738	C2739	C2740	U2833	U2834	U2835	U2836	U2505	A2505	U2431	G2361	U2292	U	U2160	G2092	C2012	U1787	U1863	U1787
C2739	C2740	C2741	U2837	U2838	U2839	U2840	U2506	A2506	U2432	G2362	U2293	U	U2161	G2093	C2013	U1788	U1864	U1788
C2740	C2741	C2742	U2841	U2842	U2843	U2844	U2507	A2507	U2433	G2363	U2294	U	U2162	G2094	C2014	U1789	U1865	U1789
C2741	C2742	C2743	U2845	U2846	U2847	U2848	U2508	A2508	U2434	G2364	U2295	U	U2163	G2095	C2015	U1790	U1866	U1790
C2742	C2743	C2744	U2849	U2850	U2851	U2852	U2509	A2509	U2435	G2365	U2296	U	U2164	G2096	C2016	U1791	U1867	U1791
C2743	C2744	C2745	U2853	U2854	U2855	U2856	U2510	A2510	U2436	G2366	U2297	U	U2165	G2097	C2017	U1792	U1868	U1792
C2744	C2745	C2746	U2857	U2858	U2859	U2860	U2511	A2511	U2437	G2367	U2298	U	U2166	G2098	C2018	U1793	U1869	U1793
C2745	C2746	C2747	U2861	U2862	U2863	U2864	U2512	A2512	U2438	G2368	U2299	U	U2167	G2099	C2019	U1794	U1870	U1794
C2746	C2747	C2748	U2865	U2866	U2867	U2868	U2513	A2513	U2439	G2369	U2300	U	U2168	G2100	C2020	U1795	U1871	U1795
C2747	C2748	C2749	U2869	U2870	U2871													



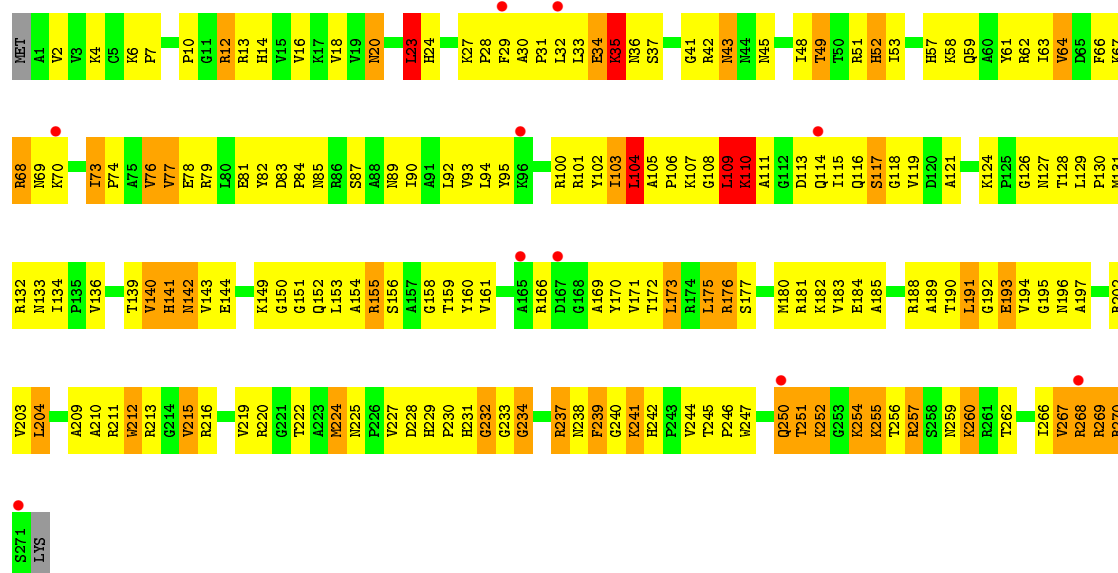
• Molecule 35: 5S ribosomal RNA

Chain BB: 36% 50% 14%



• Molecule 36: 50S ribosomal protein L2

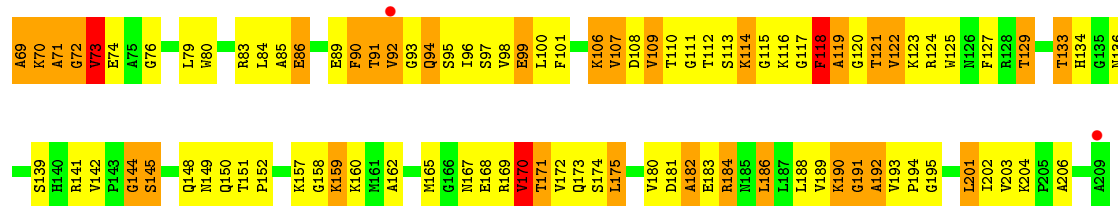
Chain BC: 4% 32% 51% 15% ..



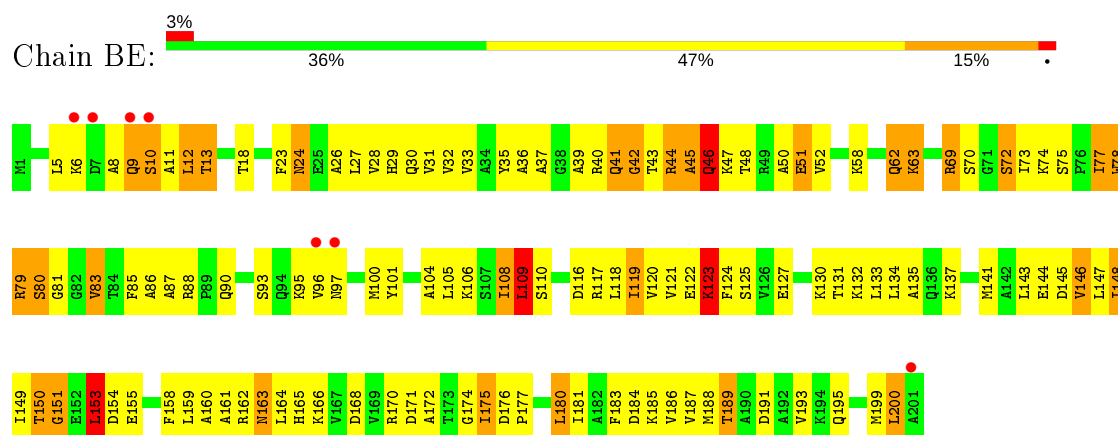
• Molecule 37: 50S ribosomal protein L3

Chain BD: 33% 47% 19%

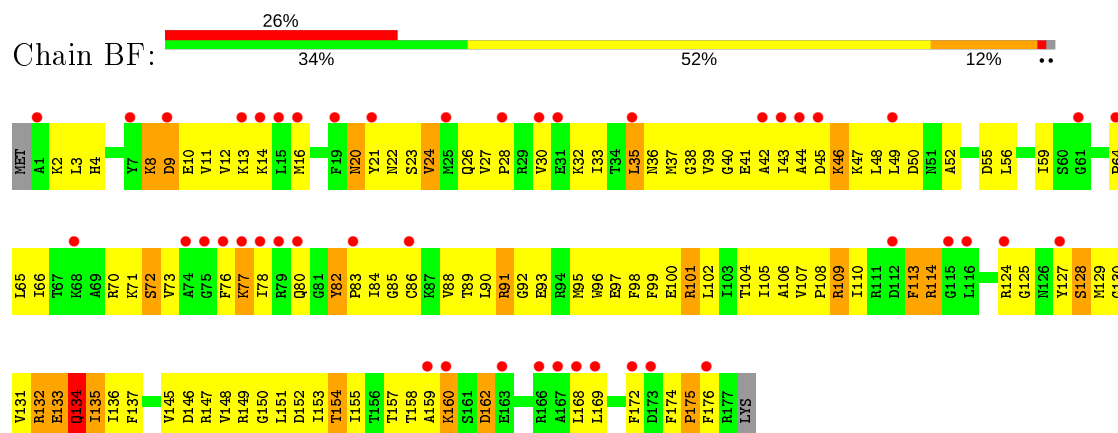




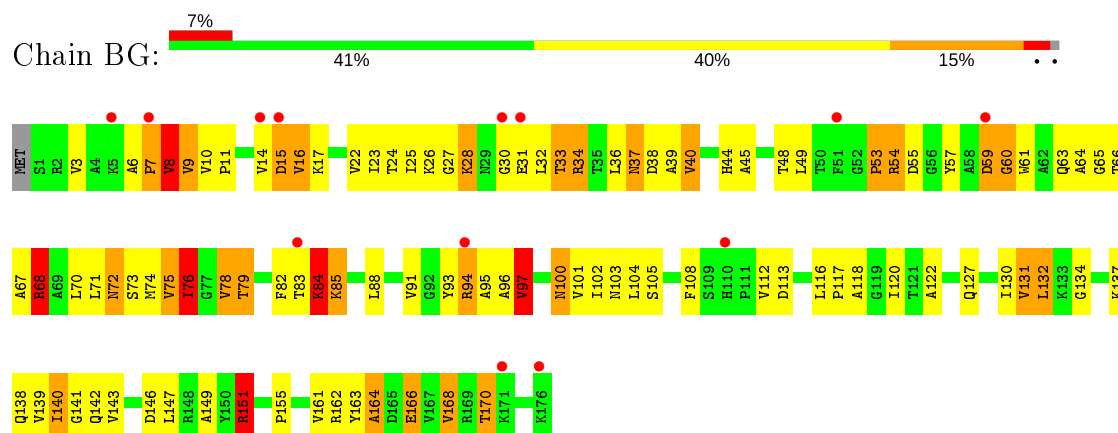
• Molecule 38: 50S ribosomal protein L4



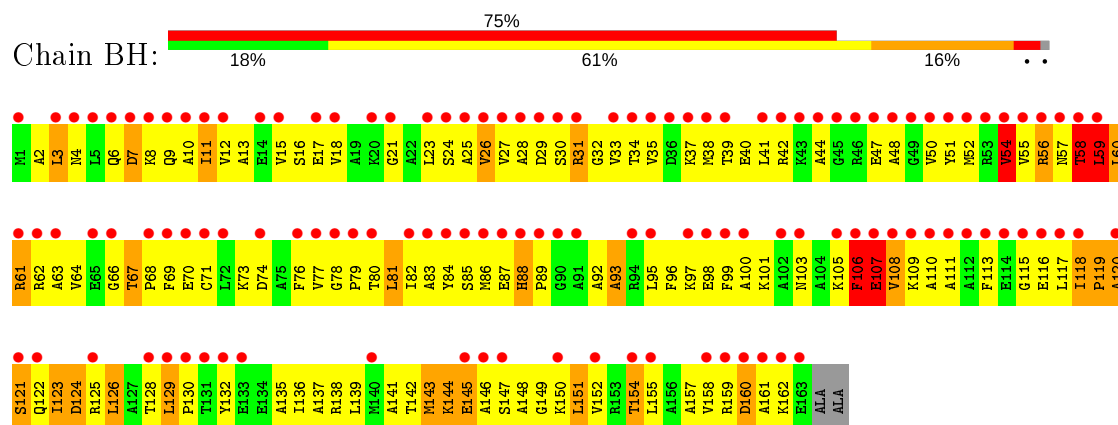
• Molecule 39: 50S ribosomal protein L5



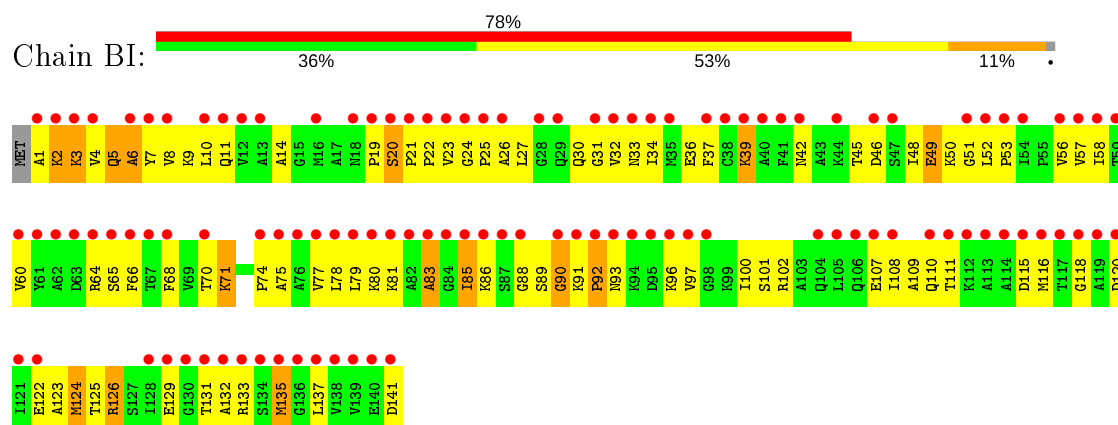
• Molecule 40: 50S ribosomal protein L6



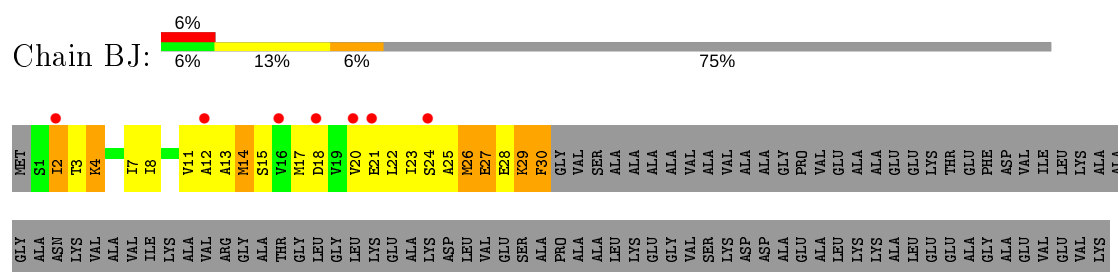
Chain BH:



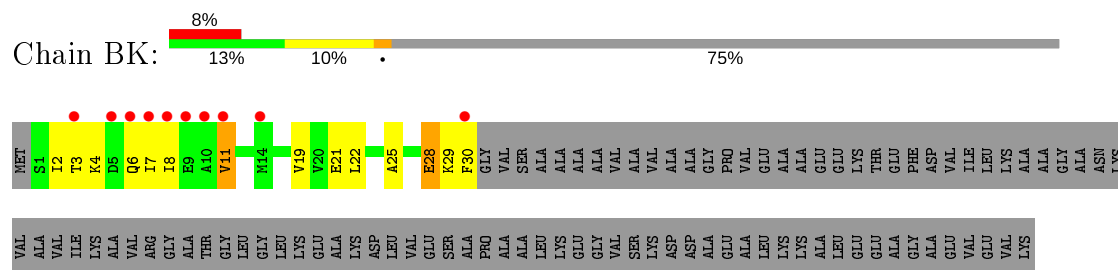
Chain BI:



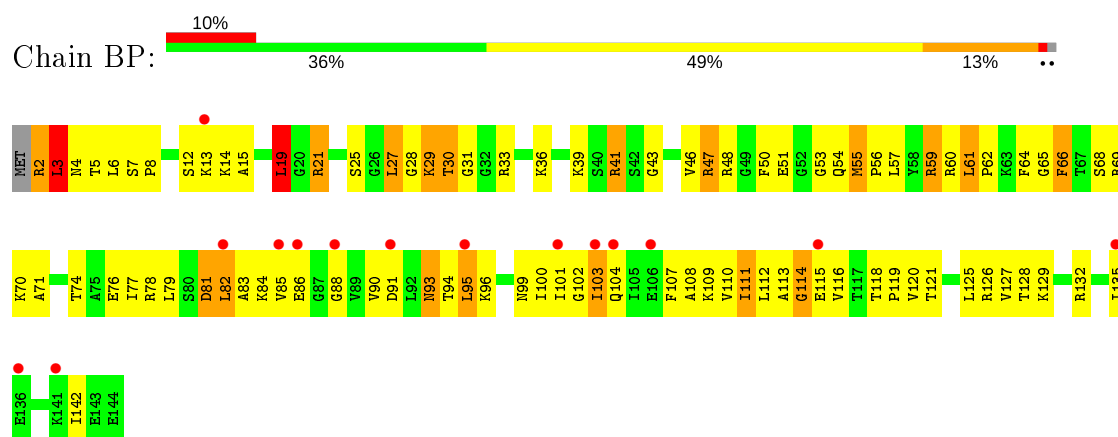
Chain B.J:



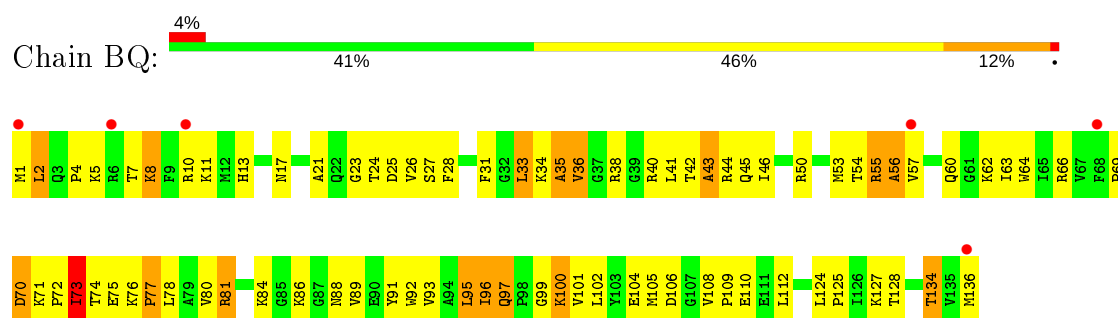
Chain BK:



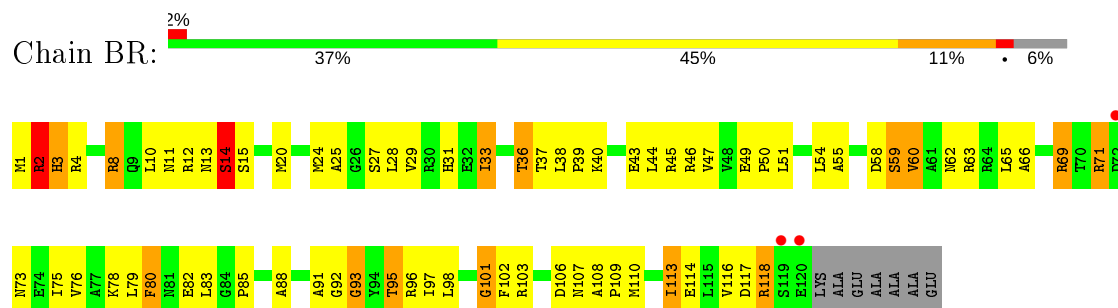
WORLDWIDE
PDB
PROTEIN DATA BANK



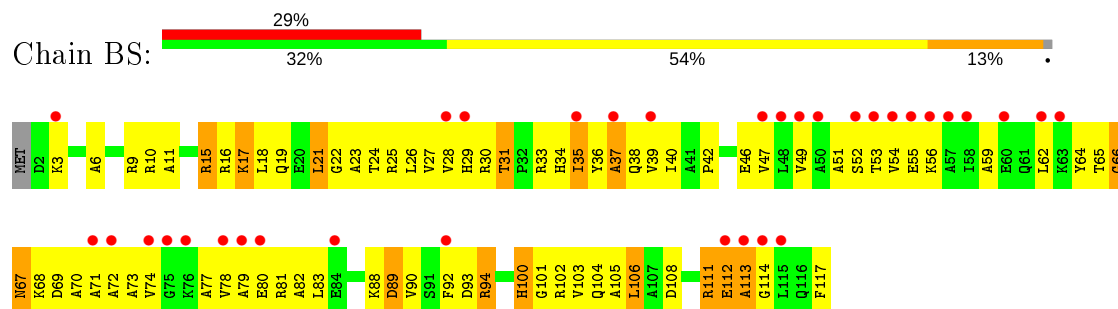
• Molecule 47: 50S ribosomal protein L16



• Molecule 48: 50S ribosomal protein L17

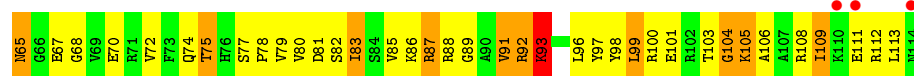


• Molecule 49: 50S ribosomal protein L18

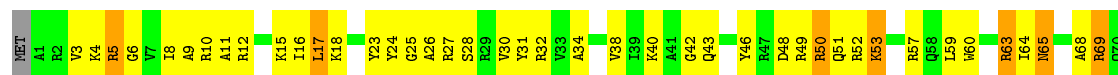


• Molecule 50: 50S ribosomal protein L19

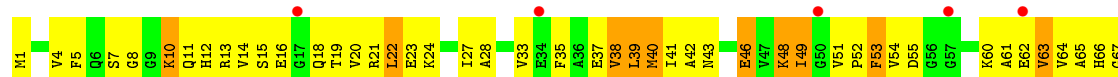




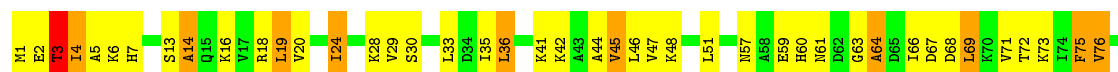
• Molecule 51: 50S ribosomal protein L20



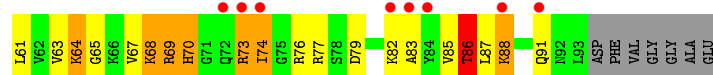
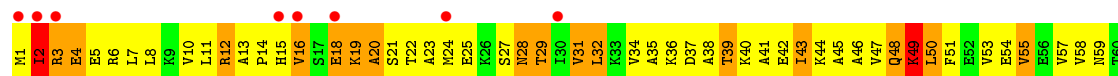
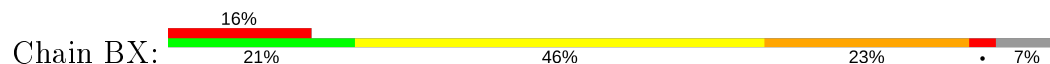
• Molecule 52: 50S ribosomal protein L21



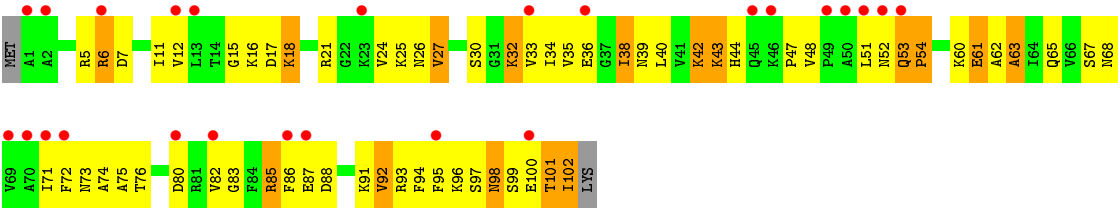
• Molecule 53: 50S ribosomal protein L22



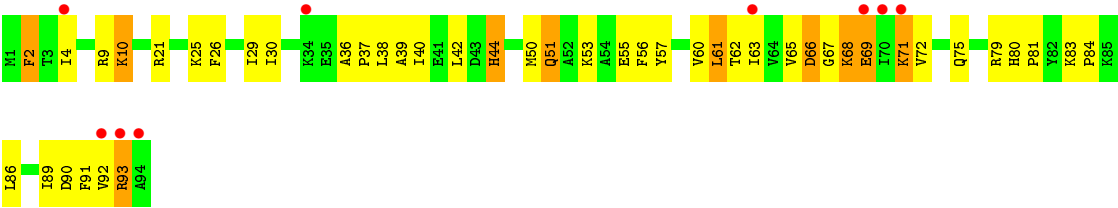
• Molecule 54: 50S ribosomal protein L23



• 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 59.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 99.9 (59.36-3.00)	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 0.226 , 0.254	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)	0.32 , 87.4	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, KBE, UAL, 5OH

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	0.44	0/36809	0.81	26/57423 (0.0%)
2	AB	0.29	0/1735	0.48	0/2338
3	AC	0.29	0/1651	0.51	0/2225
4	AD	0.29	0/1665	0.50	0/2227
5	AE	0.34	0/1118	0.58	0/1504
6	AF	0.27	0/835	0.49	0/1128
7	AG	0.23	0/1195	0.41	0/1602
8	AH	0.30	0/989	0.50	0/1326
9	AI	0.26	0/1034	0.49	0/1375
10	AJ	0.30	0/796	0.54	0/1077
11	AK	0.29	0/893	0.51	0/1205
12	AL	0.38	0/969	0.65	0/1300
13	AM	0.21	0/892	0.42	0/1193
14	AN	0.28	0/785	0.47	0/1043
15	AO	0.28	0/722	0.49	0/964
16	AP	0.30	0/659	0.48	0/884
17	AQ	0.30	0/657	0.52	0/881
18	AR	0.30	0/462	0.49	0/621
19	AS	0.23	0/652	0.42	0/877
20	AT	0.31	0/671	0.53	0/888
21	AU	0.31	0/430	0.46	0/570
22	AV	0.53	0/144	0.91	0/222
23	AW	0.47	2/4221 (0.0%)	0.73	5/5702 (0.1%)
24	AY	0.97	0/11	0.62	0/13
25	B0	0.43	0/603	0.64	0/797
26	B1	0.37	0/635	0.66	0/848
27	B2	0.31	0/510	0.55	0/677
28	B3	0.34	0/453	0.59	0/605
29	B4	0.42	0/450	0.64	0/599
30	B5	0.27	0/416	0.46	0/554
31	B6	0.42	0/380	0.64	0/498
32	B7	0.37	0/513	0.57	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.42	0/303	0.65	0/397
34	BA	0.61	9/68601 (0.0%)	0.98	142/107017 (0.1%)
35	BB	0.40	0/2828	0.78	1/4410 (0.0%)
36	BC	0.42	0/2121	0.70	0/2852
37	BD	0.46	0/1586	0.70	0/2134
38	BE	0.36	0/1571	0.56	0/2113
39	BF	0.27	0/1434	0.45	0/1926
40	BG	0.34	0/1343	0.60	0/1816
41	BH	0.28	0/1244	0.53	1/1675 (0.1%)
42	BI	0.22	0/1046	0.42	0/1410
43	BJ	0.28	0/227	0.52	0/304
43	BK	0.25	0/227	0.44	0/304
43	BL	0.27	0/227	0.49	0/304
43	BM	0.25	0/227	0.42	0/304
44	BN	0.41	0/1152	0.66	0/1551
45	BO	0.47	0/947	0.70	0/1268
46	BP	0.35	0/1054	0.64	0/1403
47	BQ	0.38	0/1093	0.61	0/1460
48	BR	0.42	0/973	0.64	0/1301
49	BS	0.32	0/902	0.51	0/1209
50	BT	0.43	0/929	0.67	0/1242
51	BU	0.42	0/960	0.58	0/1278
52	BV	0.36	0/829	0.62	0/1107
53	BW	0.45	0/863	0.63	0/1156
54	BX	0.40	0/744	0.65	0/994
55	BY	0.38	0/787	0.60	0/1051
56	BZ	0.32	0/766	0.50	0/1025
All	All	0.50	11/158939 (0.0%)	0.84	175/236853 (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	20.78	1.86	1.61
34	BA	2183	A	O3'-P	15.69	1.79	1.61
34	BA	974	G	O3'-P	-15.38	1.42	1.61
34	BA	973	A	O3'-P	-13.70	1.44	1.61
34	BA	974	G	N7-C5	-6.57	1.35	1.39

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	2183	A	O3'-P-O5'	-12.34	80.55	104.00
34	BA	2183	A	OP2-P-O3'	12.19	132.01	105.20
34	BA	752	A	C5-N7-C8	-8.85	99.48	103.90
34	BA	2106	U	OP2-P-O3'	8.38	123.64	105.20
34	BA	2183	A	P-O3'-C3'	-8.25	109.80	119.70

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	1452	0
2	AB	1704	0	1732	189	0
3	AC	1624	0	1699	162	4
4	AD	1643	0	1710	196	0
5	AE	1105	0	1148	135	0
6	AF	817	0	808	102	0
7	AG	1181	0	1240	70	0
8	AH	979	0	1034	91	0
9	AI	1022	0	1070	126	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	97	0
11	AK	877	0	887	104	0
12	AL	955	0	1019	123	0
13	AM	883	0	944	96	0
14	AN	774	0	827	90	0
15	AO	714	0	737	45	0
16	AP	649	0	666	63	0
17	AQ	648	0	691	62	0
18	AR	455	0	478	41	0
19	AS	637	0	665	70	0
20	AT	665	0	714	60	0
21	AU	425	0	449	67	0
22	AV	129	0	65	9	0
23	AW	4144	0	4127	284	0
24	AY	48	0	40	31	0
25	B0	596	0	610	166	0
26	B1	625	0	655	54	0
27	B2	509	0	543	40	0
28	B3	449	0	491	53	0
29	B4	444	0	461	33	0
30	B5	409	0	440	39	0
31	B6	377	0	418	20	0
32	B7	504	0	574	49	0
33	B8	302	0	340	40	0
34	BA	61252	0	30808	2053	4
35	BB	2529	0	1281	94	0
36	BC	2082	0	2157	226	0
37	BD	1565	0	1616	201	0
38	BE	1552	0	1619	151	0
39	BF	1410	0	1447	142	0
40	BG	1323	0	1374	134	0
41	BH	1230	0	1282	253	0
42	BI	1032	0	1088	85	0
43	BJ	227	0	237	48	0
43	BK	227	0	237	23	0
43	BL	227	0	237	38	0
43	BM	227	0	237	47	0
44	BN	1129	0	1162	147	0
45	BO	938	0	1012	117	0
46	BP	1045	0	1117	108	0
47	BQ	1074	0	1157	79	0
48	BR	960	0	1000	87	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	123	0
51	BU	947	0	1022	108	0
52	BV	816	0	839	96	0
53	BW	856	0	922	55	0
54	BX	738	0	807	110	0
55	BY	779	0	834	74	0
56	BZ	753	0	780	54	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	8115	4

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 33.

The worst 5 of 8115 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

All (4) 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:NE	34:BA:2157:G:OP1[4_445]	1.68	0.52
3:AC:131:ARG:NH2	34:BA:2156:G:O3'[4_445]	1.80	0.40
3:AC:131:ARG:CZ	34:BA:2157:G:P[4_445]	2.10	0.10

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	1
3	AC	204/233 (88%)	156 (76%)	32 (16%)	16 (8%)	1	6
4	AD	203/206 (98%)	134 (66%)	45 (22%)	24 (12%)	0	2
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	12
8	AH	127/130 (98%)	96 (76%)	27 (21%)	4 (3%)	4	26
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	3
11	AK	115/129 (89%)	82 (71%)	25 (22%)	8 (7%)	1	8

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%)	1	5
13	AM	112/118 (95%)	78 (70%)	27 (24%)	7 (6%)	1	10
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	24
16	AP	80/82 (98%)	57 (71%)	16 (20%)	7 (9%)	1	4
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	14
19	AS	77/92 (84%)	60 (78%)	14 (18%)	3 (4%)	3	22
20	AT	83/87 (95%)	59 (71%)	20 (24%)	4 (5%)	2	17
21	AU	49/71 (69%)	24 (49%)	19 (39%)	6 (12%)	0	2
23	AW	523/529 (99%)	381 (73%)	82 (16%)	60 (12%)	0	2
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%)	3	21
27	B2	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	1	5
28	B3	56/59 (95%)	46 (82%)	5 (9%)	5 (9%)	1	4
29	B4	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	7
30	B5	48/55 (87%)	41 (85%)	3 (6%)	4 (8%)	1	5
31	B6	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	2	18
32	B7	62/65 (95%)	53 (86%)	6 (10%)	3 (5%)	2	17
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	2
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	1
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	8
43	BL	28/121 (23%)	22 (79%)	4 (14%)	2 (7%)	1	8

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	8
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%)	1	4
48	BR	118/127 (93%)	86 (73%)	20 (17%)	12 (10%)	0	3
49	BS	114/117 (97%)	90 (79%)	14 (12%)	10 (9%)	1	4
50	BT	112/115 (97%)	74 (66%)	21 (19%)	17 (15%)	0	1
51	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	12
52	BV	101/103 (98%)	75 (74%)	18 (18%)	8 (8%)	1	6
53	BW	108/116 (93%)	89 (82%)	15 (14%)	4 (4%)	3	22
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	10
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%)	145 (81%)	35 (19%)	1	7
3	AC	170/190 (90%)	146 (86%)	24 (14%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	152 (88%)	20 (12%)	5	24
5	AE	113/126 (90%)	95 (84%)	18 (16%)	2	12
6	AF	87/112 (78%)	73 (84%)	14 (16%)	2	11
7	AG	124/129 (96%)	121 (98%)	3 (2%)	49	77
8	AH	104/105 (99%)	94 (90%)	10 (10%)	8	32
9	AI	105/107 (98%)	92 (88%)	13 (12%)	4	21
10	AJ	86/90 (96%)	70 (81%)	16 (19%)	1	8
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	9
12	AL	103/104 (99%)	89 (86%)	14 (14%)	3	17
13	AM	92/96 (96%)	87 (95%)	5 (5%)	22	58
14	AN	79/84 (94%)	71 (90%)	8 (10%)	7	29
15	AO	76/77 (99%)	66 (87%)	10 (13%)	4	19
16	AP	65/65 (100%)	57 (88%)	8 (12%)	4	21
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	9
18	AR	48/65 (74%)	44 (92%)	4 (8%)	11	40
19	AS	70/79 (89%)	64 (91%)	6 (9%)	10	38
20	AT	65/66 (98%)	60 (92%)	5 (8%)	13	44
21	AU	44/61 (72%)	37 (84%)	7 (16%)	2	12
23	AW	447/453 (99%)	381 (85%)	66 (15%)	3	14
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%)	56 (84%)	11 (16%)	2	11
27	B2	55/55 (100%)	46 (84%)	9 (16%)	2	11
28	B3	48/49 (98%)	39 (81%)	9 (19%)	1	8
29	B4	47/48 (98%)	40 (85%)	7 (15%)	3	14
30	B5	45/49 (92%)	42 (93%)	3 (7%)	16	50
31	B6	38/38 (100%)	34 (90%)	4 (10%)	7	28
32	B7	51/52 (98%)	48 (94%)	3 (6%)	19	54
33	B8	34/34 (100%)	32 (94%)	2 (6%)	19	54
36	BC	216/218 (99%)	177 (82%)	39 (18%)	1	8
37	BD	164/164 (100%)	143 (87%)	21 (13%)	4	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BE	165/165 (100%)	138 (84%)	27 (16%)	2	11
39	BF	148/150 (99%)	136 (92%)	12 (8%)	11	42
40	BG	137/138 (99%)	116 (85%)	21 (15%)	2	13
41	BH	123/123 (100%)	109 (89%)	14 (11%)	5	24
42	BI	109/110 (99%)	101 (93%)	8 (7%)	14	46
43	BJ	26/85 (31%)	23 (88%)	3 (12%)	5	24
43	BK	26/85 (31%)	26 (100%)	0	100	100
43	BL	26/85 (31%)	25 (96%)	1 (4%)	33	67
43	BM	26/85 (31%)	24 (92%)	2 (8%)	13	44
44	BN	116/116 (100%)	94 (81%)	22 (19%)	1	8
45	BO	103/104 (99%)	80 (78%)	23 (22%)	1	4
46	BP	102/103 (99%)	85 (83%)	17 (17%)	2	10
47	BQ	109/109 (100%)	91 (84%)	18 (16%)	2	10
48	BR	100/103 (97%)	88 (88%)	12 (12%)	5	22
49	BS	86/87 (99%)	76 (88%)	10 (12%)	5	24
50	BT	99/100 (99%)	81 (82%)	18 (18%)	1	8
51	BU	89/90 (99%)	77 (86%)	12 (14%)	4	18
52	BV	84/84 (100%)	74 (88%)	10 (12%)	5	22
53	BW	93/99 (94%)	73 (78%)	20 (22%)	1	5
54	BX	80/84 (95%)	66 (82%)	14 (18%)	2	9
55	BY	83/85 (98%)	74 (89%)	9 (11%)	6	27
56	BZ	78/78 (100%)	74 (95%)	4 (5%)	24	60
All	All	5228/5666 (92%)	4511 (86%)	717 (14%)	3	17

5 of 717 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	42	THR
36	BC	173	LEU
52	BV	37	GLU
26	B1	10	ARG
29	B4	27	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
27	B2	20	ASN
36	BC	43	ASN
54	BX	48	GLN
27	B2	41	HIS
31	B6	13	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1531/1533 (99%)	298 (19%)	45 (2%)
22	AV	5/27 (18%)	3 (60%)	0
34	BA	2849/2903 (98%)	570 (20%)	95 (3%)
35	BB	117/118 (99%)	22 (18%)	3 (2%)
All	All	4502/4581 (98%)	893 (19%)	143 (3%)

5 of 893 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	442	G
34	BA	859	G
34	BA	2726	A
34	BA	479	A
34	BA	627	A

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	DPP	AY	2	24	3,5,6	1.21	1 (33%)	1,5,7	0.16	0
24	UAL	AY	5	24	7,8,9	2.46	2 (28%)	5,9,11	1.45	1 (20%)
24	KBE	AY	1	24	8,8,9	0.59	0	7,8,10	1.30	1 (14%)
24	5OH	AY	6	24	8,12,13	0.60	0	3,16,18	0.80	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	DPP	AY	2	24	-	0/2/4/6	-
24	UAL	AY	5	24	-	0/3/7/9	-
24	KBE	AY	1	24	-	1/7/7/8	-
24	5OH	AY	6	24	-	0/2/18/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	5	UAL	C-CA	5.10	1.53	1.45
24	AY	5	UAL	C1-N1	-3.10	1.35	1.40
24	AY	2	DPP	O-C	2.06	1.28	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	1	KBE	CB-CA-C	2.80	116.38	112.25
24	AY	5	UAL	O-C-CA	-2.33	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	2	DPP	1	0
24	AY	5	UAL	4	0
24	AY	1	KBE	17	0
24	AY	6	5OH	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	28,34,34	2.74	8 (28%)	30,54,54	2.47	10 (33%)

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	-	10/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AW	602	GNP	C5-C6	-8.18	1.38	1.52
58	AW	602	GNP	C4-N9	-8.15	1.36	1.47
58	AW	602	GNP	PG-O1G	4.81	1.53	1.46
58	AW	602	GNP	C6-N1	3.63	1.39	1.33
58	AW	602	GNP	C5-C4	-2.54	1.37	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AW	602	GNP	C4-C5-N7	7.63	112.57	102.46
58	AW	602	GNP	C5-C6-N1	-5.27	111.69	118.19
58	AW	602	GNP	PA-O3A-PB	-4.70	116.08	132.62
58	AW	602	GNP	O2B-PB-O1B	3.49	117.24	109.92
58	AW	602	GNP	O3G-PG-O2G	3.32	116.48	107.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

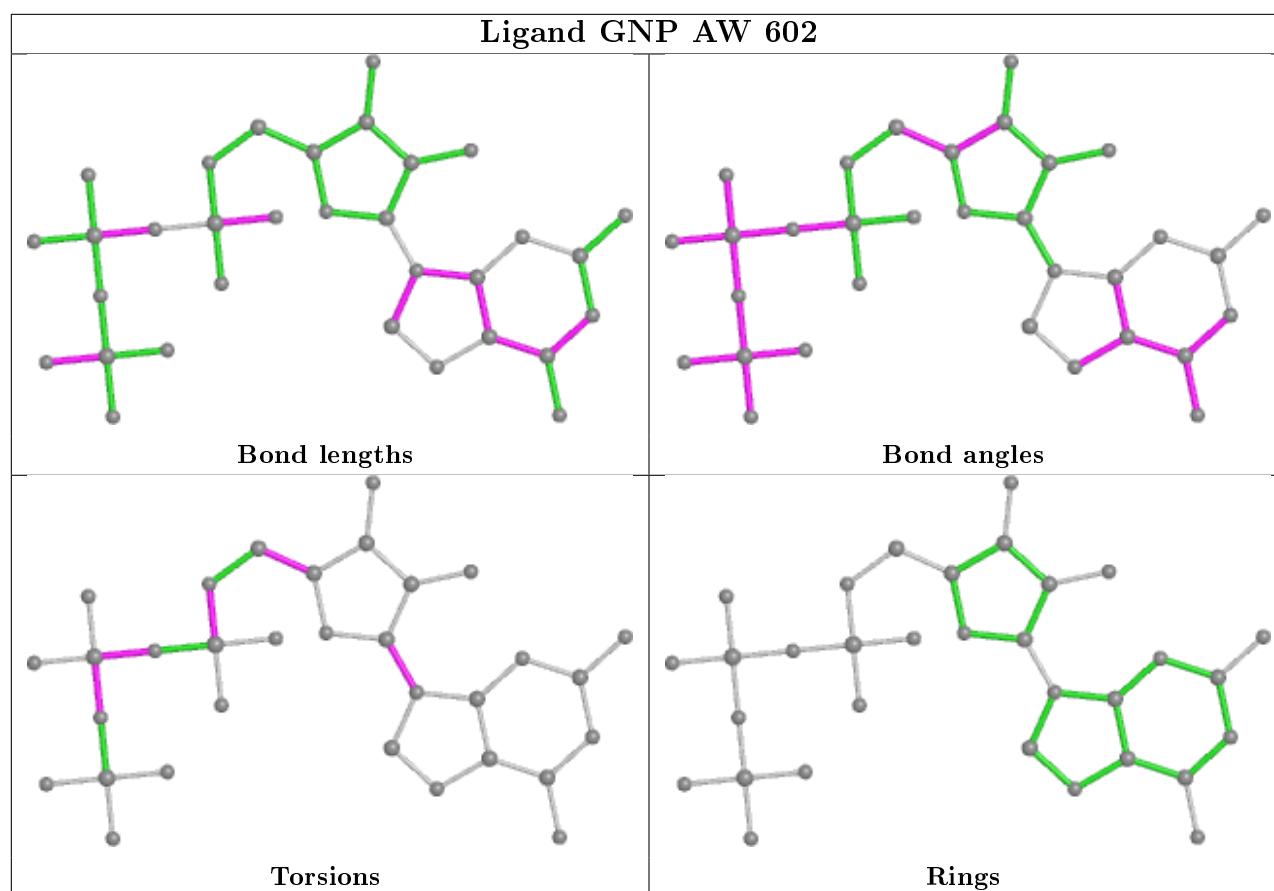
Mol	Chain	Res	Type	Atoms
58	AW	602	GNP	PG-N3B-PB-O1B
58	AW	602	GNP	PG-N3B-PB-O3A
58	AW	602	GNP	PA-O3A-PB-O1B
58	AW	602	GNP	PA-O3A-PB-O2B
58	AW	602	GNP	C5'-O5'-PA-O3A

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 [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
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%)	0.45	121 (7%) 12 6	51, 102, 197, 245	0
2	AB	218/241 (90%)	1.47	66 (30%) 0 0	91, 120, 142, 158	0
3	AC	206/233 (88%)	0.55	20 (9%) 7 4	75, 114, 132, 139	0
4	AD	205/206 (99%)	1.36	60 (29%) 0 0	86, 110, 132, 147	0
5	AE	150/167 (89%)	0.22	4 (2%) 54 39	73, 94, 129, 143	0
6	AF	100/131 (76%)	0.95	20 (20%) 1 1	98, 122, 135, 145	0
7	AG	151/156 (96%)	2.26	78 (51%) 0 0	107, 144, 159, 163	0
8	AH	129/130 (99%)	0.66	9 (6%) 16 9	77, 97, 121, 139	0
9	AI	127/130 (97%)	1.62	37 (29%) 0 0	77, 122, 148, 159	0
10	AJ	98/103 (95%)	1.22	19 (19%) 1 1	89, 106, 143, 156	0
11	AK	117/129 (90%)	0.61	9 (7%) 13 7	73, 105, 133, 150	0
12	AL	123/124 (99%)	0.58	5 (4%) 37 24	55, 74, 111, 143	0
13	AM	114/118 (96%)	3.29	70 (61%) 0 0	137, 149, 163, 165	0
14	AN	96/101 (95%)	2.49	42 (43%) 0 0	79, 128, 152, 160	0
15	AO	88/89 (98%)	0.51	7 (7%) 12 6	79, 101, 131, 142	0
16	AP	82/82 (100%)	1.59	28 (34%) 0 0	72, 95, 131, 147	0
17	AQ	80/84 (95%)	1.94	30 (37%) 0 0	78, 111, 136, 147	0
18	AR	55/75 (73%)	1.19	10 (18%) 1 1	77, 101, 126, 165	0
19	AS	79/92 (85%)	4.25	59 (74%) 0 0	131, 153, 159, 164	0
20	AT	85/87 (97%)	0.96	12 (14%) 2 2	80, 105, 126, 142	0
21	AU	51/71 (71%)	2.06	24 (47%) 0 0	106, 132, 153, 157	0
22	AV	6/27 (22%)	5.58	6 (100%) 0 0	181, 198, 202, 206	0
23	AW	525/529 (99%)	0.59	49 (9%) 8 5	47, 99, 188, 267	0
24	AY	2/6 (33%)	-0.12	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%)	1.02	10 (12%)	3 2	62, 87, 115, 129	0
26	B1	77/78 (98%)	0.60	5 (6%)	18 11	55, 71, 124, 126	0
27	B2	63/63 (100%)	0.18	4 (6%)	20 11	69, 101, 126, 140	0
28	B3	58/59 (98%)	0.86	10 (17%)	1 1	63, 75, 121, 129	0
29	B4	56/57 (98%)	0.23	4 (7%)	16 9	42, 63, 97, 125	0
30	B5	50/55 (90%)	3.26	37 (74%)	0 0	114, 128, 137, 151	0
31	B6	46/46 (100%)	0.42	2 (4%)	35 22	43, 56, 77, 114	0
32	B7	64/65 (98%)	0.37	0	100 100	57, 68, 83, 90	0
33	B8	38/38 (100%)	0.52	0	100 100	61, 78, 90, 105	0
34	BA	2853/2903 (98%)	0.29	133 (4%)	31 19	35, 67, 195, 445	0
35	BB	118/118 (100%)	0.02	0	100 100	61, 106, 152, 188	0
36	BC	271/273 (99%)	0.27	10 (3%)	41 26	36, 66, 83, 108	0
37	BD	209/209 (100%)	0.02	3 (1%)	75 63	37, 57, 89, 99	0
38	BE	201/201 (100%)	0.18	7 (3%)	44 28	37, 76, 109, 131	0
39	BF	177/179 (98%)	1.32	46 (25%)	0 0	106, 128, 152, 165	0
40	BG	176/177 (99%)	0.41	13 (7%)	14 8	54, 80, 117, 131	0
41	BH	163/165 (98%)	4.72	124 (76%)	0 0	80, 145, 163, 185	1 (0%)
42	BI	141/142 (99%)	3.87	111 (78%)	0 0	135, 157, 169, 176	0
43	BJ	30/121 (24%)	1.37	7 (23%)	0 0	126, 137, 143, 145	0
43	BK	30/121 (24%)	1.65	10 (33%)	0 0	133, 146, 152, 156	0
43	BL	30/121 (24%)	4.12	23 (76%)	0 0	132, 148, 158, 163	0
43	BM	30/121 (24%)	2.71	14 (46%)	0 0	128, 142, 149, 151	0
44	BN	142/142 (100%)	0.47	7 (4%)	29 17	45, 65, 91, 117	0
45	BO	122/123 (99%)	0.24	3 (2%)	57 43	41, 61, 84, 104	0
46	BP	143/144 (99%)	0.61	15 (10%)	6 3	41, 84, 112, 132	0
47	BQ	136/136 (100%)	0.42	6 (4%)	34 21	47, 70, 100, 126	0
48	BR	120/127 (94%)	0.31	3 (2%)	57 43	40, 56, 72, 138	0
49	BS	116/117 (99%)	1.43	34 (29%)	0 0	81, 100, 121, 128	0
50	BT	114/115 (99%)	0.25	5 (4%)	34 21	48, 71, 112, 121	0
51	BU	117/118 (99%)	0.10	3 (2%)	56 40	37, 59, 94, 108	0
52	BV	103/103 (100%)	0.35	5 (4%)	29 17	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%)	-0.04	1 (0%) 84 75	41, 54, 82, 127	0
54	BX	93/100 (93%)	1.03	16 (17%) 1 1	50, 81, 134, 144	0
55	BY	102/104 (98%)	1.30	25 (24%) 0 0	63, 84, 126, 141	0
56	BZ	94/94 (100%)	0.63	9 (9%) 8 4	68, 94, 113, 126	0
All	All	10891/11580 (94%)	0.77	1490 (13%) 3 2	35, 89, 165, 445	1 (0%)

The worst 5 of 1490 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	BH	88	HIS	21.4
34	BA	2903	U	21.0
19	AS	55	GLN	17.4
41	BH	84	TYR	17.1
41	BH	89	PRO	17.0

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	KBE	AY	1	9/10	0.51	0.60	78,79,82,82	0
24	UAL	AY	5	9/10	0.72	0.31	81,82,83,84	0
24	DPP	AY	2	6/7	0.81	0.31	79,82,82,84	0
24	5OH	AY	6	12/13	0.81	0.30	84,89,92,94	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
57	MG	AW	601	1/1	0.43	0.15	36,36,36,36	0
57	MG	AA	1686	1/1	0.44	0.62	93,93,93,93	0
57	MG	BA	3317	1/1	0.44	0.36	88,88,88,88	0
57	MG	AA	1685	1/1	0.46	0.24	64,64,64,64	0
57	MG	BA	3333	1/1	0.50	0.83	77,77,77,77	0
57	MG	BA	3204	1/1	0.53	0.53	72,72,72,72	0
57	MG	BA	3332	1/1	0.55	0.23	96,96,96,96	0
57	MG	BA	3210	1/1	0.60	0.39	73,73,73,73	0
57	MG	BA	3219	1/1	0.63	0.75	69,69,69,69	0
57	MG	BA	3338	1/1	0.64	0.13	61,61,61,61	0
57	MG	BA	3288	1/1	0.65	0.18	95,95,95,95	0
57	MG	AA	1670	1/1	0.65	0.35	62,62,62,62	0
57	MG	BA	3306	1/1	0.66	0.35	67,67,67,67	0
57	MG	BA	3242	1/1	0.69	0.27	72,72,72,72	0
57	MG	AA	1657	1/1	0.69	0.36	83,83,83,83	0
57	MG	BA	3295	1/1	0.69	0.20	57,57,57,57	0
57	MG	AA	1687	1/1	0.69	0.82	81,81,81,81	0
57	MG	BA	3349	1/1	0.69	0.34	79,79,79,79	0
57	MG	BA	3348	1/1	0.69	0.29	67,67,67,67	0
57	MG	BA	3202	1/1	0.70	0.35	57,57,57,57	0
57	MG	BA	3345	1/1	0.70	0.43	67,67,67,67	0
57	MG	BB	203	1/1	0.70	0.19	51,51,51,51	0
57	MG	BA	3280	1/1	0.72	0.36	73,73,73,73	0
57	MG	BD	301	1/1	0.72	0.22	49,49,49,49	0
57	MG	BA	3216	1/1	0.73	0.49	63,63,63,63	0
57	MG	BA	3312	1/1	0.73	0.26	56,56,56,56	0
57	MG	BA	3313	1/1	0.73	0.35	67,67,67,67	0
57	MG	AA	1701	1/1	0.74	0.16	79,79,79,79	0
57	MG	BA	3355	1/1	0.75	0.24	69,69,69,69	0
57	MG	AA	1669	1/1	0.75	0.17	71,71,71,71	0
57	MG	BA	3353	1/1	0.76	0.53	73,73,73,73	0
57	MG	AA	1658	1/1	0.76	0.47	61,61,61,61	0
57	MG	BA	3284	1/1	0.77	0.33	73,73,73,73	0
57	MG	BA	3311	1/1	0.77	0.22	48,48,48,48	0
57	MG	BA	3297	1/1	0.77	0.31	49,49,49,49	0
57	MG	BA	3172	1/1	0.77	0.19	53,53,53,53	0
57	MG	BA	3336	1/1	0.78	0.29	86,86,86,86	0
57	MG	AA	1667	1/1	0.78	0.15	87,87,87,87	0
57	MG	BA	3233	1/1	0.78	0.48	46,46,46,46	0
57	MG	BA	3356	1/1	0.78	0.23	61,61,61,61	0
57	MG	AA	1671	1/1	0.79	0.16	53,53,53,53	0
57	MG	BA	3303	1/1	0.79	0.38	56,56,56,56	0
57	MG	BA	3321	1/1	0.80	0.14	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1631	1/1	0.80	0.33	60,60,60,60	0
57	MG	BD	303	1/1	0.80	0.20	57,57,57,57	0
57	MG	BB	201	1/1	0.80	0.33	54,54,54,54	0
57	MG	BA	3327	1/1	0.80	0.24	64,64,64,64	0
57	MG	BB	208	1/1	0.81	0.29	59,59,59,59	0
57	MG	BA	3319	1/1	0.81	0.20	68,68,68,68	0
57	MG	BA	3298	1/1	0.81	0.26	76,76,76,76	0
57	MG	BA	3331	1/1	0.81	0.33	64,64,64,64	0
57	MG	AA	1678	1/1	0.81	0.53	65,65,65,65	0
57	MG	BA	3291	1/1	0.81	0.51	58,58,58,58	0
57	MG	AA	1626	1/1	0.81	0.19	45,45,45,45	0
57	MG	BA	3150	1/1	0.81	0.39	53,53,53,53	0
57	MG	BA	3240	1/1	0.81	0.52	56,56,56,56	0
57	MG	AA	1654	1/1	0.81	0.31	58,58,58,58	0
57	MG	BA	3316	1/1	0.81	0.32	61,61,61,61	0
57	MG	BA	3322	1/1	0.82	0.20	62,62,62,62	0
57	MG	BA	3185	1/1	0.82	0.28	52,52,52,52	0
57	MG	BA	3334	1/1	0.82	0.26	56,56,56,56	0
57	MG	BA	3350	1/1	0.82	0.25	80,80,80,80	0
57	MG	BA	3192	1/1	0.82	0.44	59,59,59,59	0
57	MG	BA	3294	1/1	0.82	0.27	43,43,43,43	0
57	MG	BA	3302	1/1	0.82	0.53	68,68,68,68	0
57	MG	BA	3215	1/1	0.82	0.12	53,53,53,53	0
57	MG	AA	1637	1/1	0.82	0.09	54,54,54,54	0
57	MG	BA	3225	1/1	0.82	0.41	60,60,60,60	0
57	MG	BA	3346	1/1	0.82	0.56	83,83,83,83	0
57	MG	BA	3207	1/1	0.82	0.36	54,54,54,54	0
57	MG	BC	301	1/1	0.82	0.38	53,53,53,53	0
57	MG	BA	3195	1/1	0.83	0.15	47,47,47,47	0
57	MG	AM	201	1/1	0.83	0.12	80,80,80,80	0
57	MG	AA	1652	1/1	0.83	0.26	60,60,60,60	0
57	MG	BA	3232	1/1	0.83	0.33	54,54,54,54	0
57	MG	BA	3223	1/1	0.83	1.05	75,75,75,75	0
57	MG	AL	201	1/1	0.83	0.30	54,54,54,54	0
57	MG	BA	3271	1/1	0.83	0.48	53,53,53,53	0
57	MG	AA	1679	1/1	0.83	0.30	62,62,62,62	0
57	MG	AA	1688	1/1	0.83	0.07	77,77,77,77	0
57	MG	BA	3357	1/1	0.83	0.22	81,81,81,81	0
57	MG	BA	3343	1/1	0.84	0.07	71,71,71,71	0
57	MG	BA	3337	1/1	0.84	0.27	55,55,55,55	0
57	MG	BA	3281	1/1	0.84	0.64	73,73,73,73	0
57	MG	AA	1700	1/1	0.84	0.35	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1668	1/1	0.84	0.27	51,51,51,51	0
57	MG	AA	1691	1/1	0.84	0.38	63,63,63,63	0
57	MG	AA	1647	1/1	0.84	0.25	60,60,60,60	0
57	MG	BA	3272	1/1	0.84	0.26	55,55,55,55	0
57	MG	BA	3285	1/1	0.84	0.26	75,75,75,75	0
57	MG	AA	1693	1/1	0.84	0.28	56,56,56,56	0
57	MG	BA	3170	1/1	0.84	0.38	52,52,52,52	0
57	MG	BA	3328	1/1	0.84	0.12	71,71,71,71	0
57	MG	BA	3323	1/1	0.85	0.29	64,64,64,64	0
57	MG	AA	1672	1/1	0.85	0.17	52,52,52,52	0
57	MG	AA	1663	1/1	0.85	0.26	74,74,74,74	0
57	MG	BA	3305	1/1	0.85	0.19	71,71,71,71	0
57	MG	BA	3125	1/1	0.85	0.53	53,53,53,53	0
57	MG	AA	1699	1/1	0.85	0.37	49,49,49,49	0
57	MG	BA	3169	1/1	0.85	0.26	39,39,39,39	0
57	MG	AA	1646	1/1	0.85	0.18	50,50,50,50	0
57	MG	BA	3177	1/1	0.85	0.48	59,59,59,59	0
57	MG	AA	1694	1/1	0.85	0.11	75,75,75,75	0
57	MG	BA	3257	1/1	0.85	0.31	48,48,48,48	0
57	MG	BA	3181	1/1	0.85	0.27	44,44,44,44	0
57	MG	AA	1627	1/1	0.86	0.27	40,40,40,40	0
57	MG	AF	201	1/1	0.86	0.33	65,65,65,65	0
57	MG	BA	3211	1/1	0.86	0.54	48,48,48,48	0
57	MG	BB	207	1/1	0.86	0.12	47,47,47,47	0
57	MG	BA	3296	1/1	0.86	0.29	60,60,60,60	0
57	MG	AA	1639	1/1	0.86	0.17	49,49,49,49	0
57	MG	BA	3131	1/1	0.86	0.23	40,40,40,40	0
57	MG	BA	3239	1/1	0.86	0.17	71,71,71,71	0
57	MG	BA	3324	1/1	0.86	0.24	59,59,59,59	0
57	MG	BA	3160	1/1	0.86	0.35	49,49,49,49	0
57	MG	BA	3151	1/1	0.86	0.33	47,47,47,47	0
57	MG	AA	1633	1/1	0.87	0.29	53,53,53,53	0
57	MG	AA	1655	1/1	0.87	0.26	60,60,60,60	0
57	MG	BA	3259	1/1	0.87	0.10	69,69,69,69	0
57	MG	BA	3104	1/1	0.87	0.25	45,45,45,45	0
57	MG	BA	3189	1/1	0.87	0.12	51,51,51,51	0
57	MG	BD	302	1/1	0.87	0.48	53,53,53,53	0
57	MG	BA	3127	1/1	0.87	0.27	38,38,38,38	0
57	MG	AA	1689	1/1	0.87	0.28	69,69,69,69	0
57	MG	BA	3196	1/1	0.87	0.54	46,46,46,46	0
57	MG	BA	3148	1/1	0.87	0.23	50,50,50,50	0
57	MG	BA	3105	1/1	0.87	0.42	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1696	1/1	0.87	0.24	89,89,89,89	0
57	MG	AA	1675	1/1	0.87	0.18	57,57,57,57	0
57	MG	BA	3159	1/1	0.87	0.49	49,49,49,49	0
57	MG	BA	3246	1/1	0.87	0.27	48,48,48,48	0
57	MG	AA	1641	1/1	0.87	0.24	67,67,67,67	0
57	MG	BA	3314	1/1	0.87	0.42	56,56,56,56	0
57	MG	BA	3206	1/1	0.87	0.24	52,52,52,52	0
57	MG	BA	3262	1/1	0.88	0.29	85,85,85,85	0
57	MG	BE	301	1/1	0.88	0.09	67,67,67,67	0
57	MG	BA	3097	1/1	0.88	0.41	48,48,48,48	0
57	MG	AA	1648	1/1	0.88	0.13	54,54,54,54	0
57	MG	BA	3282	1/1	0.88	0.25	55,55,55,55	0
57	MG	BA	3214	1/1	0.88	0.23	43,43,43,43	0
57	MG	AA	1644	1/1	0.88	0.18	49,49,49,49	0
57	MG	BA	3146	1/1	0.88	0.33	40,40,40,40	0
57	MG	BA	3320	1/1	0.88	0.21	52,52,52,52	0
57	MG	BA	3137	1/1	0.88	0.57	42,42,42,42	0
57	MG	BA	3227	1/1	0.88	0.25	63,63,63,63	0
57	MG	BA	3267	1/1	0.88	0.21	52,52,52,52	0
57	MG	BA	3132	1/1	0.89	0.26	52,52,52,52	0
57	MG	BA	3299	1/1	0.89	0.17	64,64,64,64	0
57	MG	BA	3255	1/1	0.89	0.34	66,66,66,66	0
57	MG	BA	3220	1/1	0.89	0.32	56,56,56,56	0
57	MG	BA	3165	1/1	0.89	0.50	52,52,52,52	0
57	MG	AA	1606	1/1	0.89	0.37	45,45,45,45	0
57	MG	AA	1651	1/1	0.89	0.30	51,51,51,51	0
57	MG	BA	3252	1/1	0.89	0.33	49,49,49,49	0
57	MG	BA	3075	1/1	0.89	0.13	43,43,43,43	0
57	MG	AA	1677	1/1	0.89	0.48	57,57,57,57	0
57	MG	BA	3286	1/1	0.89	0.20	48,48,48,48	0
57	MG	BA	3275	1/1	0.89	0.12	59,59,59,59	0
57	MG	BA	3238	1/1	0.89	0.17	50,50,50,50	0
57	MG	AA	1684	1/1	0.89	0.50	60,60,60,60	0
57	MG	BA	3351	1/1	0.89	0.19	58,58,58,58	0
57	MG	BA	3228	1/1	0.89	0.23	42,42,42,42	0
57	MG	BA	3201	1/1	0.89	0.20	47,47,47,47	0
57	MG	AA	1702	1/1	0.89	0.32	58,58,58,58	0
57	MG	AA	1623	1/1	0.90	0.29	42,42,42,42	0
57	MG	BA	3300	1/1	0.90	0.55	69,69,69,69	0
57	MG	BA	3065	1/1	0.90	0.36	46,46,46,46	0
57	MG	BA	3354	1/1	0.90	0.12	62,62,62,62	0
57	MG	BA	3093	1/1	0.90	0.24	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1683	1/1	0.90	0.22	63,63,63,63	0
57	MG	BB	205	1/1	0.90	0.12	79,79,79,79	0
57	MG	AA	1604	1/1	0.90	0.50	42,42,42,42	0
57	MG	BA	3116	1/1	0.90	0.24	41,41,41,41	0
57	MG	BA	3091	1/1	0.90	0.40	42,42,42,42	0
57	MG	AA	1682	1/1	0.90	0.12	76,76,76,76	0
57	MG	BQ	201	1/1	0.90	0.17	44,44,44,44	0
57	MG	BA	3344	1/1	0.90	0.14	71,71,71,71	0
57	MG	BA	3274	1/1	0.90	0.12	52,52,52,52	0
57	MG	BA	3253	1/1	0.90	0.14	65,65,65,65	0
57	MG	BA	3293	1/1	0.90	0.38	53,53,53,53	0
57	MG	AA	1692	1/1	0.90	0.16	67,67,67,67	0
57	MG	BA	3235	1/1	0.90	0.22	64,64,64,64	0
57	MG	BA	3352	1/1	0.90	0.29	61,61,61,61	0
57	MG	BA	3138	1/1	0.90	0.34	58,58,58,58	0
57	MG	BA	3264	1/1	0.90	0.20	67,67,67,67	0
57	MG	BA	3197	1/1	0.90	0.16	38,38,38,38	0
57	MG	BA	3047	1/1	0.90	0.42	51,51,51,51	0
57	MG	BA	3222	1/1	0.91	0.14	50,50,50,50	0
57	MG	BA	3270	1/1	0.91	0.29	59,59,59,59	0
57	MG	AA	1681	1/1	0.91	0.15	38,38,38,38	0
57	MG	BA	3261	1/1	0.91	0.22	63,63,63,63	0
57	MG	BA	3342	1/1	0.91	0.26	54,54,54,54	0
57	MG	BA	3028	1/1	0.91	0.36	26,26,26,26	0
57	MG	BA	3318	1/1	0.91	0.31	57,57,57,57	0
57	MG	BB	202	1/1	0.91	0.24	43,43,43,43	0
57	MG	BA	3260	1/1	0.91	0.24	50,50,50,50	0
57	MG	BA	3174	1/1	0.91	0.26	49,49,49,49	0
57	MG	BA	3164	1/1	0.91	0.14	45,45,45,45	0
57	MG	AA	1635	1/1	0.91	0.29	58,58,58,58	0
57	MG	BA	3256	1/1	0.91	0.19	56,56,56,56	0
57	MG	B0	103	1/1	0.91	0.53	54,54,54,54	0
57	MG	BA	3208	1/1	0.91	0.26	62,62,62,62	0
57	MG	BA	3335	1/1	0.91	0.17	58,58,58,58	0
57	MG	BA	3130	1/1	0.91	0.43	41,41,41,41	0
57	MG	BA	3175	1/1	0.91	0.15	44,44,44,44	0
57	MG	AA	1656	1/1	0.91	0.15	73,73,73,73	0
57	MG	BA	3266	1/1	0.91	0.30	56,56,56,56	0
57	MG	BA	3292	1/1	0.91	0.28	54,54,54,54	0
57	MG	BA	3229	1/1	0.91	0.09	46,46,46,46	0
57	MG	BB	206	1/1	0.91	0.08	65,65,65,65	0
57	MG	BA	3268	1/1	0.91	0.28	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3139	1/1	0.92	0.42	43,43,43,43	0
57	MG	BX	201	1/1	0.92	0.29	47,47,47,47	0
57	MG	BA	3017	1/1	0.92	0.34	30,30,30,30	0
57	MG	BA	3247	1/1	0.92	0.17	61,61,61,61	0
57	MG	BA	3213	1/1	0.92	0.32	46,46,46,46	0
57	MG	AA	1674	1/1	0.92	0.14	55,55,55,55	0
57	MG	BA	3187	1/1	0.92	0.10	56,56,56,56	0
57	MG	AA	1680	1/1	0.92	0.07	55,55,55,55	0
57	MG	BA	3279	1/1	0.92	0.11	50,50,50,50	0
57	MG	AH	201	1/1	0.92	0.21	50,50,50,50	0
57	MG	BA	3089	1/1	0.92	0.07	52,52,52,52	0
57	MG	BA	3070	1/1	0.92	0.34	44,44,44,44	0
57	MG	BA	3289	1/1	0.92	0.17	62,62,62,62	0
57	MG	BA	3205	1/1	0.92	0.21	50,50,50,50	0
57	MG	AA	1625	1/1	0.92	0.22	40,40,40,40	0
57	MG	BA	3188	1/1	0.92	0.27	51,51,51,51	0
57	MG	BA	3025	1/1	0.92	0.31	32,32,32,32	0
57	MG	BA	3308	1/1	0.92	0.44	82,82,82,82	0
57	MG	BA	3087	1/1	0.92	0.46	42,42,42,42	0
57	MG	BA	3198	1/1	0.92	0.15	60,60,60,60	0
57	MG	AA	1610	1/1	0.92	0.32	45,45,45,45	0
57	MG	AA	1638	1/1	0.92	0.20	55,55,55,55	0
57	MG	AA	1676	1/1	0.92	0.41	52,52,52,52	0
57	MG	BA	3226	1/1	0.92	0.24	51,51,51,51	0
57	MG	BT	201	1/1	0.92	0.12	40,40,40,40	0
57	MG	BA	3263	1/1	0.92	0.23	53,53,53,53	0
57	MG	BA	3249	1/1	0.92	0.09	49,49,49,49	0
57	MG	BA	3030	1/1	0.92	0.27	38,38,38,38	0
57	MG	BA	3265	1/1	0.92	0.32	45,45,45,45	0
57	MG	BA	3241	1/1	0.92	0.25	57,57,57,57	0
57	MG	BA	3144	1/1	0.93	0.12	68,68,68,68	0
57	MG	BA	3031	1/1	0.93	0.39	25,25,25,25	0
57	MG	AA	1690	1/1	0.93	0.29	83,83,83,83	0
57	MG	AA	1650	1/1	0.93	0.23	67,67,67,67	0
57	MG	BA	3200	1/1	0.93	0.40	44,44,44,44	0
57	MG	BA	3244	1/1	0.93	0.46	76,76,76,76	0
57	MG	BA	3140	1/1	0.93	0.16	46,46,46,46	0
57	MG	BA	3161	1/1	0.93	0.21	42,42,42,42	0
57	MG	BA	3083	1/1	0.93	0.35	47,47,47,47	0
57	MG	BA	3325	1/1	0.93	0.36	59,59,59,59	0
57	MG	BA	3109	1/1	0.93	0.13	38,38,38,38	0
57	MG	BA	3145	1/1	0.93	0.23	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3110	1/1	0.93	0.30	38,38,38,38	0
57	MG	BA	3248	1/1	0.93	0.17	52,52,52,52	0
57	MG	BA	3231	1/1	0.93	0.09	56,56,56,56	0
57	MG	BA	3167	1/1	0.93	0.41	48,48,48,48	0
57	MG	BA	3133	1/1	0.93	0.27	45,45,45,45	0
57	MG	AA	1617	1/1	0.93	0.19	47,47,47,47	0
57	MG	BA	3171	1/1	0.93	0.27	57,57,57,57	0
57	MG	BA	3136	1/1	0.93	0.65	53,53,53,53	0
57	MG	BA	3152	1/1	0.93	0.07	41,41,41,41	0
57	MG	BA	3278	1/1	0.93	0.32	48,48,48,48	0
57	MG	AA	1659	1/1	0.93	0.12	55,55,55,55	0
57	MG	BA	3108	1/1	0.93	0.19	42,42,42,42	0
57	MG	BA	3064	1/1	0.93	0.22	24,24,24,24	0
57	MG	BA	3147	1/1	0.93	0.22	46,46,46,46	0
57	MG	AA	1602	1/1	0.93	0.31	37,37,37,37	0
57	MG	BA	3037	1/1	0.93	0.45	36,36,36,36	0
57	MG	B4	101	1/1	0.93	0.42	40,40,40,40	0
57	MG	BA	3179	1/1	0.93	0.15	46,46,46,46	0
57	MG	AA	1613	1/1	0.93	0.18	58,58,58,58	0
57	MG	BA	3048	1/1	0.93	0.39	40,40,40,40	0
57	MG	BA	3154	1/1	0.93	0.56	43,43,43,43	0
57	MG	BA	3142	1/1	0.93	0.22	50,50,50,50	0
57	MG	BA	3050	1/1	0.93	0.40	33,33,33,33	0
57	MG	BA	3277	1/1	0.93	0.25	42,42,42,42	0
57	MG	BA	3176	1/1	0.93	0.28	50,50,50,50	0
57	MG	AA	1643	1/1	0.93	0.39	56,56,56,56	0
57	MG	BA	3341	1/1	0.93	0.53	57,57,57,57	0
57	MG	BA	3168	1/1	0.93	0.15	32,32,32,32	0
57	MG	AA	1661	1/1	0.93	0.25	49,49,49,49	0
57	MG	BA	3234	1/1	0.93	0.47	49,49,49,49	0
57	MG	BB	204	1/1	0.93	0.12	53,53,53,53	0
57	MG	BA	3287	1/1	0.93	0.23	83,83,83,83	0
57	MG	BA	3014	1/1	0.94	0.22	27,27,27,27	0
57	MG	BA	3180	1/1	0.94	0.12	45,45,45,45	0
57	MG	AA	1634	1/1	0.94	0.34	55,55,55,55	0
57	MG	BA	3061	1/1	0.94	0.27	48,48,48,48	0
57	MG	BA	3173	1/1	0.94	0.11	36,36,36,36	0
57	MG	AA	1621	1/1	0.94	0.39	57,57,57,57	0
57	MG	BA	3184	1/1	0.94	0.14	37,37,37,37	0
57	MG	AA	1622	1/1	0.94	0.29	42,42,42,42	0
57	MG	BA	3347	1/1	0.94	0.14	76,76,76,76	0
57	MG	BA	3007	1/1	0.94	0.37	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	B0	101	1/1	0.94	0.11	23,23,23,23	0
57	MG	BA	3067	1/1	0.94	0.29	35,35,35,35	0
57	MG	BA	3330	1/1	0.94	0.16	83,83,83,83	0
57	MG	BA	3016	1/1	0.94	0.38	39,39,39,39	0
57	MG	AA	1645	1/1	0.94	0.44	62,62,62,62	0
57	MG	BA	3141	1/1	0.94	0.19	54,54,54,54	0
57	MG	BA	3290	1/1	0.94	0.10	56,56,56,56	0
57	MG	BA	3315	1/1	0.94	0.19	63,63,63,63	0
57	MG	BA	3149	1/1	0.94	0.32	42,42,42,42	0
57	MG	BA	3062	1/1	0.94	0.33	42,42,42,42	0
57	MG	AA	1624	1/1	0.94	0.45	51,51,51,51	0
57	MG	BA	3158	1/1	0.94	0.26	35,35,35,35	0
57	MG	BA	3329	1/1	0.94	0.24	58,58,58,58	0
57	MG	BA	3096	1/1	0.94	0.37	44,44,44,44	0
57	MG	BA	3121	1/1	0.94	0.48	39,39,39,39	0
57	MG	BA	3060	1/1	0.94	0.39	27,27,27,27	0
57	MG	AA	1665	1/1	0.94	0.53	56,56,56,56	0
57	MG	AA	1607	1/1	0.94	0.33	33,33,33,33	0
57	MG	BA	3099	1/1	0.94	0.46	44,44,44,44	0
57	MG	BA	3128	1/1	0.94	0.29	33,33,33,33	0
57	MG	BA	3304	1/1	0.94	0.46	50,50,50,50	0
57	MG	BA	3218	1/1	0.94	0.22	50,50,50,50	0
57	MG	BA	3078	1/1	0.94	0.42	32,32,32,32	0
57	MG	BA	3250	1/1	0.94	0.64	66,66,66,66	0
57	MG	BA	3019	1/1	0.94	0.23	15,15,15,15	0
57	MG	BA	3072	1/1	0.94	0.22	36,36,36,36	0
57	MG	BA	3076	1/1	0.95	0.19	36,36,36,36	0
57	MG	AA	1636	1/1	0.95	0.16	36,36,36,36	0
57	MG	BA	3301	1/1	0.95	0.23	64,64,64,64	0
57	MG	BA	3115	1/1	0.95	0.24	37,37,37,37	0
57	MG	AA	1603	1/1	0.95	0.44	42,42,42,42	0
57	MG	BA	3209	1/1	0.95	0.10	42,42,42,42	0
57	MG	BA	3254	1/1	0.95	0.22	59,59,59,59	0
57	MG	AA	1662	1/1	0.95	0.34	57,57,57,57	0
57	MG	AA	1630	1/1	0.95	0.44	48,48,48,48	0
57	MG	AA	1629	1/1	0.95	0.26	41,41,41,41	0
57	MG	BA	3276	1/1	0.95	0.31	58,58,58,58	0
57	MG	BA	3118	1/1	0.95	0.26	40,40,40,40	0
57	MG	AA	1612	1/1	0.95	0.22	29,29,29,29	0
57	MG	BA	3135	1/1	0.95	0.15	45,45,45,45	0
57	MG	AA	1619	1/1	0.95	0.18	40,40,40,40	0
57	MG	BA	3038	1/1	0.95	0.19	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1698	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3340	1/1	0.95	0.49	61,61,61,61	0
57	MG	BA	3022	1/1	0.95	0.29	28,28,28,28	0
57	MG	BN	201	1/1	0.95	0.30	51,51,51,51	0
57	MG	BA	3178	1/1	0.95	0.26	49,49,49,49	0
57	MG	BA	3310	1/1	0.95	0.17	75,75,75,75	0
57	MG	BA	3221	1/1	0.95	0.37	43,43,43,43	0
57	MG	BA	3114	1/1	0.95	0.33	32,32,32,32	0
57	MG	BA	3193	1/1	0.95	0.48	61,61,61,61	0
57	MG	B2	101	1/1	0.95	0.12	49,49,49,49	0
57	MG	BA	3199	1/1	0.95	0.43	42,42,42,42	0
57	MG	BA	3036	1/1	0.95	0.28	43,43,43,43	0
57	MG	BA	3190	1/1	0.95	0.58	43,43,43,43	0
57	MG	BA	3026	1/1	0.95	0.31	24,24,24,24	0
57	MG	AL	202	1/1	0.95	0.15	73,73,73,73	0
57	MG	BA	3077	1/1	0.95	0.57	41,41,41,41	0
57	MG	BA	3023	1/1	0.95	0.41	39,39,39,39	0
57	MG	AA	1605	1/1	0.95	0.24	38,38,38,38	0
57	MG	BA	3251	1/1	0.95	0.24	49,49,49,49	0
57	MG	BA	3237	1/1	0.95	0.14	51,51,51,51	0
57	MG	BA	3217	1/1	0.95	0.06	56,56,56,56	0
57	MG	BA	3157	1/1	0.95	0.51	46,46,46,46	0
57	MG	BA	3269	1/1	0.95	0.26	51,51,51,51	0
57	MG	BA	3074	1/1	0.95	0.40	44,44,44,44	0
57	MG	BA	3124	1/1	0.95	0.56	42,42,42,42	0
57	MG	BA	3134	1/1	0.95	0.63	49,49,49,49	0
57	MG	BA	3183	1/1	0.95	0.26	48,48,48,48	0
57	MG	BA	3243	1/1	0.95	0.07	62,62,62,62	0
57	MG	BA	3080	1/1	0.95	0.23	43,43,43,43	0
57	MG	BA	3088	1/1	0.95	0.27	36,36,36,36	0
57	MG	AA	1616	1/1	0.95	0.35	37,37,37,37	0
57	MG	AA	1673	1/1	0.95	0.48	84,84,84,84	0
57	MG	BA	3129	1/1	0.95	0.21	43,43,43,43	0
57	MG	BA	3156	1/1	0.95	0.18	41,41,41,41	0
57	MG	BA	3095	1/1	0.95	0.28	42,42,42,42	0
57	MG	BA	3307	1/1	0.95	0.22	52,52,52,52	0
58	GNP	AW	602	32/32	0.95	0.16	58,71,81,83	0
57	MG	AA	1653	1/1	0.96	0.17	41,41,41,41	0
57	MG	AA	1632	1/1	0.96	0.44	40,40,40,40	0
57	MG	AA	1620	1/1	0.96	0.16	52,52,52,52	0
57	MG	BA	3035	1/1	0.96	0.33	26,26,26,26	0
57	MG	BA	3081	1/1	0.96	0.39	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3123	1/1	0.96	0.31	36,36,36,36	0
57	MG	BA	3051	1/1	0.96	0.26	33,33,33,33	0
57	MG	BA	3098	1/1	0.96	0.13	47,47,47,47	0
57	MG	BA	3186	1/1	0.96	0.24	47,47,47,47	0
57	MG	BA	3245	1/1	0.96	0.50	46,46,46,46	0
57	MG	BA	3063	1/1	0.96	0.45	32,32,32,32	0
57	MG	BA	3041	1/1	0.96	0.29	27,27,27,27	0
57	MG	BA	3339	1/1	0.96	0.15	76,76,76,76	0
57	MG	AA	1695	1/1	0.96	0.10	62,62,62,62	0
57	MG	BA	3032	1/1	0.96	0.54	38,38,38,38	0
57	MG	BA	3283	1/1	0.96	0.33	25,25,25,25	0
57	MG	BR	201	1/1	0.96	0.15	69,69,69,69	0
57	MG	BA	3102	1/1	0.96	0.30	36,36,36,36	0
57	MG	BA	3071	1/1	0.96	0.39	35,35,35,35	0
57	MG	AA	1611	1/1	0.96	0.40	44,44,44,44	0
57	MG	BA	3224	1/1	0.96	0.13	41,41,41,41	0
57	MG	BA	3101	1/1	0.96	0.23	43,43,43,43	0
57	MG	BA	3044	1/1	0.96	0.42	37,37,37,37	0
57	MG	AA	1608	1/1	0.96	0.19	59,59,59,59	0
57	MG	BB	209	1/1	0.96	0.34	36,36,36,36	0
57	MG	BA	3162	1/1	0.96	0.11	56,56,56,56	0
57	MG	AA	1697	1/1	0.96	0.11	64,64,64,64	0
57	MG	BA	3230	1/1	0.96	0.21	46,46,46,46	0
57	MG	AA	1666	1/1	0.96	0.36	62,62,62,62	0
57	MG	BO	201	1/1	0.96	0.17	41,41,41,41	0
57	MG	AA	1649	1/1	0.96	0.39	49,49,49,49	0
57	MG	BA	3086	1/1	0.97	0.44	43,43,43,43	0
57	MG	BA	3027	1/1	0.97	0.43	40,40,40,40	0
57	MG	BA	3045	1/1	0.97	0.46	35,35,35,35	0
57	MG	BA	3009	1/1	0.97	0.33	14,14,14,14	0
57	MG	BA	3182	1/1	0.97	0.57	48,48,48,48	0
57	MG	BA	3018	1/1	0.97	0.25	16,16,16,16	0
57	MG	BA	3153	1/1	0.97	0.26	59,59,59,59	0
57	MG	BA	3001	1/1	0.97	0.42	42,42,42,42	0
57	MG	BA	3273	1/1	0.97	0.57	72,72,72,72	0
57	MG	BA	3155	1/1	0.97	0.69	51,51,51,51	0
57	MG	BA	3020	1/1	0.97	0.41	29,29,29,29	0
57	MG	BA	3122	1/1	0.97	0.21	38,38,38,38	0
57	MG	BA	3068	1/1	0.97	0.30	28,28,28,28	0
57	MG	BA	3049	1/1	0.97	0.24	31,31,31,31	0
57	MG	AA	1614	1/1	0.97	0.18	42,42,42,42	0
57	MG	AA	1660	1/1	0.97	0.17	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3021	1/1	0.97	0.34	18,18,18,18	0
57	MG	BR	202	1/1	0.97	0.18	51,51,51,51	0
57	MG	BA	3079	1/1	0.97	0.68	44,44,44,44	0
57	MG	BA	3194	1/1	0.97	0.24	49,49,49,49	0
57	MG	BA	3112	1/1	0.97	0.27	41,41,41,41	0
57	MG	BA	3117	1/1	0.97	0.21	46,46,46,46	0
57	MG	BA	3212	1/1	0.97	0.21	45,45,45,45	0
57	MG	BA	3191	1/1	0.97	0.10	57,57,57,57	0
57	MG	BA	3326	1/1	0.97	0.14	42,42,42,42	0
57	MG	AA	1615	1/1	0.97	0.29	40,40,40,40	0
57	MG	BA	3094	1/1	0.97	0.19	47,47,47,47	0
57	MG	BA	3034	1/1	0.97	0.30	36,36,36,36	0
57	MG	BA	3163	1/1	0.97	0.21	49,49,49,49	0
57	MG	BA	3126	1/1	0.97	0.26	31,31,31,31	0
57	MG	BA	3012	1/1	0.97	0.43	18,18,18,18	0
57	MG	BA	3059	1/1	0.97	0.20	43,43,43,43	0
57	MG	BA	3008	1/1	0.97	0.29	22,22,22,22	0
57	MG	BA	3029	1/1	0.97	0.39	28,28,28,28	0
57	MG	BA	3054	1/1	0.97	0.43	36,36,36,36	0
57	MG	AA	1609	1/1	0.97	0.49	40,40,40,40	0
57	MG	BA	3040	1/1	0.97	0.42	43,43,43,43	0
57	MG	BA	3056	1/1	0.97	0.22	26,26,26,26	0
57	MG	BA	3103	1/1	0.97	0.33	28,28,28,28	0
57	MG	AA	1618	1/1	0.97	0.27	49,49,49,49	0
57	MG	BA	3003	1/1	0.97	0.42	18,18,18,18	0
57	MG	BA	3106	1/1	0.97	0.23	37,37,37,37	0
57	MG	BA	3120	1/1	0.97	0.09	31,31,31,31	0
57	MG	AA	1640	1/1	0.97	0.09	41,41,41,41	0
57	MG	BA	3042	1/1	0.98	0.33	27,27,27,27	0
57	MG	BA	3111	1/1	0.98	0.23	29,29,29,29	0
57	MG	BD	304	1/1	0.98	0.41	28,28,28,28	0
57	MG	BA	3203	1/1	0.98	0.31	50,50,50,50	0
57	MG	BA	3058	1/1	0.98	0.32	35,35,35,35	0
57	MG	BD	305	1/1	0.98	0.16	16,16,16,16	0
57	MG	BA	3258	1/1	0.98	0.14	50,50,50,50	0
57	MG	BA	3055	1/1	0.98	0.42	24,24,24,24	0
57	MG	BA	3024	1/1	0.98	0.42	32,32,32,32	0
57	MG	BA	3100	1/1	0.98	0.43	36,36,36,36	0
57	MG	BA	3004	1/1	0.98	0.25	21,21,21,21	0
57	MG	BA	3015	1/1	0.98	0.58	38,38,38,38	0
57	MG	BA	3085	1/1	0.98	0.23	40,40,40,40	0
57	MG	BA	3236	1/1	0.98	0.21	46,46,46,46	0

Continued on next page...

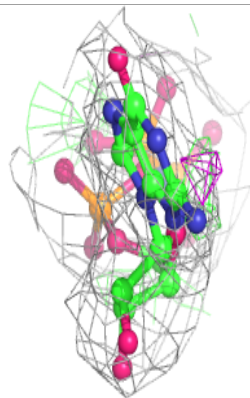
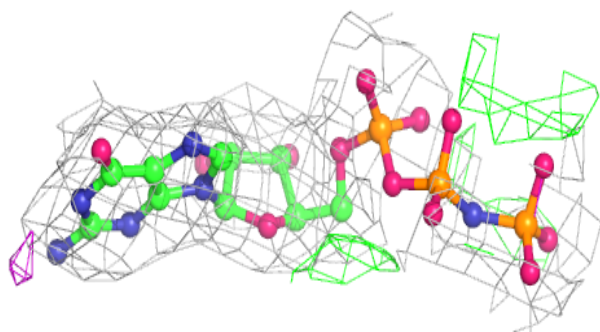
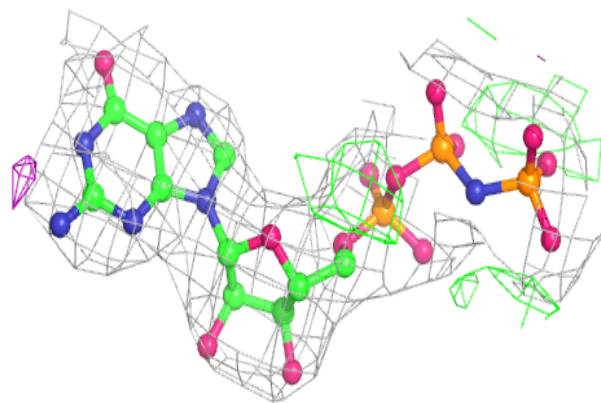
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3046	1/1	0.98	0.42	27,27,27,27	0
57	MG	BA	3309	1/1	0.98	0.14	62,62,62,62	0
57	MG	AA	1628	1/1	0.98	0.28	44,44,44,44	0
57	MG	BA	3082	1/1	0.98	0.38	36,36,36,36	0
57	MG	B0	102	1/1	0.98	0.30	33,33,33,33	0
57	MG	BA	3092	1/1	0.98	0.54	43,43,43,43	0
57	MG	BA	3090	1/1	0.98	0.46	40,40,40,40	0
57	MG	AA	1642	1/1	0.98	0.28	53,53,53,53	0
57	MG	BA	3005	1/1	0.98	0.25	20,20,20,20	0
57	MG	BA	3073	1/1	0.98	0.49	42,42,42,42	0
57	MG	BA	3039	1/1	0.98	0.40	31,31,31,31	0
57	MG	AA	1664	1/1	0.98	0.20	41,41,41,41	0
57	MG	BA	3002	1/1	0.98	0.20	13,13,13,13	0
57	MG	BA	3057	1/1	0.98	0.30	33,33,33,33	0
57	MG	BA	3066	1/1	0.98	0.49	41,41,41,41	0
57	MG	BA	3107	1/1	0.98	0.31	36,36,36,36	0
57	MG	BA	3119	1/1	0.98	0.26	29,29,29,29	0
57	MG	AA	1601	1/1	0.98	0.27	22,22,22,22	0
57	MG	BA	3143	1/1	0.98	0.19	32,32,32,32	0
57	MG	BA	3013	1/1	0.99	0.38	20,20,20,20	0
57	MG	BA	3053	1/1	0.99	0.51	31,31,31,31	0
57	MG	BA	3069	1/1	0.99	0.24	39,39,39,39	0
57	MG	BA	3011	1/1	0.99	0.50	23,23,23,23	0
57	MG	BA	3010	1/1	0.99	0.28	33,33,33,33	0
57	MG	BA	3052	1/1	0.99	0.38	39,39,39,39	0
57	MG	BA	3084	1/1	0.99	0.32	21,21,21,21	0
57	MG	BA	3006	1/1	0.99	0.37	22,22,22,22	0
57	MG	BA	3043	1/1	0.99	0.46	26,26,26,26	0
57	MG	BA	3033	1/1	0.99	0.42	25,25,25,25	0
57	MG	BA	3166	1/1	0.99	0.07	50,50,50,50	0
57	MG	BA	3113	1/1	0.99	0.27	34,34,34,34	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.