wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 10:29 PM EST

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

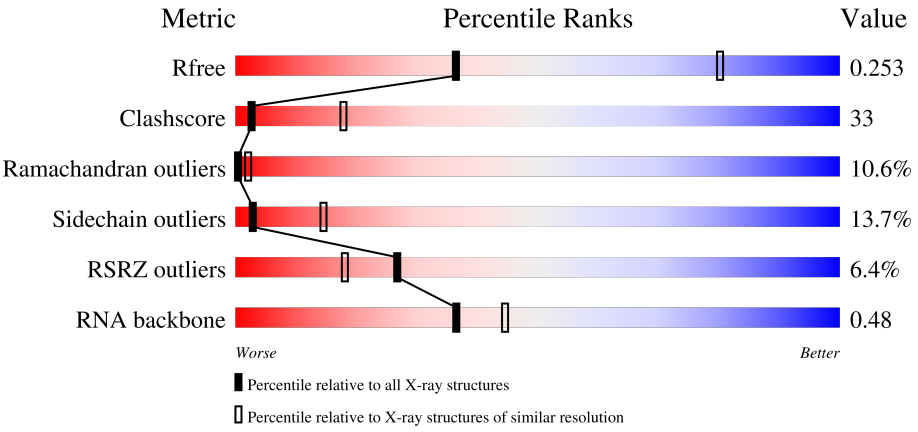
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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.



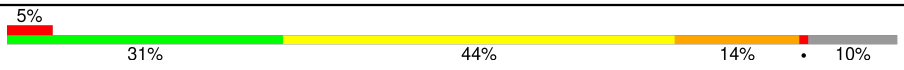
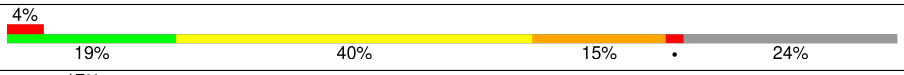
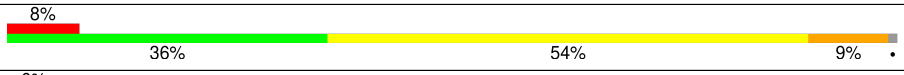
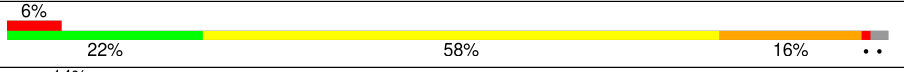
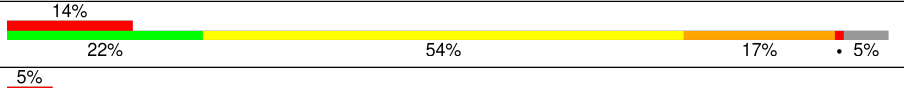
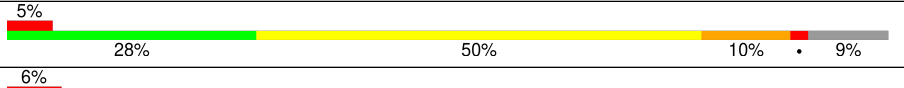
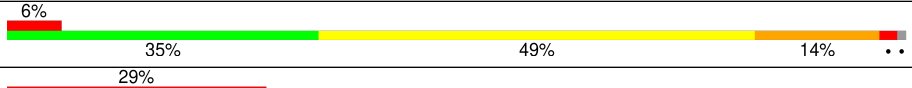
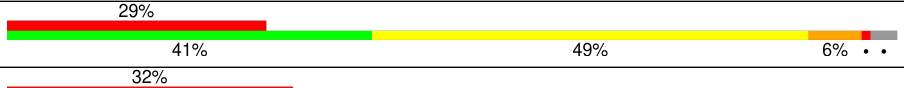
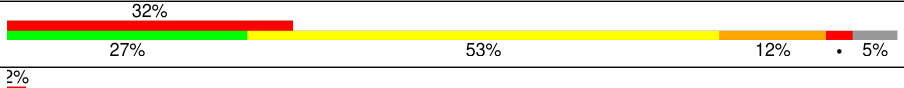
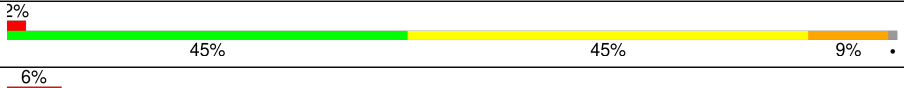
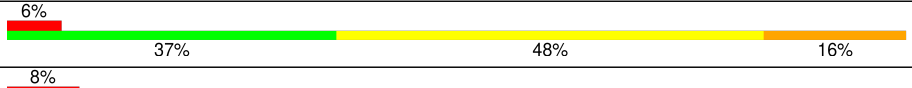
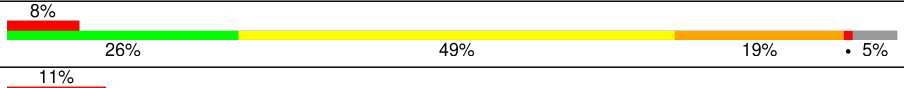
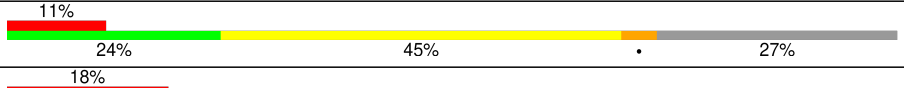
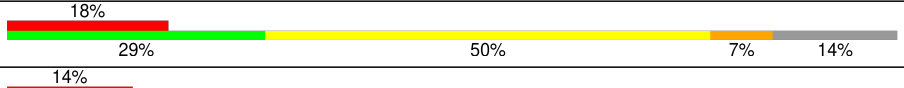
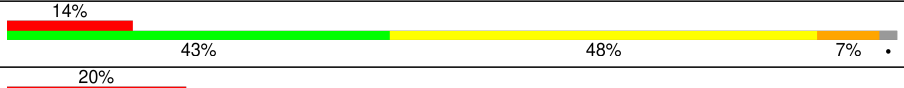
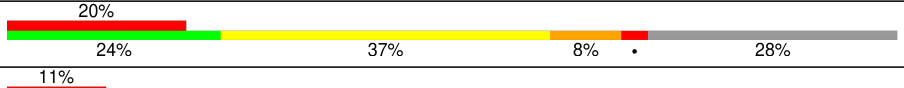
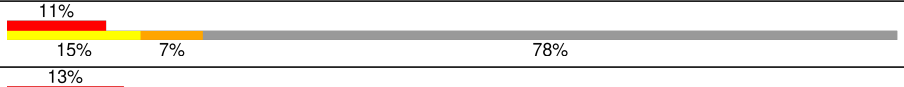
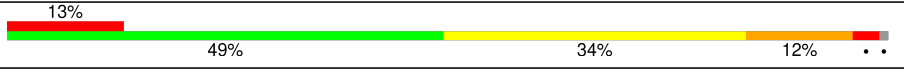
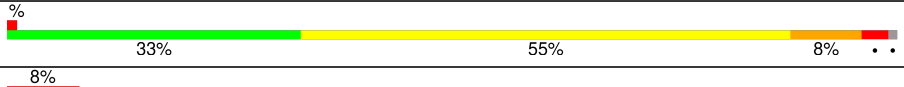
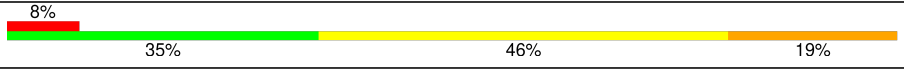
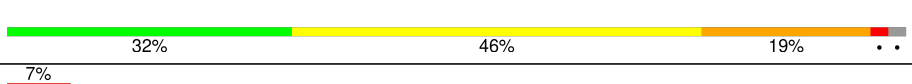
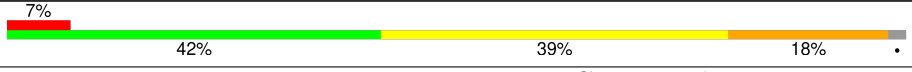
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 28% 56% 16%
2	AB	241	8% 25% 45% 17% 10%
3	AC	233	5% 30% 44% 13% 12%
4	AD	206	15% 27% 57% 15%

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	11% 29% 53% 7% 9%
31	B6	46	7% 65% 26% 9%
32	B7	65	2% 51% 43%
33	B8	38	3% 34% 50% 16%
34	BA	2903	% 34% 49% 14%
35	BB	118	36% 50% 14%
36	BC	273	4% 32% 51% 15%
37	BD	209	2% 33% 47% 19%
38	BE	201	3% 36% 47% 15%
39	BF	179	5% 34% 52% 12%
40	BG	177	3% 41% 40% 15%
41	BH	165	34% 18% 61% 16%
42	BI	142	33% 36% 53% 11%
43	BJ	121	3% 6% 13% 6% 75%
43	BK	121	5% 13% 10% 75%
43	BL	121	12% 7% 16% 75%
43	BM	121	3% 7% 15% 75%
44	BN	142	7% 30% 52% 14%
45	BO	123	3% 26% 51% 20%
46	BP	144	3% 36% 49% 12%
47	BQ	136	% 41% 46% 12%
48	BR	127	% 37% 45% 11% 6%
49	BS	117	3% 32% 54% 13%
50	BT	115	3% 29% 47% 21%
51	BU	118	3% 37% 49% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	BV	103	3% 31% 54% 15%
53	BW	116	44% 37% 12% 5%
54	BX	100	5% 21% 46% 23% 7%
55	BY	104	7% 37% 46% 15%
56	BZ	94	2% 52% 37% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	KBE	AY	1	-	-	X	-
24	UAL	AY	5	-	-	X	-
24	5OH	AY	6	-	-	X	-
57	MG	BA	3349	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	P			
1	AA	1532	32873	14661	6031	10649	1532	0	0	0

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

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	1624	1028	305	288	3	0	0	0

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	150	1105	687	211	201	6	0	0	0

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

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

- 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	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).

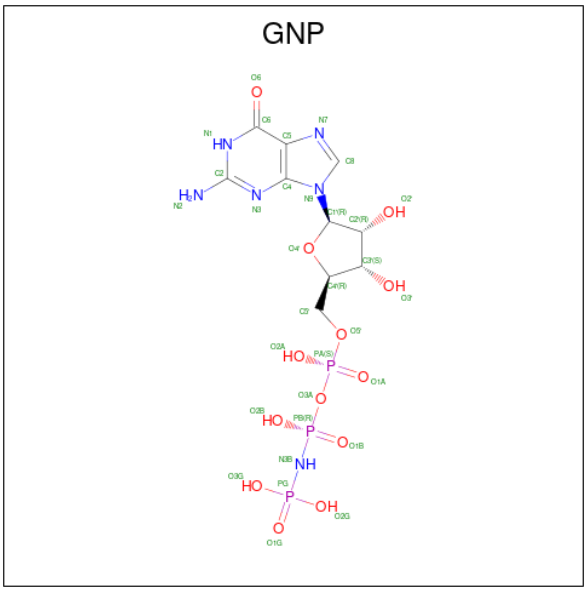
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	102	Total	Mg	0	0
			102	102		
57	AF	1	Total	Mg	0	0
			1	1		
57	AH	1	Total	Mg	0	0
			1	1		
57	AL	2	Total	Mg	0	0
			2	2		
57	AM	1	Total	Mg	0	0
			1	1		
57	AW	1	Total	Mg	0	0
			1	1		
57	B0	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

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

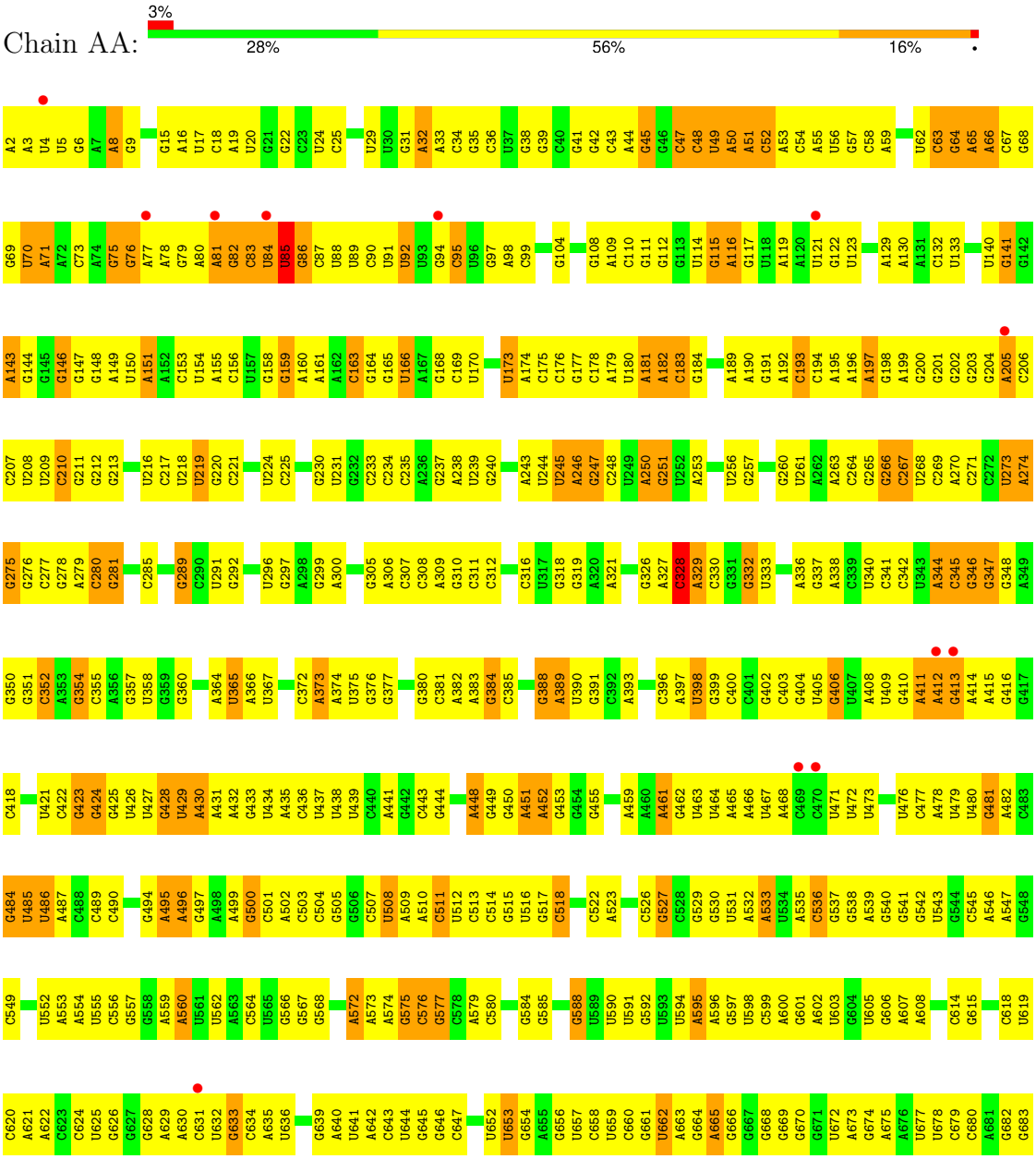
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AW	2	Total	O	0	0
			2	2		
59	B8	1	Total	O	0	0
			1	1		
59	BA	8	Total	O	0	0
			8	8		
59	BC	2	Total	O	0	0
			2	2		
59	BD	1	Total	O	0	0
			1	1		
59	BF	1	Total	O	0	0
			1	1		
59	BG	1	Total	O	0	0
			1	1		
59	BW	1	Total	O	0	0
			1	1		

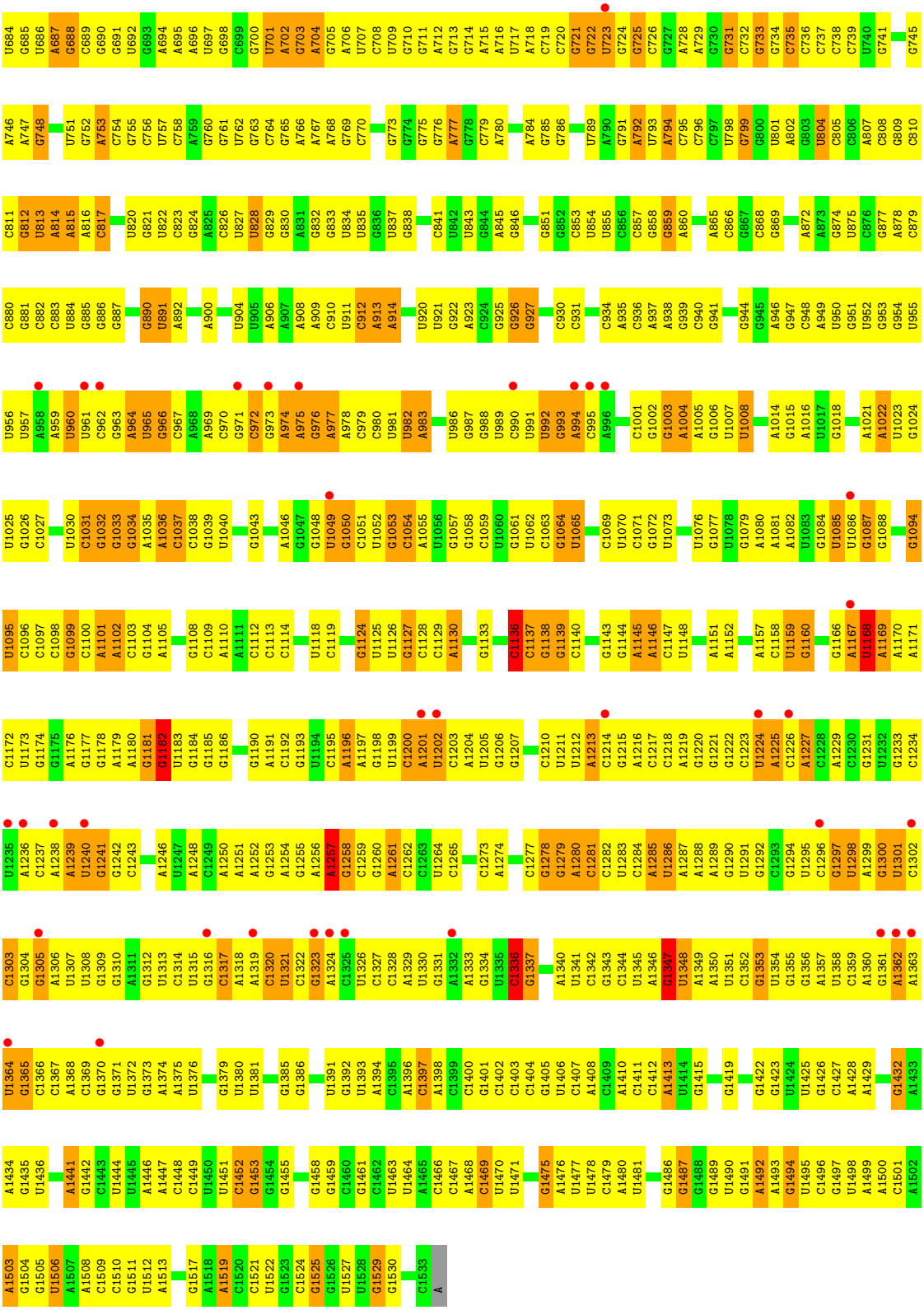
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

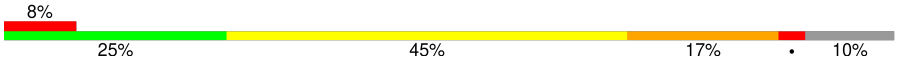
Chain AA:

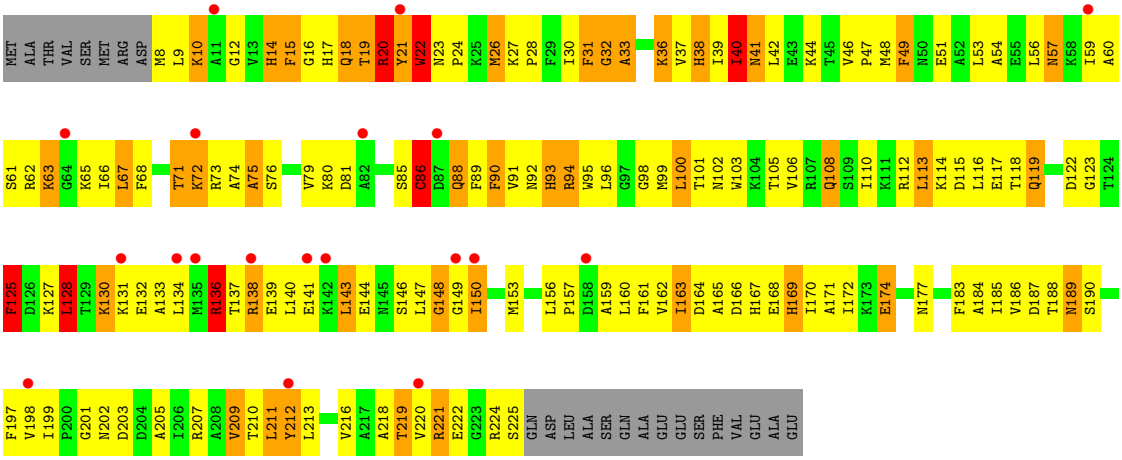




• Molecule 2: 30S ribosomal protein S2

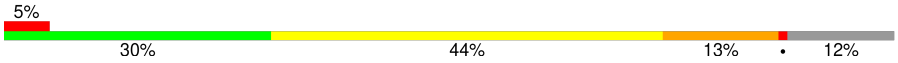
Chain AB:

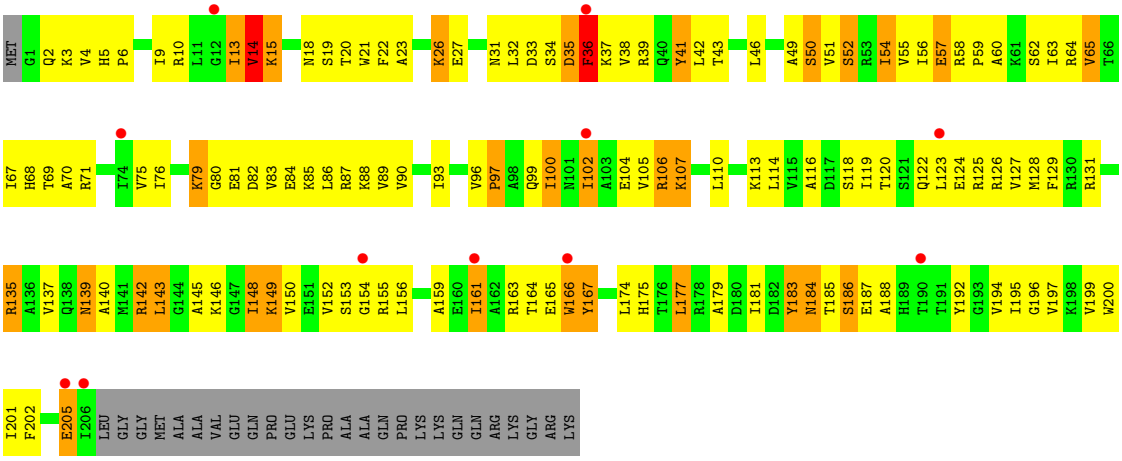




• Molecule 3: 30S ribosomal protein S3

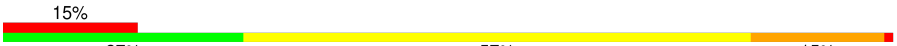
Chain AC:

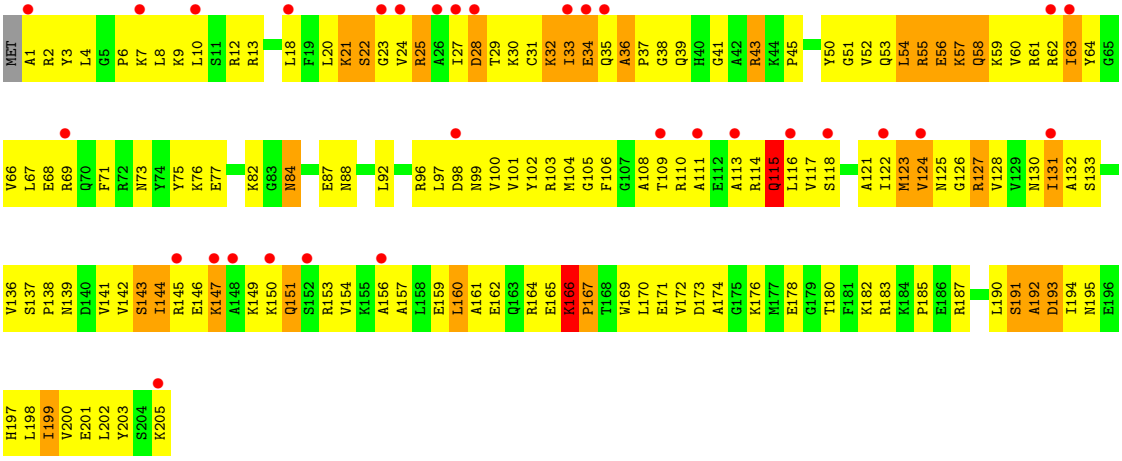




• Molecule 4: 30S ribosomal protein S4

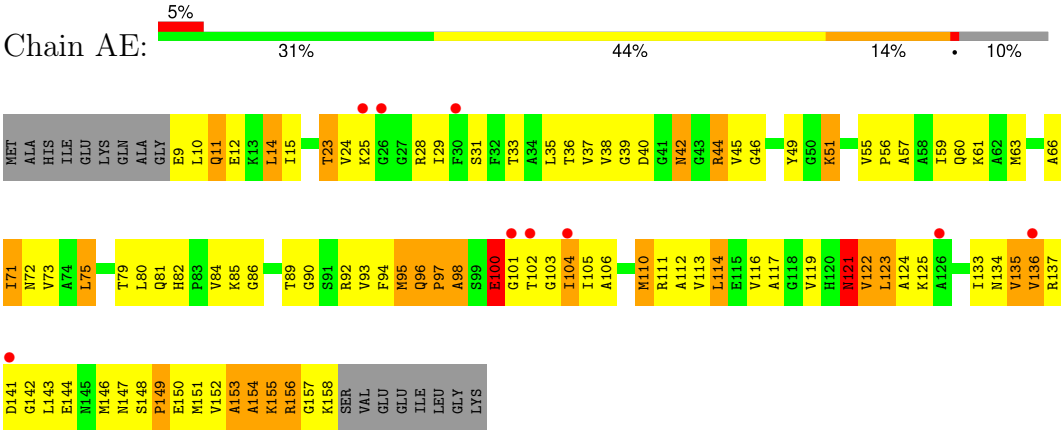
Chain AD:





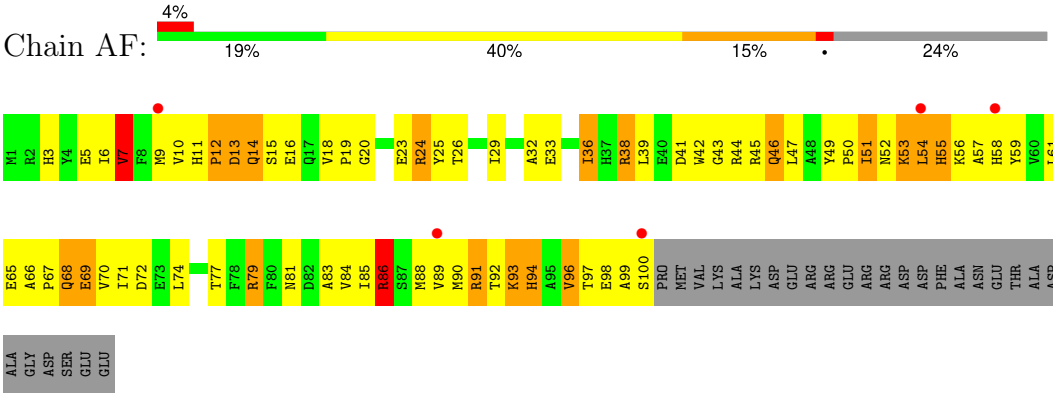
• Molecule 5: 30S ribosomal protein S5

Chain AE:



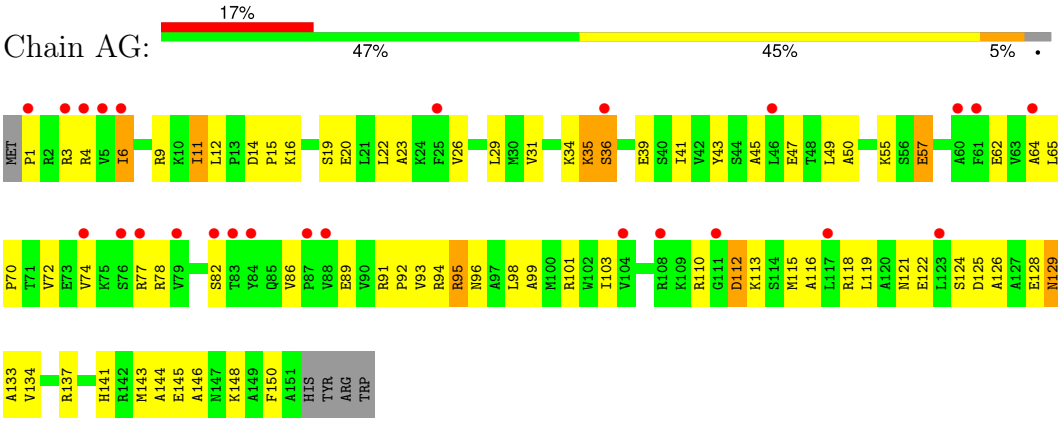
• Molecule 6: 30S ribosomal protein S6 1

Chain AF:



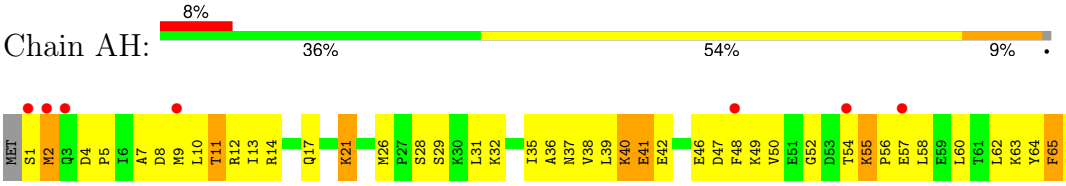
• Molecule 7: 30S ribosomal protein S7

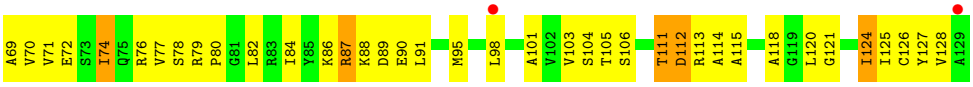
Chain AG:



• Molecule 8: 30S ribosomal protein S8

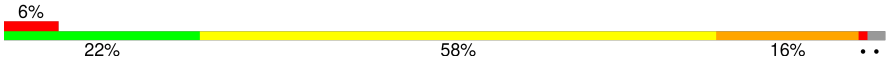
Chain AH:

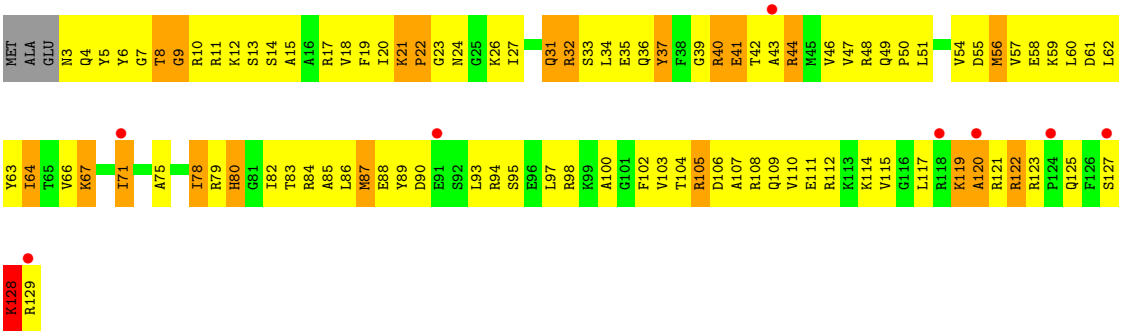




• Molecule 9: 30S ribosomal protein S9

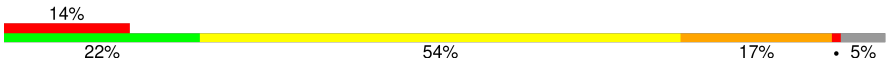
Chain AI:

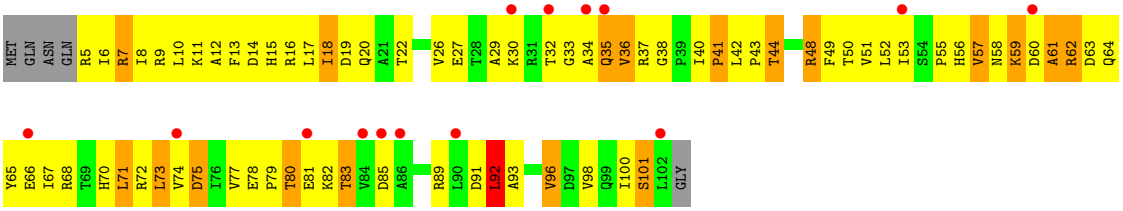




• Molecule 10: 30S ribosomal protein S10

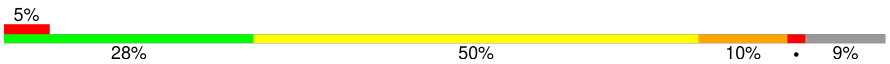
Chain AJ:

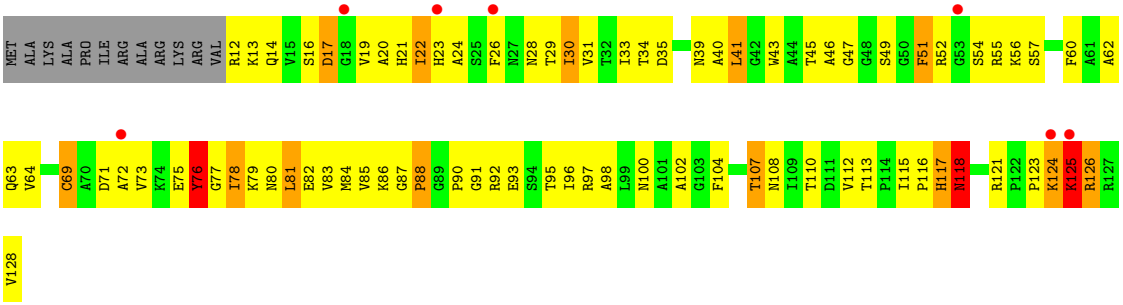




• Molecule 11: 30S ribosomal protein S11

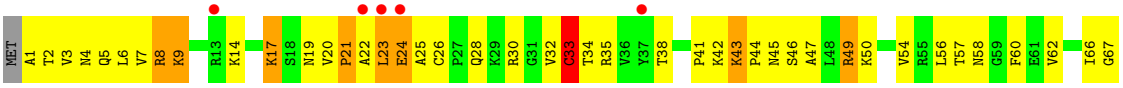
Chain AK:

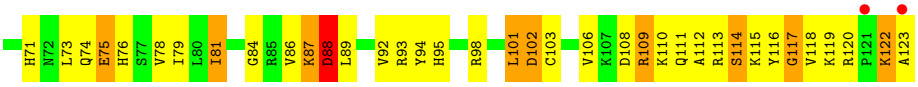




• Molecule 12: 30S ribosomal protein S12 1

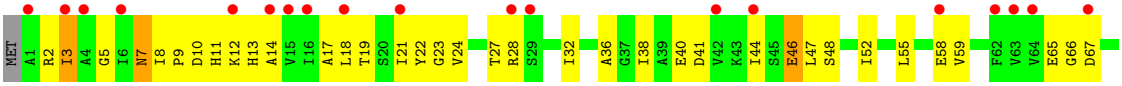
Chain AL:

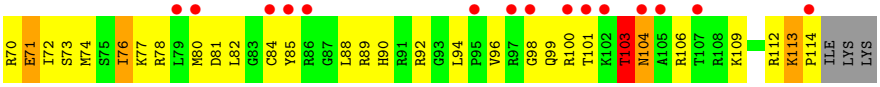




• Molecule 13: 30S ribosomal protein S13

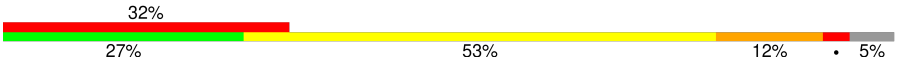
Chain AM:

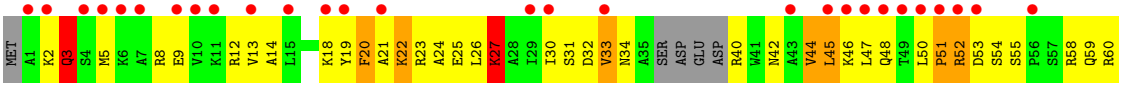


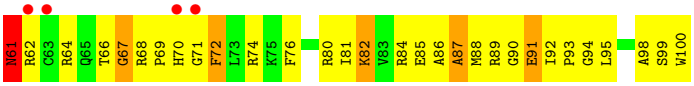


• Molecule 14: 30S ribosomal protein S14

Chain AN:

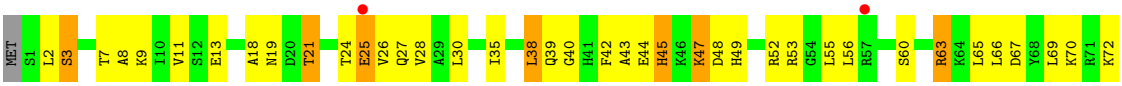


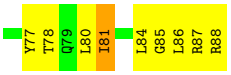




• Molecule 15: 30S ribosomal protein S15 1

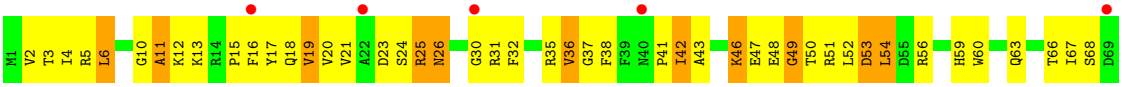
Chain AO:

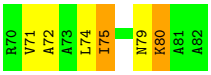




• Molecule 16: 30S ribosomal protein S16

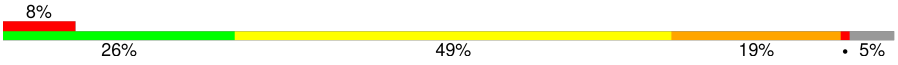
Chain AP:

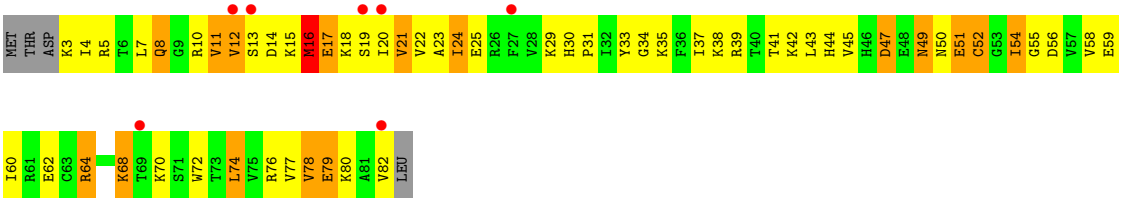




• Molecule 17: 30S ribosomal protein S17

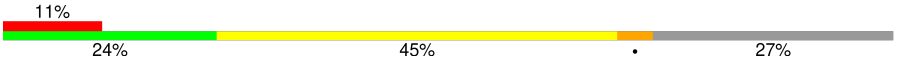
Chain AQ:

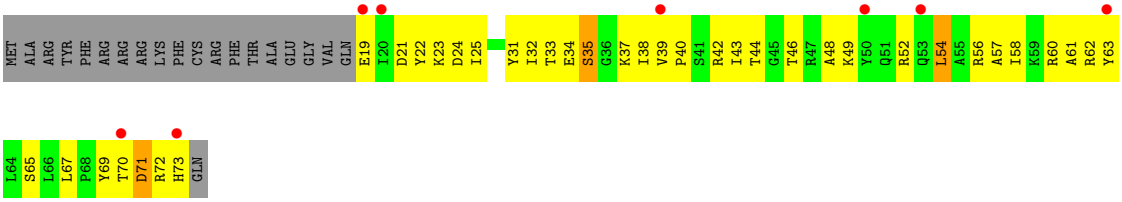




• Molecule 18: 30S ribosomal protein S18

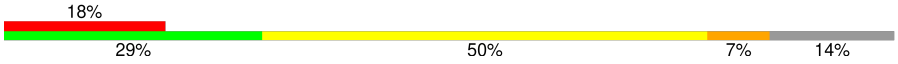
Chain AR:

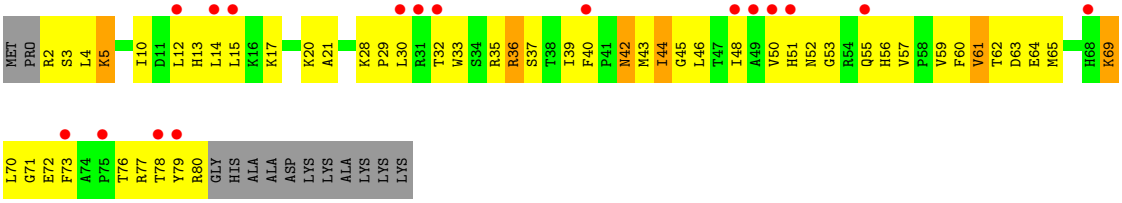




• Molecule 19: 30S ribosomal protein S19

Chain AS:



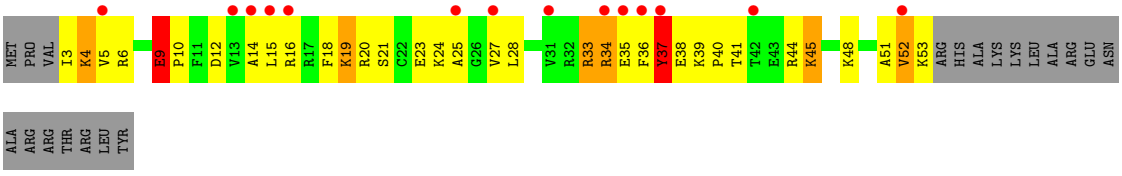


• Molecule 20: 30S ribosomal protein S20

Chain AT:

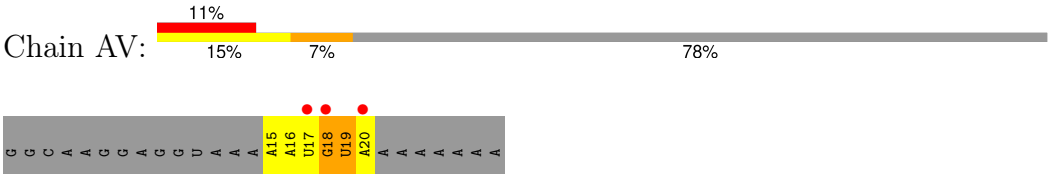
• Molecule 21: 30S ribosomal protein S21

Chain AU:



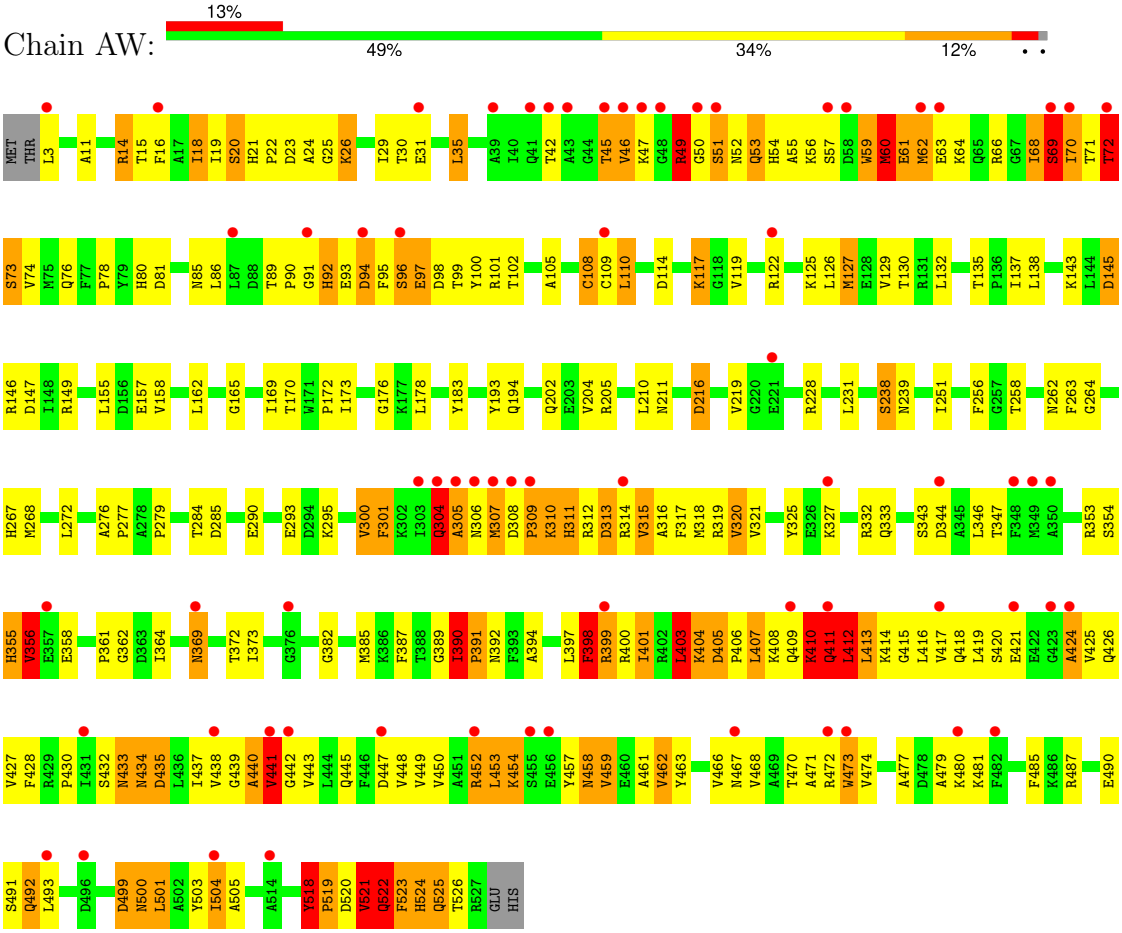
• Molecule 22: messenger RNA

Chain AV:



• Molecule 23: Peptide chain release factor 3

Chain AW:

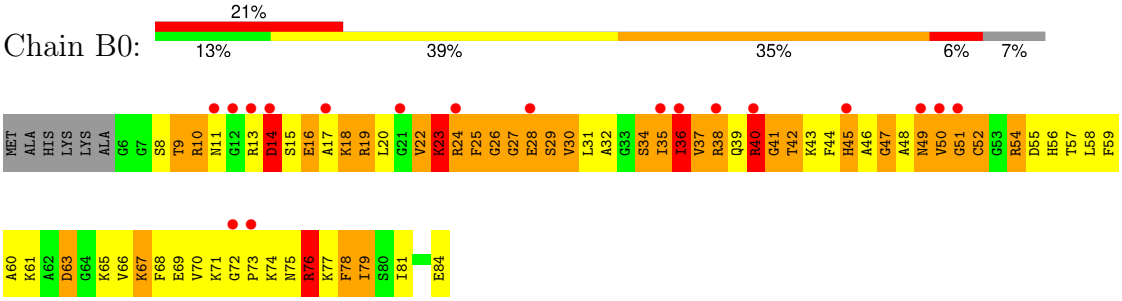


• Molecule 24: Viomycin

Chain AY:

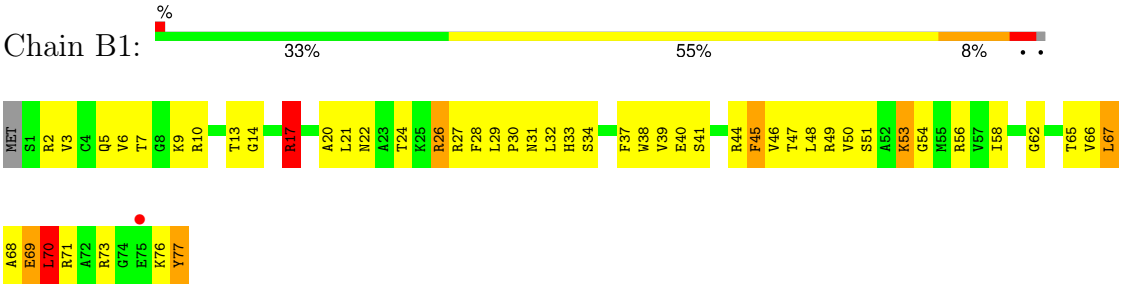
• Molecule 25: 50S ribosomal protein L27

Chain B0:



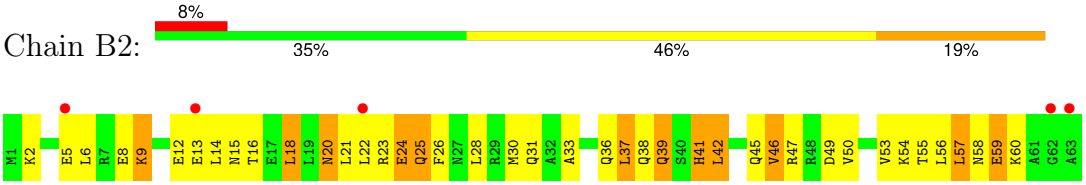
• Molecule 26: 50S ribosomal protein L28

Chain B1:



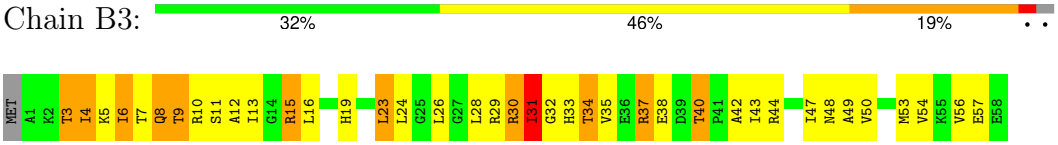
• Molecule 27: 50S ribosomal protein L29

Chain B2:



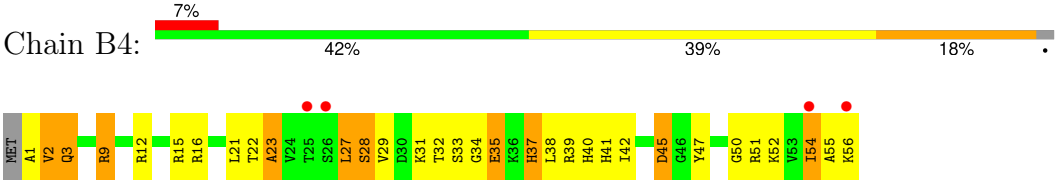
• Molecule 28: 50S ribosomal protein L30

Chain B3:



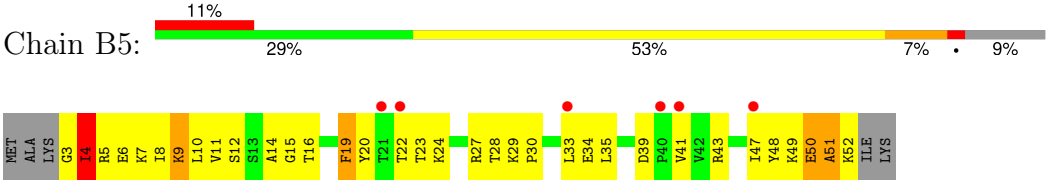
• Molecule 29: 50S ribosomal protein L32

Chain B4:



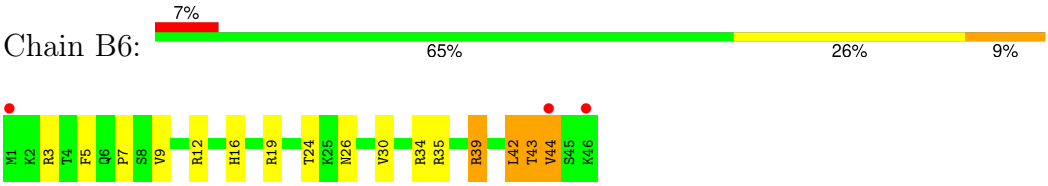
• Molecule 30: 50S ribosomal protein L33

Chain B5:



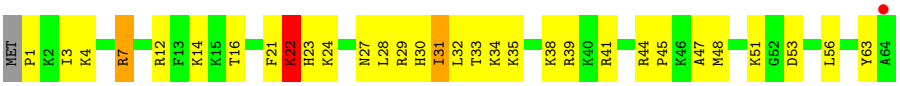
• Molecule 31: 50S ribosomal protein L34

Chain B6:



• Molecule 32: 50S ribosomal protein L35

Chain B7:

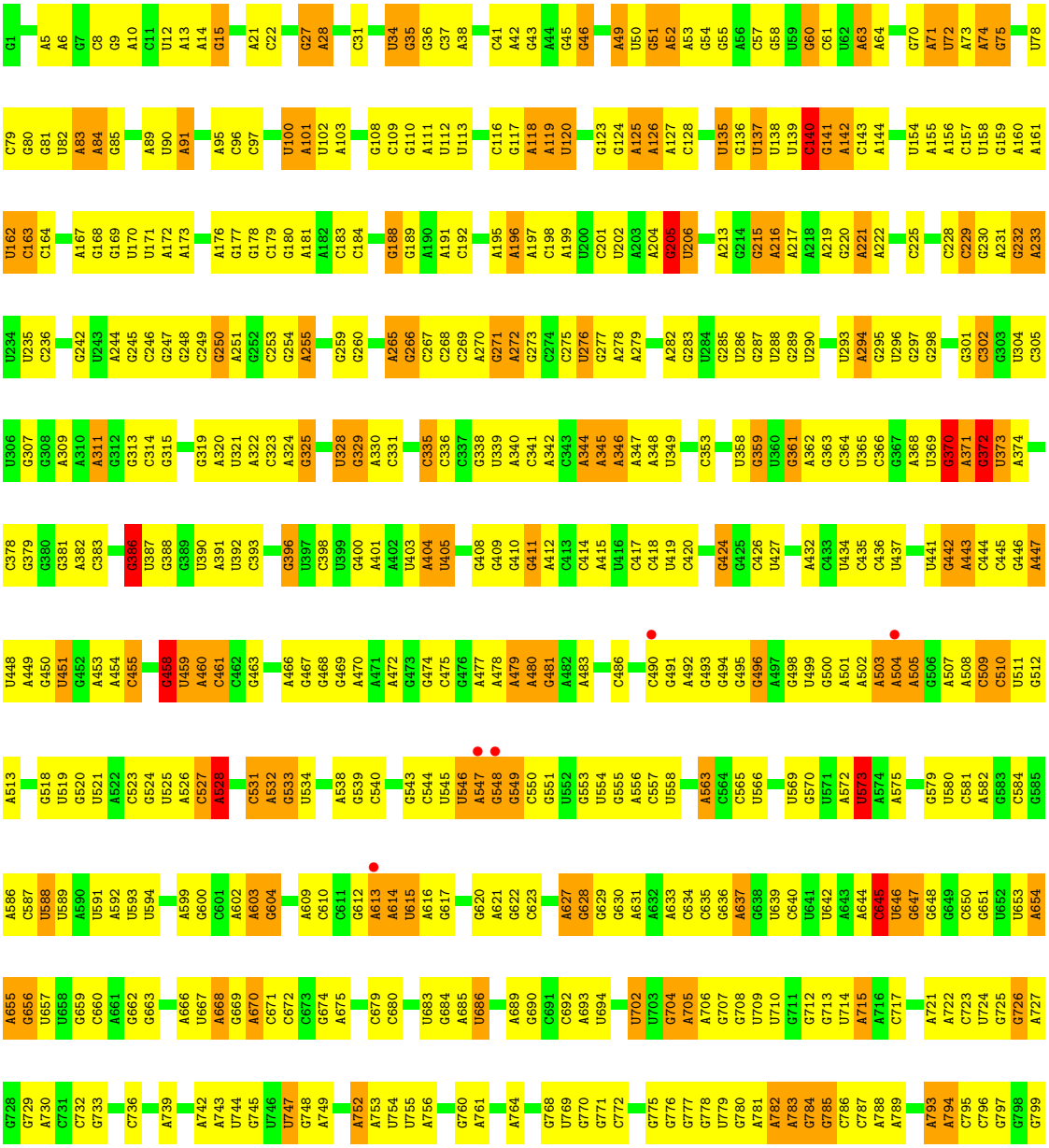


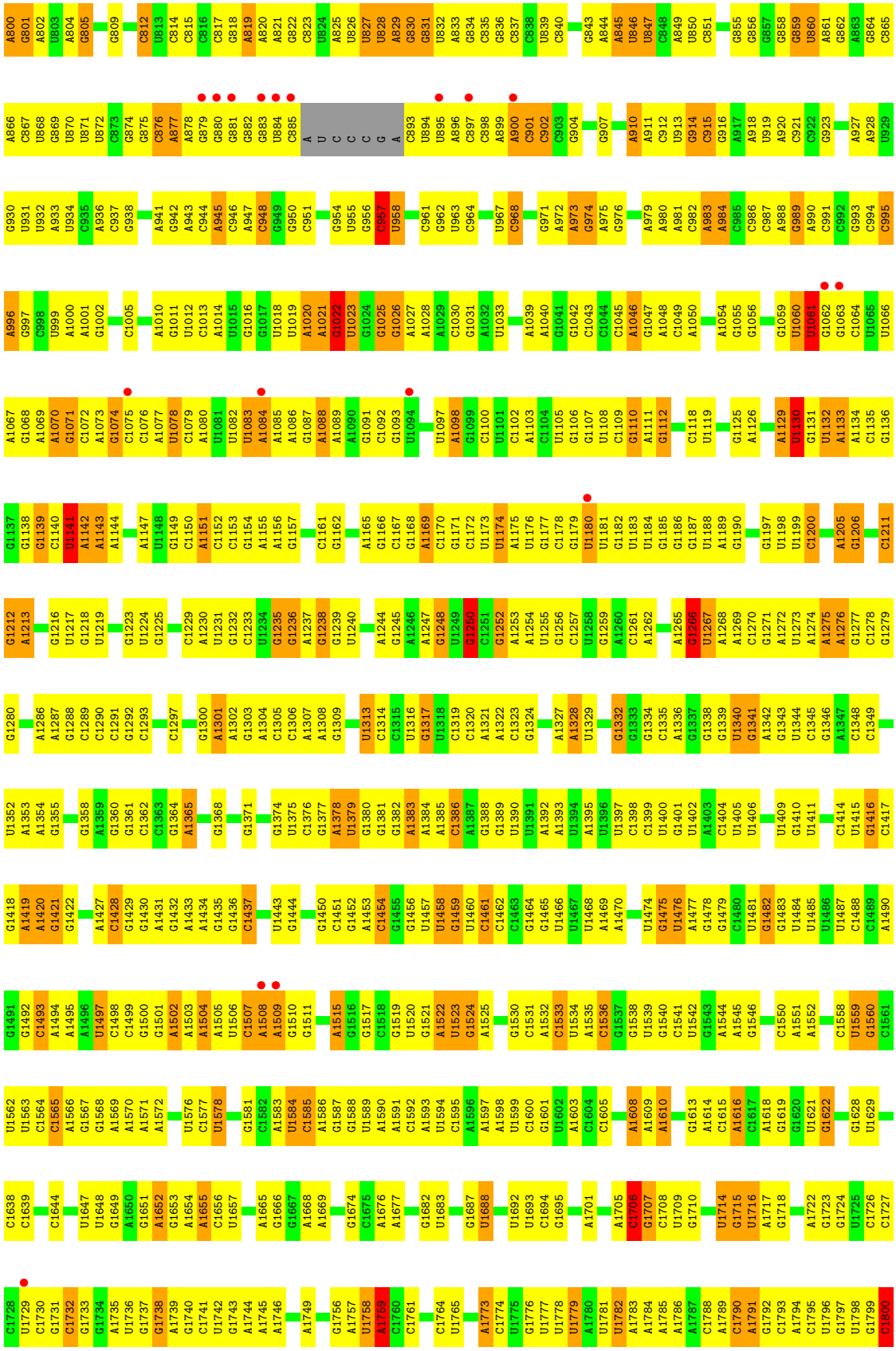
• Molecule 33: 50S ribosomal protein L36 1

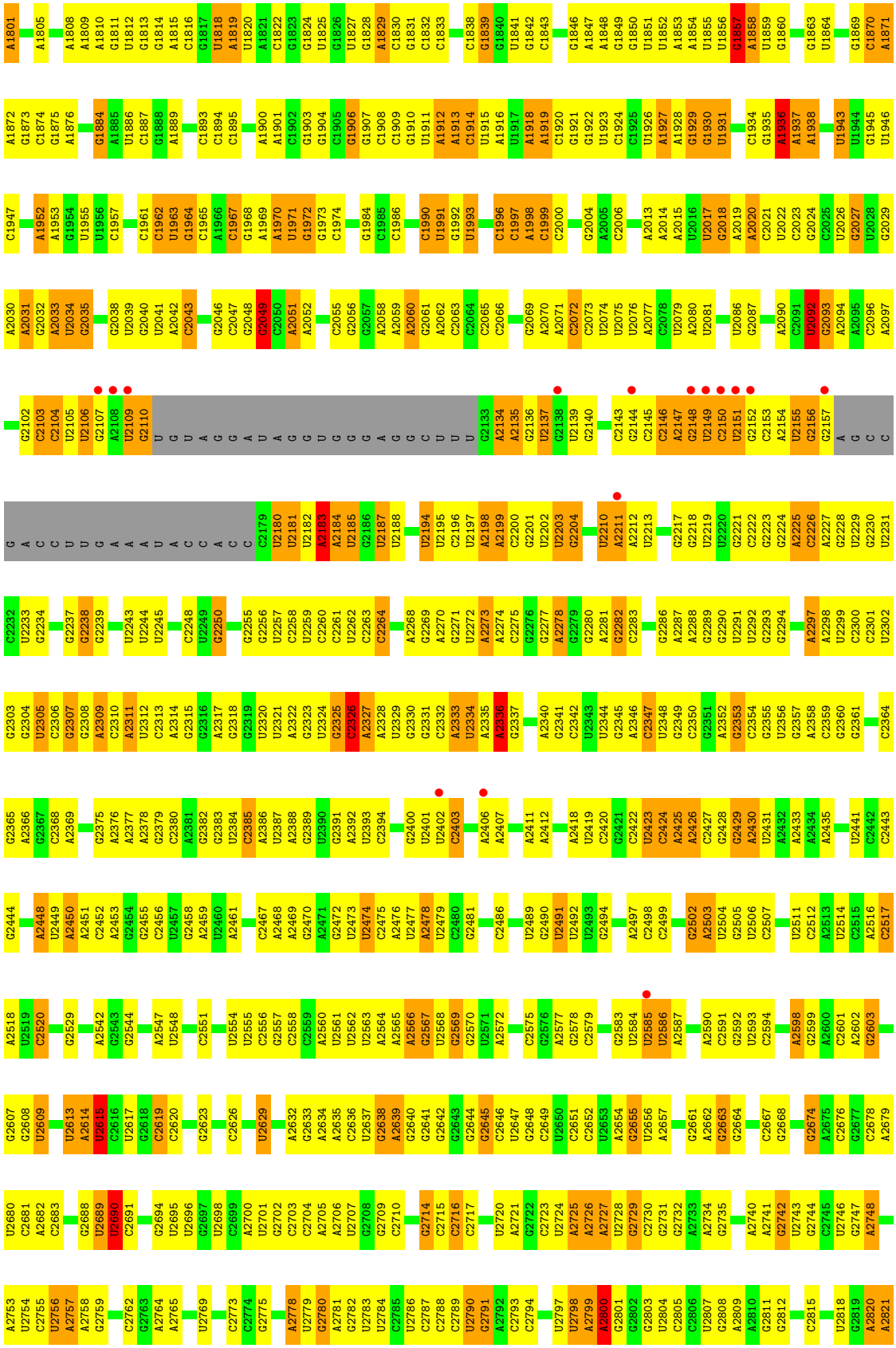
Chain B8:

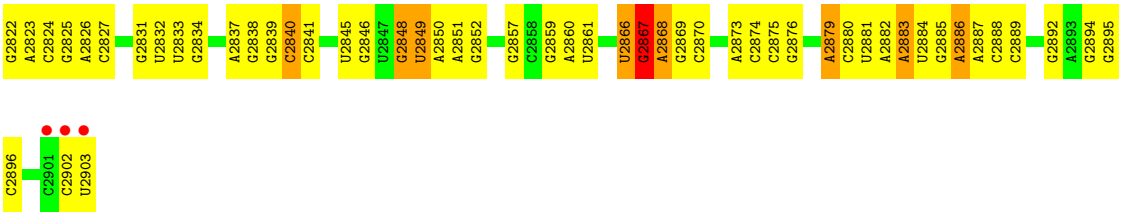
• Molecule 34: 23S rRNA

Chain BA:



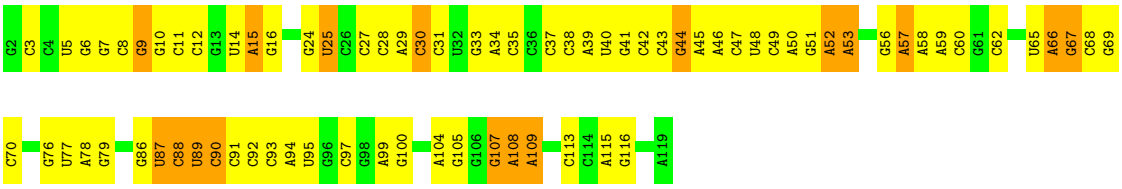

A800 G801 A802 U803 A804 G805 G809 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 G822 C823 U824 A825 U826 U827 U828 A829 G830 G831 U832 A833 G834 C835 G836 C837 C838 U839 C840 G843 A844 A845 U846 U847 C848 A849 U850 C851 G855 G856 G857 G858 G859 U860 A861 G862 A863 G864 C865
A866 C867 U868 G869 U870 U871 U872 C873 G874 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A U C C C G A C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 G904 G907 A910 A911 C912 U913 G914 C915 G916 A917 A918 U919 A920 C921 C922 G923 A927 A928 U929
G930 U931 U932 A933 U934 C935 A936 C937 G938 A941 G942 A943 C944 A945 C946 A947 C948 G949 G950 C951 G954 U955 G956 C957 U958 C961 G962 U963 C964 U967 C968 G971 A972 A973 G974 A975 G976 A979 A980 A981 C982 A983 A984 C985 C986 C987 A988 G989 A990 C991 C992 G993 C994 C995
A996 G997 C998 U999 A1000 A1001 G1002 C1005 A1010 G1011 U1012 C1013 A1014 U1015 G1016 G1017 U1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 A1054 G1055 G1056 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066
A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 C1118 U1119 G1125 A1126 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136
G1137 G1138 G1139 C1140 U1141 A1142 A1143 A1144 A1147 U1148 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157 C1161 G1162 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1197 U1198 U1199 C1200 A1205 G1206 C1211
G1212 A1213 G1216 U1217 G1218 U1219 G1223 U1224 G1225 C1229 A1230 U1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258 G1259 A1260 C1261 A1262 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 C1278 G1279
G1280 A1286 A1287 G1288 C1289 C1290 C1291 C1292 C1293 C1297 G1300 A1301 A1302 G1303 A1304 C1305 C1306 A1307 A1308 G1309 U1313 C1314 C1315 U1316 G1317 U1318 C1319 C1320 A1321 A1322 C1323 G1324 A1327 A1328 U1329 C1332 G1333 G1334 C1335 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1345 G1346 A1347 C1348 C1349
U1352 A1353 A1354 G1355 G1358 A1359 G1360 G1361 C1362 C1363 G1364 A1365 G1368 G1371 G1374 U1375 C1376 G1377 A1378 U1379 G1380 G1381 G1382 A1383 A1384 A1385 C1386 A1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 U1400 G1401 A1403 C1404 U1405 U1406 U1409 G1410 U1411 C1414 U1415 G1416 C1417
G1418 A1419 A1420 G1421 G1422 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1443 G1444 G1450 C1451 G1452 A1453 C1454 C1455 G1456 U1457 U1458 G1459 U1460 C1461 C1462 C1463 C1464 G1465 U1466 U1467 U1468 A1469 A1470 U1474 G1475 U1476 A1477 G1478 G1479 C1480 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490
G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 G1499 G1500 G1501 A1502 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1511 A1515 G1516 G1517 C1518 G1519 U1520 G1521 A1522 U1523 G1524 A1525 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 G1546 C1550 A1551 A1552 C1558 U1559 G1560 C1561
U1562 U1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 A1572 U1576 C1577 U1578 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1598 U1599 C1600 G1601 U1602 A1603 C1604 C1605 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1620 U1621 G1622 G1628 U1629
C1638 C1639 C1644 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654 A1655 C1656 U1657 A1665 G1666 G1667 A1668 A1669 G1674 C1675 A1676 A1677 G1682 U1683 G1687 U1688 U1692 U1693 C1694 G1695 A1701 A1705 C1706 G1707 C1708 U1709 G1710 U1714 G1715 U1716 A1717 G1718 A1722 G1723 G1724 U1725 C1726 C1727
C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 G1740 C1741 U1742 G1743 A1744 A1745 A1746 A1749 G1756 A1757 U1758 A1759 C1760 C1761 C1764 U1765 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 U1781 U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 A1794 C1795 U1796 G1797 U1798 G1799 C1800





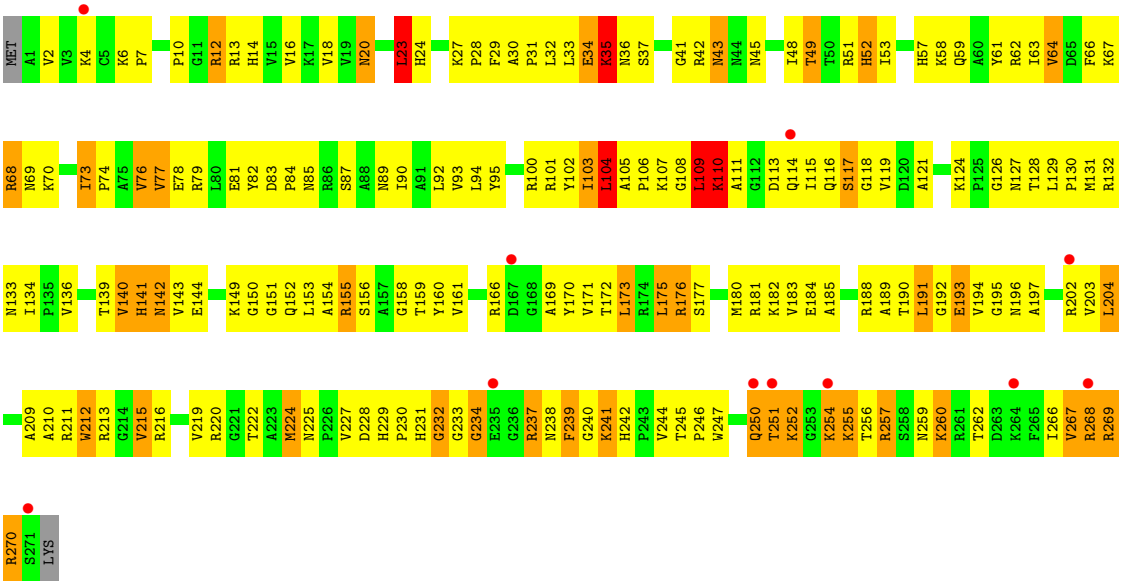
• Molecule 35: 5S ribosomal RNA

Chain BB:



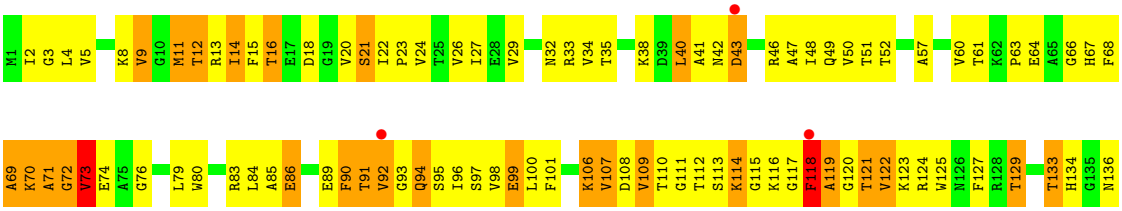
• Molecule 36: 50S ribosomal protein L2

Chain BC:

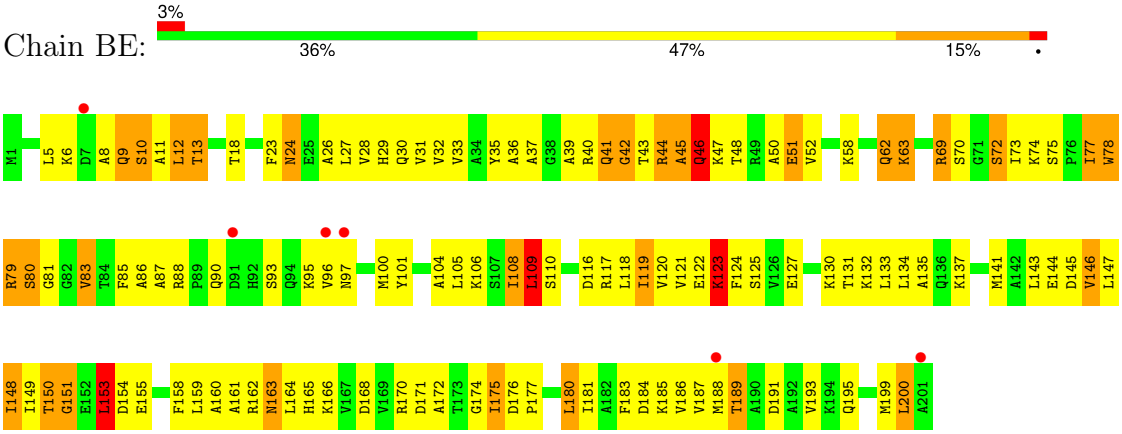


• Molecule 37: 50S ribosomal protein L3

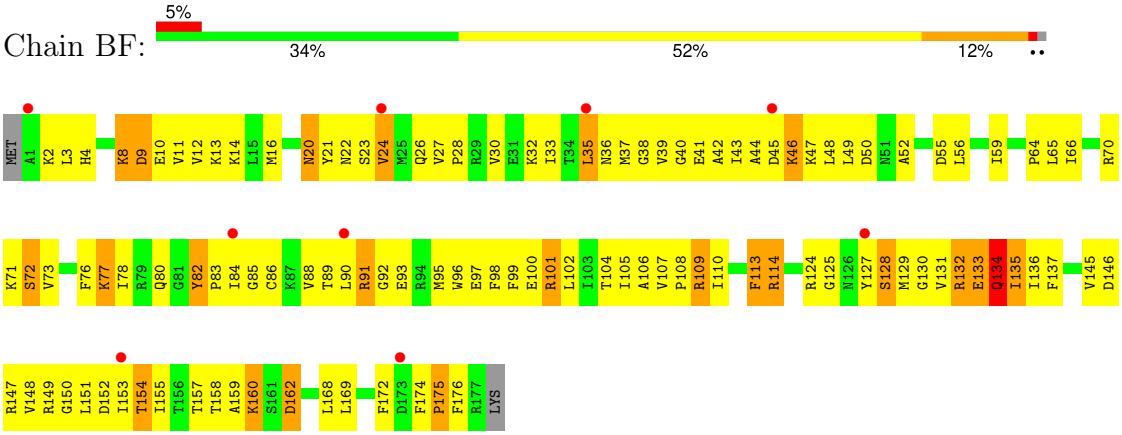
Chain BD:



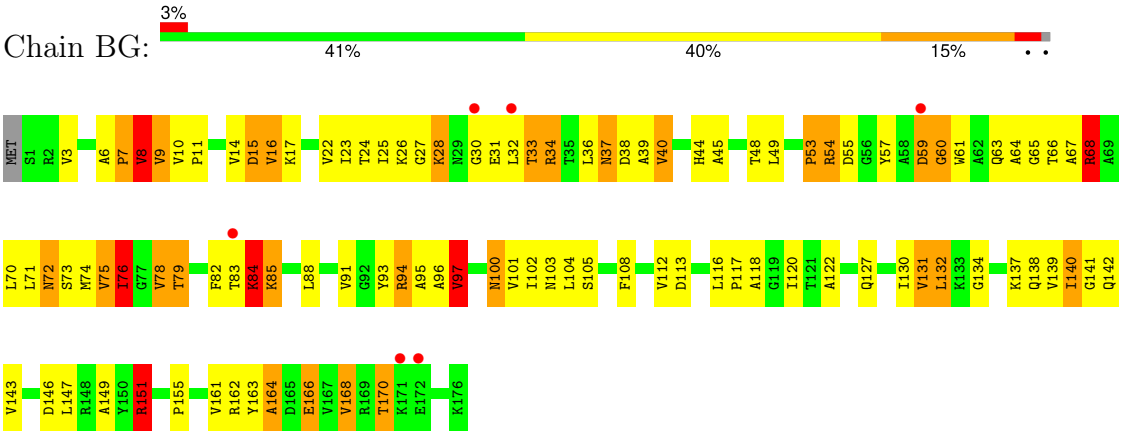
• Molecule 38: 50S ribosomal protein L4



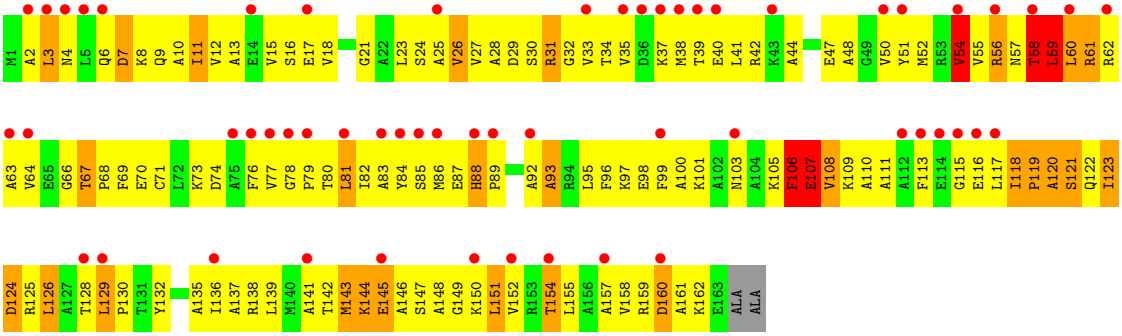
• Molecule 39: 50S ribosomal protein L5



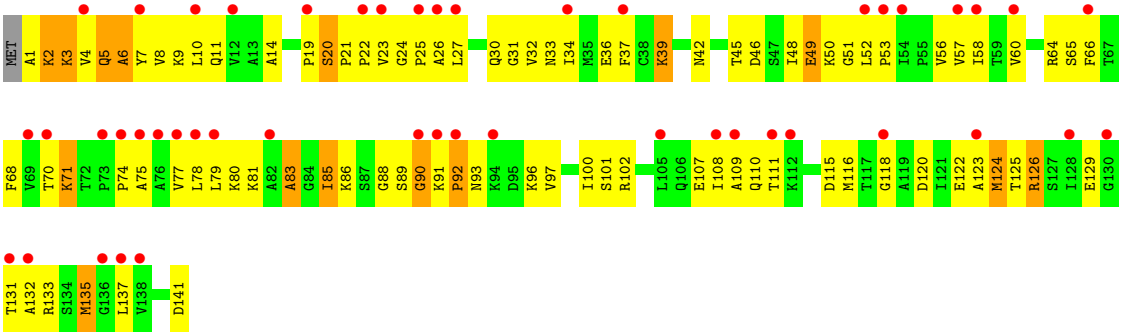
• Molecule 40: 50S ribosomal protein L6



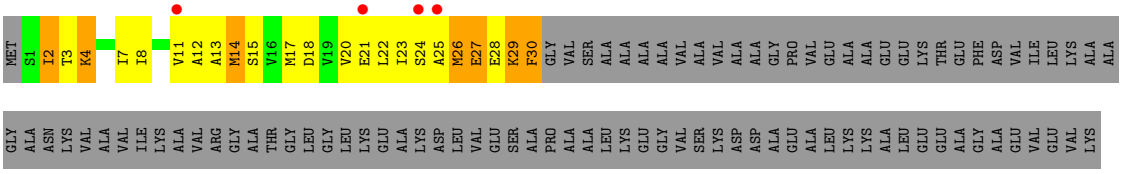
• Molecule 41: 50S ribosomal protein L10



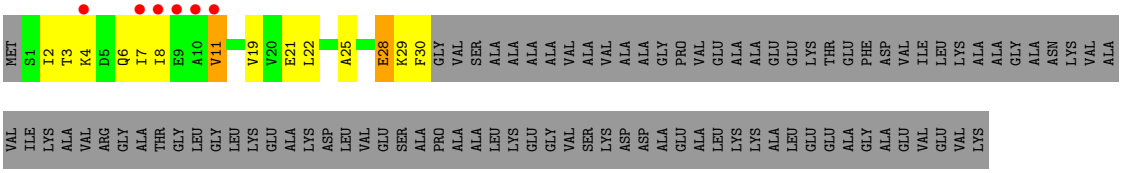
• Molecule 42: 50S ribosomal protein L11



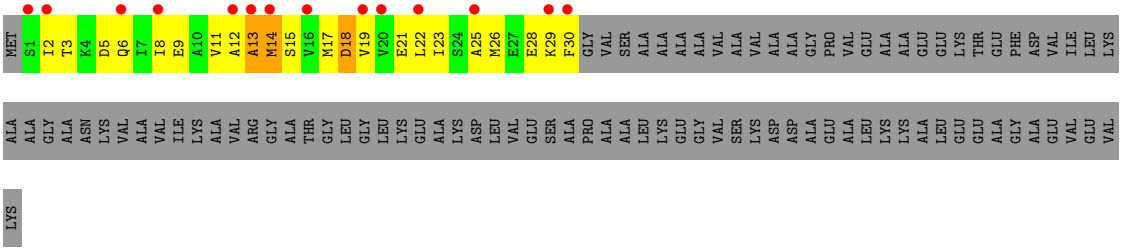
• Molecule 43: 50S ribosomal protein L7/L12



• Molecule 43: 50S ribosomal protein L7/L12

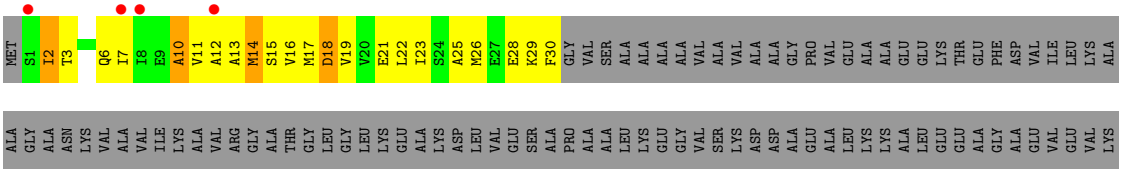


• Molecule 43: 50S ribosomal protein L7/L12



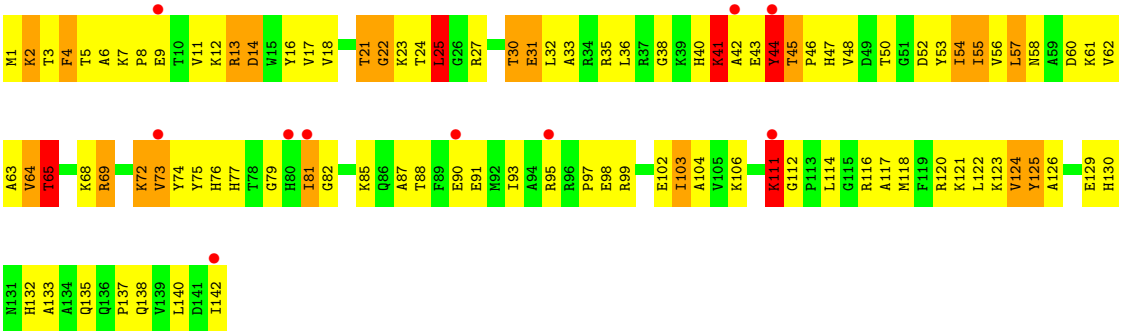
• Molecule 43: 50S ribosomal protein L7/L12

Chain BM:



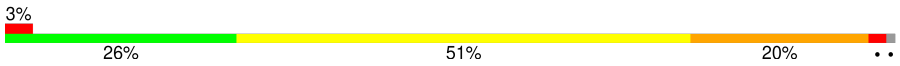
• Molecule 44: 50S ribosomal protein L13

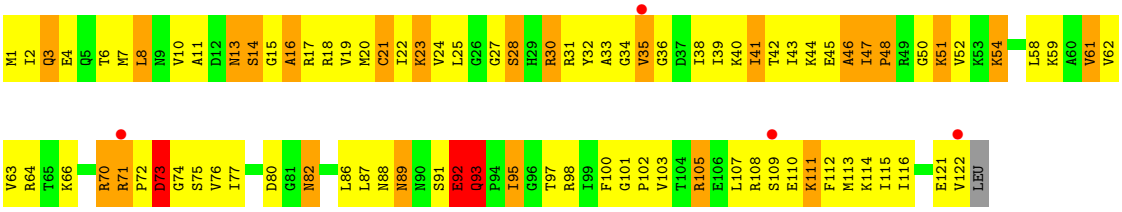
Chain BN:



• Molecule 45: 50S ribosomal protein L14

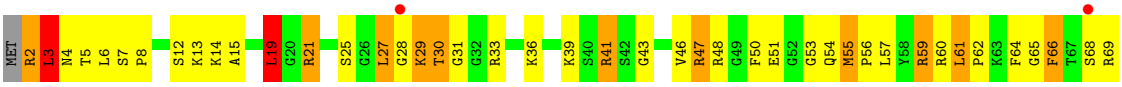
Chain BO:

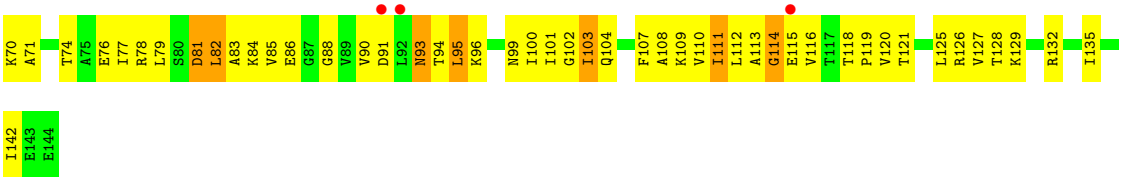




• Molecule 46: 50S ribosomal protein L15

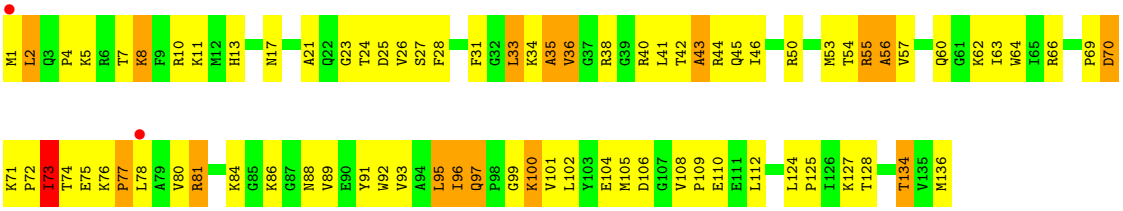
Chain BP:





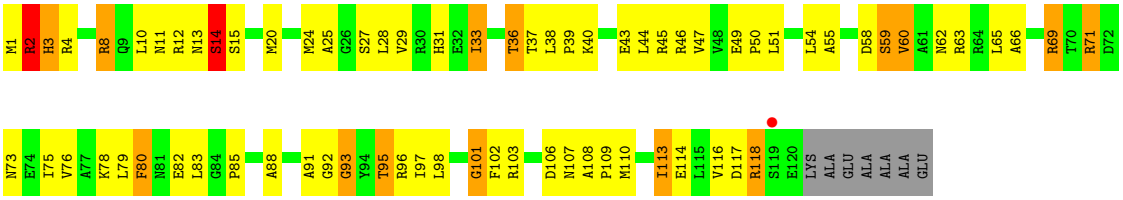
• Molecule 47: 50S ribosomal protein L16

Chain BQ:



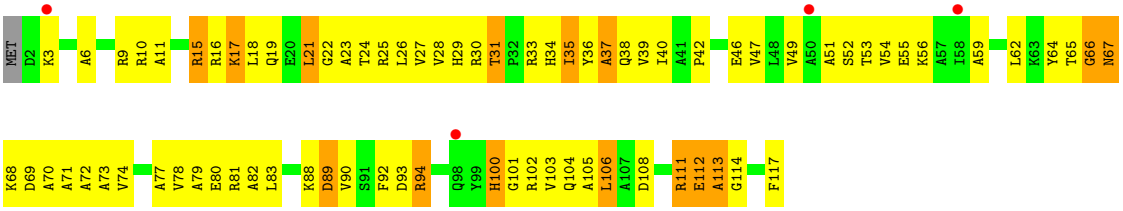
• Molecule 48: 50S ribosomal protein L17

Chain BR:



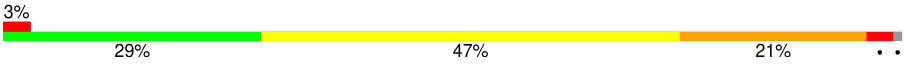
• Molecule 49: 50S ribosomal protein L18

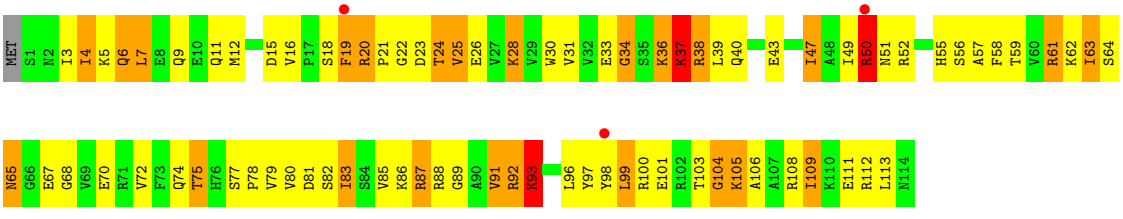
Chain BS:



• Molecule 50: 50S ribosomal protein L19

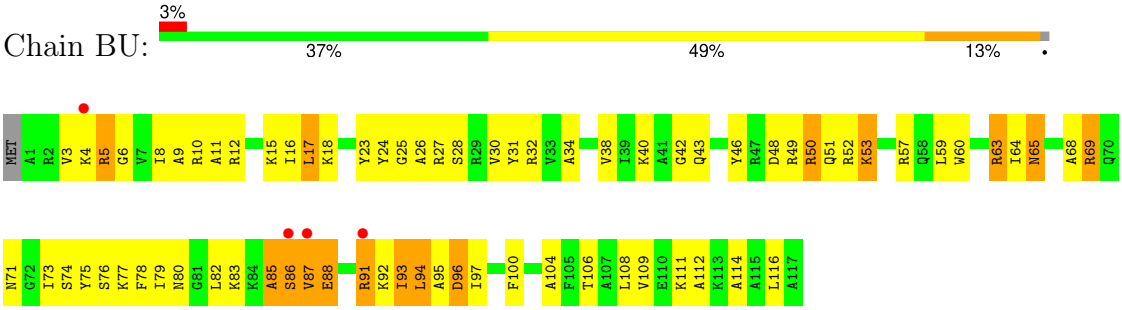
Chain BT:





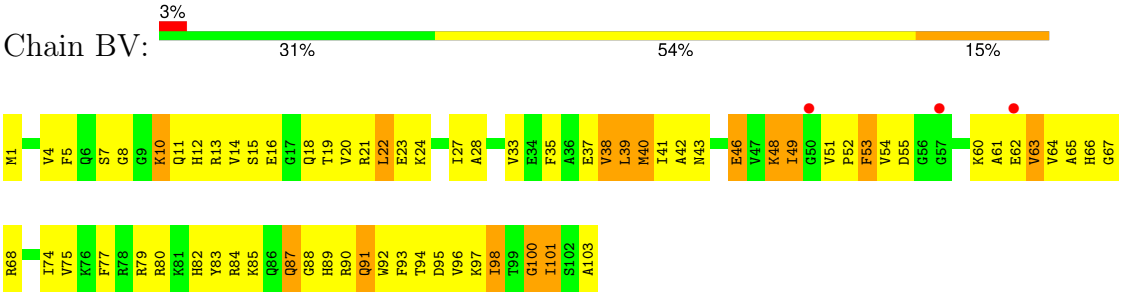
• Molecule 51: 50S ribosomal protein L20

Chain BU:



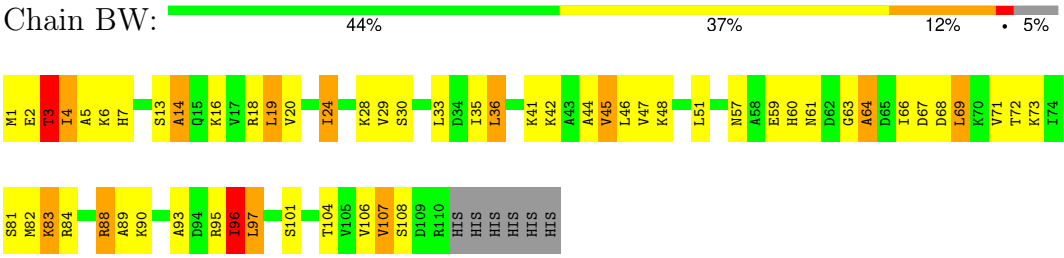
• Molecule 52: 50S ribosomal protein L21

Chain BV:



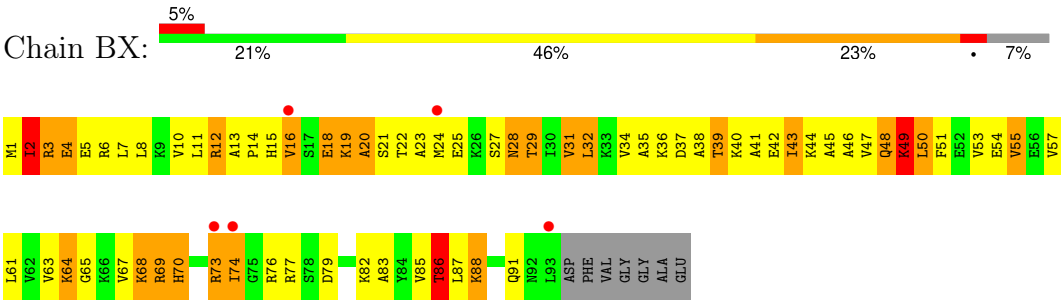
• Molecule 53: 50S ribosomal protein L22

Chain BW:



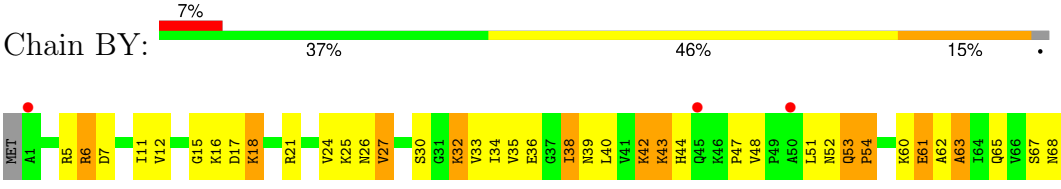
• Molecule 54: 50S ribosomal protein L23

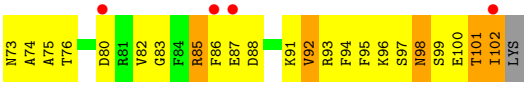
Chain BX:



• Molecule 55: 50S ribosomal protein L24 1

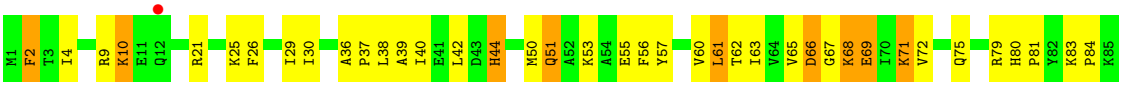
Chain BY:

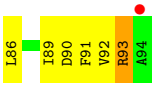




• Molecule 56: 50S ribosomal protein L25 1

Chain BZ:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 99.9 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX, CNS 1.2	Depositor
R, R_{free}	0.210 , 0.250 0.227 , 0.253	Depositor DCC
R_{free} test set	21734 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 90.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG, 5OH, DPP, UAL, KBE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.44	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(^{o})	Ideal(^{o})
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	7
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	7
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	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 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

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:131:ARG:NH2	34:BA:2157:G:P[4_445]	1.17	1.03
3:AC:131:ARG:CZ	34:BA:2157:G:OP1[4_445]	1.23	0.97
3:AC:131:ARG:NH2	34:BA:2157:G:OP1[4_445]	1.40	0.80
3:AC:131:ARG:NH2	34:BA:2157:G:O5'[4_445]	1.48	0.72
3:AC:131:ARG:NE	34:BA:2157:G:OP1[4_445]	1.68	0.52

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

5 of 664 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	22	TRP
2	AB	33	ALA
2	AB	40	ILE
2	AB	75	ALA

5.3.2 Protein sidechains (i)

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 6
3	AC	170/190 (90%)	146 (86%)	24 (14%)	3 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	AD	172/173 (99%)	152 (88%)	20 (12%)	4 21
5	AE	113/126 (90%)	95 (84%)	18 (16%)	2 10
6	AF	87/112 (78%)	73 (84%)	14 (16%)	2 9
7	AG	124/129 (96%)	121 (98%)	3 (2%)	44 71
8	AH	104/105 (99%)	94 (90%)	10 (10%)	7 28
9	AI	105/107 (98%)	92 (88%)	13 (12%)	4 18
10	AJ	86/90 (96%)	70 (81%)	16 (19%)	1 7
11	AK	90/99 (91%)	74 (82%)	16 (18%)	1 7
12	AL	103/104 (99%)	89 (86%)	14 (14%)	3 15
13	AM	92/96 (96%)	87 (95%)	5 (5%)	18 51
14	AN	79/84 (94%)	71 (90%)	8 (10%)	6 26
15	AO	76/77 (99%)	66 (87%)	10 (13%)	3 16
16	AP	65/65 (100%)	57 (88%)	8 (12%)	4 19
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	1 8
18	AR	48/65 (74%)	44 (92%)	4 (8%)	9 35
19	AS	70/79 (89%)	64 (91%)	6 (9%)	8 33
20	AT	65/66 (98%)	60 (92%)	5 (8%)	10 39
21	AU	44/61 (72%)	37 (84%)	7 (16%)	2 10
23	AW	447/453 (99%)	381 (85%)	66 (15%)	2 12
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 9
27	B2	55/55 (100%)	46 (84%)	9 (16%)	2 9
28	B3	48/49 (98%)	39 (81%)	9 (19%)	1 6
29	B4	47/48 (98%)	40 (85%)	7 (15%)	2 12
30	B5	45/49 (92%)	42 (93%)	3 (7%)	13 44
31	B6	38/38 (100%)	34 (90%)	4 (10%)	5 24
32	B7	51/52 (98%)	48 (94%)	3 (6%)	16 48
33	B8	34/34 (100%)	32 (94%)	2 (6%)	16 48
36	BC	216/218 (99%)	177 (82%)	39 (18%)	1 7
37	BD	164/164 (100%)	143 (87%)	21 (13%)	3 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	BE	165/165 (100%)	138 (84%)	27 (16%)	2 9
39	BF	148/150 (99%)	136 (92%)	12 (8%)	9 36
40	BG	137/138 (99%)	116 (85%)	21 (15%)	2 11
41	BH	123/123 (100%)	109 (89%)	14 (11%)	4 21
42	BI	109/110 (99%)	101 (93%)	8 (7%)	11 41
43	BJ	26/85 (31%)	23 (88%)	3 (12%)	4 21
43	BK	26/85 (31%)	26 (100%)	0	100 100
43	BL	26/85 (31%)	25 (96%)	1 (4%)	28 60
43	BM	26/85 (31%)	24 (92%)	2 (8%)	10 39
44	BN	116/116 (100%)	94 (81%)	22 (19%)	1 6
45	BO	103/104 (99%)	80 (78%)	23 (22%)	1 4
46	BP	102/103 (99%)	85 (83%)	17 (17%)	2 9
47	BQ	109/109 (100%)	91 (84%)	18 (16%)	2 9
48	BR	100/103 (97%)	88 (88%)	12 (12%)	4 19
49	BS	86/87 (99%)	76 (88%)	10 (12%)	4 21
50	BT	99/100 (99%)	81 (82%)	18 (18%)	1 7
51	BU	89/90 (99%)	77 (86%)	12 (14%)	3 15
52	BV	84/84 (100%)	74 (88%)	10 (12%)	4 19
53	BW	93/99 (94%)	73 (78%)	20 (22%)	1 4
54	BX	80/84 (95%)	66 (82%)	14 (18%)	1 8
55	BY	83/85 (98%)	74 (89%)	9 (11%)	5 23
56	BZ	78/78 (100%)	74 (95%)	4 (5%)	20 53
All	All	5228/5666 (92%)	4511 (86%)	717 (14%)	3 14

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

Mol	Chain	Res	Type
38	BE	170	ARG
46	BP	2	ARG
39	BF	114	ARG
38	BE	153	LEU
42	BI	126	ARG

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

Mol	Chain	Res	Type
37	BD	67	HIS
46	BP	93	ASN
38	BE	24	ASN
41	BH	103	ASN
48	BR	73	ASN

5.3.3 RNA (i)

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	1930	G
34	BA	2033	A
34	BA	2638	G
34	BA	60	G
34	BA	51	G

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	UAL	AY	5	24	6,8,9	2.53	2 (33%)	4,9,11	1.30	1 (25%)
24	DPP	AY	2	24	4,5,6	1.10	1 (25%)	1,5,7	0.18	0
24	5OH	AY	6	24	7,12,13	0.53	0	4,16,18	0.72	0
24	KBE	AY	1	24	8,8,9	0.57	0	6,8,10	1.30	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	UAL	AY	5	24	-	0/3/7/9	-
24	DPP	AY	2	24	-	0/2/4/6	-
24	5OH	AY	6	24	-	0/2/18/20	0/1/1/1
24	KBE	AY	1	24	-	1/7/7/8	-

All (3) bond length outliers are listed below:

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

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 28 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 494 ligands modelled in this entry, 493 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	GNP	AW	602	57	29,34,34	1.80	7 (24%)	33,54,54	2.80	14 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GNP	AW	602	57	-	7/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AW	602	GNP	PG-O1G	5.02	1.53	1.46
58	AW	602	GNP	PA-O3A	-4.25	1.54	1.59
58	AW	602	GNP	C6-N1	3.64	1.39	1.33
58	AW	602	GNP	PB-O3A	-2.48	1.56	1.59
58	AW	602	GNP	PA-O2A	-2.15	1.45	1.55

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	AW	602	GNP	C5-C6-N1	-8.77	111.69	123.42
58	AW	602	GNP	C2-N1-C6	6.60	125.14	115.96
58	AW	602	GNP	C2-N3-C4	-5.23	109.85	115.48
58	AW	602	GNP	C4'-O4'-C1'	-4.54	105.77	109.92
58	AW	602	GNP	O2B-PB-O1B	3.44	117.24	109.87

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

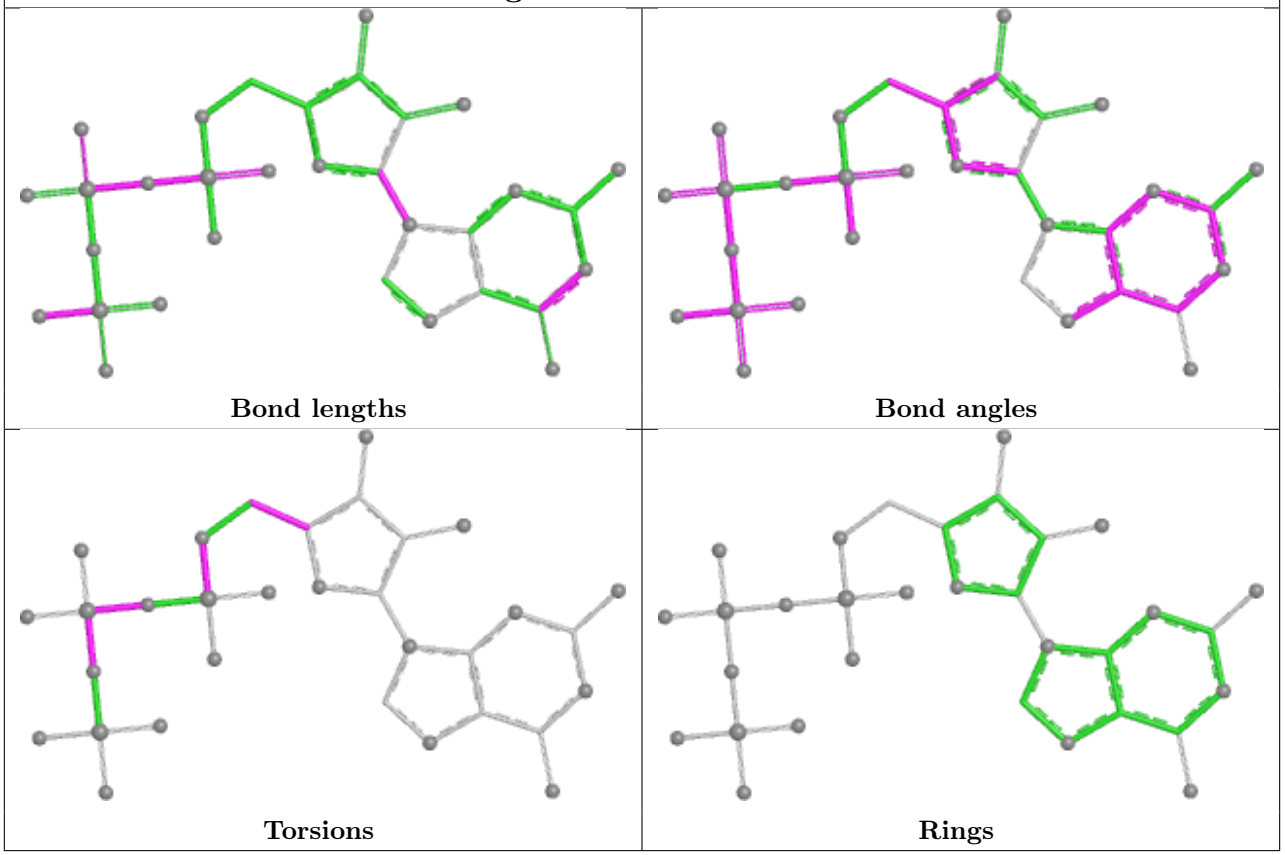
There are no ring outliers.

1 monomer is involved in 6 short contacts:

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

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

Ligand GNP AW 602



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, 95^{th} 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%)	0.29	49 (3%) 50 35	51, 102, 197, 245	0
2	AB	218/241 (90%)	0.73	19 (8%) 17 12	91, 120, 142, 158	0
3	AC	206/233 (88%)	0.47	11 (5%) 33 22	75, 114, 132, 139	0
4	AD	205/206 (99%)	0.98	31 (15%) 6 5	86, 110, 132, 147	0
5	AE	150/167 (89%)	0.60	9 (6%) 29 19	73, 94, 129, 143	0
6	AF	100/131 (76%)	0.48	5 (5%) 35 24	98, 122, 135, 145	0
7	AG	151/156 (96%)	1.16	26 (17%) 5 4	107, 144, 159, 163	0
8	AH	129/130 (99%)	0.51	10 (7%) 20 14	77, 97, 121, 139	0
9	AI	127/130 (97%)	0.83	8 (6%) 27 18	77, 122, 148, 159	0
10	AJ	98/103 (95%)	1.18	14 (14%) 7 5	89, 106, 143, 156	0
11	AK	117/129 (90%)	0.71	7 (5%) 29 19	73, 105, 133, 150	0
12	AL	123/124 (99%)	0.44	7 (5%) 30 20	55, 74, 111, 142	0
13	AM	114/118 (96%)	1.53	34 (29%) 1 1	137, 149, 163, 165	0
14	AN	96/101 (95%)	1.55	32 (33%) 1 1	79, 128, 152, 160	0
15	AO	88/89 (98%)	0.35	2 (2%) 61 44	79, 101, 131, 142	0
16	AP	82/82 (100%)	0.63	5 (6%) 28 19	72, 95, 131, 147	0
17	AQ	80/84 (95%)	1.07	7 (8%) 17 12	78, 111, 136, 147	0
18	AR	55/75 (73%)	0.85	8 (14%) 7 5	77, 100, 126, 165	0
19	AS	79/92 (85%)	1.43	17 (21%) 3 2	131, 153, 159, 164	0
20	AT	85/87 (97%)	0.98	12 (14%) 7 5	80, 105, 126, 142	0
21	AU	51/71 (71%)	1.46	14 (27%) 2 1	106, 132, 153, 157	0
22	AV	6/27 (22%)	2.19	3 (50%) 0 1	181, 198, 202, 206	0
23	AW	525/529 (99%)	0.80	67 (12%) 9 7	47, 99, 188, 267	0
24	AY	2/6 (33%)	1.24	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%)	1.23	18 (22%) 2 2	62, 87, 115, 129	0
26	B1	77/78 (98%)	0.23	1 (1%) 74 60	55, 71, 124, 126	0
27	B2	63/63 (100%)	0.55	5 (7%) 20 14	69, 101, 126, 140	0
28	B3	58/59 (98%)	0.14	0 100 100	63, 75, 121, 129	0
29	B4	56/57 (98%)	0.12	4 (7%) 23 16	42, 63, 97, 125	0
30	B5	50/55 (90%)	1.07	6 (12%) 10 7	114, 128, 137, 151	0
31	B6	46/46 (100%)	0.14	3 (6%) 26 18	43, 56, 77, 114	0
32	B7	64/65 (98%)	0.22	1 (1%) 70 55	57, 68, 83, 90	0
33	B8	38/38 (100%)	0.55	1 (2%) 57 41	61, 78, 90, 105	0
34	BA	2853/2903 (98%)	-0.27	41 (1%) 73 58	35, 67, 195, 445	0
35	BB	118/118 (100%)	0.04	0 100 100	61, 106, 152, 188	0
36	BC	271/273 (99%)	0.11	11 (4%) 42 28	36, 66, 83, 108	0
37	BD	209/209 (100%)	-0.09	4 (1%) 66 50	37, 57, 89, 99	0
38	BE	201/201 (100%)	0.14	6 (2%) 52 37	37, 76, 109, 131	0
39	BF	177/179 (98%)	0.79	9 (5%) 34 23	106, 128, 152, 165	0
40	BG	176/177 (99%)	0.28	6 (3%) 48 34	54, 80, 116, 131	0
41	BH	163/165 (98%)	1.80	56 (34%) 1 1	55, 145, 163, 185	1 (0%)
42	BI	141/142 (99%)	1.67	47 (33%) 1 1	135, 157, 169, 176	0
43	BJ	30/121 (24%)	1.12	4 (13%) 8 6	126, 137, 143, 145	0
43	BK	30/121 (24%)	1.24	6 (20%) 3 3	133, 146, 152, 156	0
43	BL	30/121 (24%)	2.01	14 (46%) 0 1	132, 148, 158, 163	0
43	BM	30/121 (24%)	1.06	4 (13%) 8 6	128, 142, 149, 151	0
44	BN	142/142 (100%)	0.15	10 (7%) 24 17	45, 65, 91, 117	0
45	BO	122/123 (99%)	0.04	4 (3%) 49 34	41, 61, 84, 104	0
46	BP	143/144 (99%)	0.44	5 (3%) 47 33	41, 84, 112, 132	0
47	BQ	136/136 (100%)	-0.03	2 (1%) 71 56	47, 70, 100, 126	0
48	BR	120/127 (94%)	-0.24	1 (0%) 82 70	40, 56, 72, 138	0
49	BS	116/117 (99%)	0.54	4 (3%) 48 34	81, 100, 121, 128	0
50	BT	114/115 (99%)	0.12	3 (2%) 57 41	48, 71, 112, 121	0
51	BU	117/118 (99%)	0.02	4 (3%) 48 34	37, 59, 94, 108	0
52	BV	103/103 (100%)	0.28	3 (2%) 54 38	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%)	-0.25	0 100 100	41, 54, 82, 127	0
54	BX	93/100 (93%)	0.41	5 (5%) 32 22	50, 81, 134, 144	0
55	BY	102/104 (98%)	0.52	7 (6%) 24 17	63, 84, 126, 141	0
56	BZ	94/94 (100%)	0.17	2 (2%) 63 47	68, 94, 113, 126	0
All	All	10891/11580 (94%)	0.32	694 (6%) 27 18	35, 89, 165, 445	1 (0%)

The worst 5 of 694 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	AK	125	LYS	9.6
43	BL	22	LEU	9.6
23	AW	424	ALA	7.2
4	AD	24	VAL	6.8
2	AB	150	ILE	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	UAL	AY	5	9/10	0.66	0.16	81,82,83,84	0
24	KBE	AY	1	9/10	0.69	0.25	78,79,82,82	0
24	5OH	AY	6	12/13	0.75	0.20	84,89,92,94	0
24	DPP	AY	2	6/7	0.85	0.18	79,82,82,84	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3281	1/1	0.59	0.24	73,73,73,73	0
57	MG	BA	3141	1/1	0.62	0.24	54,54,54,54	0
57	MG	BA	3242	1/1	0.65	0.18	72,72,72,72	0
57	MG	BA	3350	1/1	0.66	0.22	80,80,80,80	0
57	MG	BA	3317	1/1	0.67	0.34	88,88,88,88	0
57	MG	BA	3306	1/1	0.67	0.21	67,67,67,67	0
57	MG	BA	3349	1/1	0.68	0.41	79,79,79,79	0
57	MG	AA	1700	1/1	0.71	0.30	65,65,65,65	0
57	MG	AA	1680	1/1	0.71	0.20	55,55,55,55	0
57	MG	BA	3346	1/1	0.72	0.28	83,83,83,83	0
57	MG	AA	1701	1/1	0.72	0.19	79,79,79,79	0
57	MG	BA	3343	1/1	0.72	0.16	71,71,71,71	0
57	MG	AA	1687	1/1	0.73	0.21	81,81,81,81	0
57	MG	BA	3330	1/1	0.73	0.17	83,83,83,83	0
57	MG	BA	3357	1/1	0.74	0.18	81,81,81,81	0
57	MG	AA	1696	1/1	0.75	0.19	89,89,89,89	0
57	MG	BA	3305	1/1	0.77	0.23	71,71,71,71	0
57	MG	B0	103	1/1	0.77	0.13	54,54,54,54	0
57	MG	BA	3214	1/1	0.77	0.13	43,43,43,43	0
57	MG	BA	3298	1/1	0.77	0.23	76,76,76,76	0
57	MG	BA	3355	1/1	0.77	0.21	69,69,69,69	0
57	MG	BA	3334	1/1	0.77	0.16	56,56,56,56	0
57	MG	BA	3348	1/1	0.78	0.10	67,67,67,67	0
57	MG	AA	1686	1/1	0.78	0.17	93,93,93,93	0
57	MG	BA	3270	1/1	0.78	0.24	59,59,59,59	0
57	MG	BA	3352	1/1	0.78	0.17	61,61,61,61	0
57	MG	AA	1659	1/1	0.78	0.08	55,55,55,55	0
57	MG	BA	3284	1/1	0.78	0.20	73,73,73,73	0
57	MG	BA	3311	1/1	0.79	0.13	48,48,48,48	0
57	MG	BA	3065	1/1	0.79	0.28	46,46,46,46	0
57	MG	AA	1679	1/1	0.80	0.23	62,62,62,62	0
57	MG	BA	3232	1/1	0.80	0.20	54,54,54,54	0
57	MG	BA	3333	1/1	0.80	0.30	77,77,77,77	0
57	MG	BA	3104	1/1	0.80	0.18	45,45,45,45	0
57	MG	AA	1662	1/1	0.80	0.25	57,57,57,57	0
57	MG	BA	3205	1/1	0.80	0.16	50,50,50,50	0
57	MG	BB	205	1/1	0.80	0.34	79,79,79,79	0
57	MG	BA	3321	1/1	0.81	0.15	73,73,73,73	0
57	MG	AW	601	1/1	0.81	0.10	36,36,36,36	0
57	MG	BA	3332	1/1	0.81	0.15	96,96,96,96	0
57	MG	BA	3177	1/1	0.81	0.28	59,59,59,59	0
57	MG	AA	1649	1/1	0.81	0.25	49,49,49,49	0
57	MG	BA	3312	1/1	0.81	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BB	203	1/1	0.81	0.10	51,51,51,51	0
57	MG	BA	3262	1/1	0.81	0.42	85,85,85,85	0
57	MG	BD	303	1/1	0.81	0.07	57,57,57,57	0
57	MG	AA	1621	1/1	0.82	0.26	57,57,57,57	0
57	MG	AA	1668	1/1	0.82	0.12	51,51,51,51	0
57	MG	BA	3001	1/1	0.82	0.33	42,42,42,42	0
57	MG	AA	1689	1/1	0.82	0.40	69,69,69,69	0
57	MG	BA	3216	1/1	0.82	0.22	63,63,63,63	0
57	MG	BA	3299	1/1	0.82	0.20	64,64,64,64	0
57	MG	BA	3219	1/1	0.82	0.29	69,69,69,69	0
57	MG	AM	201	1/1	0.82	0.10	80,80,80,80	0
57	MG	BA	3105	1/1	0.82	0.25	49,49,49,49	0
57	MG	AA	1632	1/1	0.83	0.21	40,40,40,40	0
57	MG	AA	1671	1/1	0.83	0.13	53,53,53,53	0
57	MG	BA	3243	1/1	0.83	0.17	62,62,62,62	0
57	MG	BA	3244	1/1	0.83	0.26	76,76,76,76	0
57	MG	BA	3117	1/1	0.83	0.19	46,46,46,46	0
57	MG	AA	1651	1/1	0.83	0.13	51,51,51,51	0
57	MG	BA	3152	1/1	0.83	0.09	41,41,41,41	0
57	MG	BA	3174	1/1	0.83	0.15	49,49,49,49	0
57	MG	AA	1657	1/1	0.83	0.11	83,83,83,83	0
57	MG	BA	3184	1/1	0.83	0.09	37,37,37,37	0
57	MG	AA	1633	1/1	0.83	0.26	53,53,53,53	0
57	MG	AA	1638	1/1	0.83	0.12	55,55,55,55	0
57	MG	AA	1667	1/1	0.83	0.11	87,87,87,87	0
57	MG	AA	1694	1/1	0.83	0.14	75,75,75,75	0
57	MG	BA	3316	1/1	0.83	0.18	61,61,61,61	0
57	MG	BA	3223	1/1	0.83	0.39	75,75,75,75	0
57	MG	AA	1645	1/1	0.84	0.15	62,62,62,62	0
57	MG	BA	3170	1/1	0.84	0.15	52,52,52,52	0
57	MG	AA	1646	1/1	0.84	0.17	50,50,50,50	0
57	MG	AA	1639	1/1	0.84	0.13	49,49,49,49	0
57	MG	BA	3335	1/1	0.84	0.14	58,58,58,58	0
57	MG	AA	1683	1/1	0.84	0.08	63,63,63,63	0
57	MG	BA	3148	1/1	0.84	0.17	50,50,50,50	0
57	MG	BA	3211	1/1	0.84	0.19	48,48,48,48	0
57	MG	BO	201	1/1	0.84	0.14	41,41,41,41	0
57	MG	BA	3354	1/1	0.85	0.08	62,62,62,62	0
57	MG	BA	3075	1/1	0.85	0.09	43,43,43,43	0
57	MG	BA	3201	1/1	0.85	0.20	47,47,47,47	0
57	MG	BA	3125	1/1	0.85	0.31	53,53,53,53	0
57	MG	AA	1672	1/1	0.85	0.07	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BB	208	1/1	0.85	0.13	59,59,59,59	0
57	MG	AA	1658	1/1	0.85	0.26	61,61,61,61	0
57	MG	BA	3179	1/1	0.85	0.18	46,46,46,46	0
57	MG	BA	3169	1/1	0.86	0.17	39,39,39,39	0
57	MG	AA	1656	1/1	0.86	0.21	73,73,73,73	0
57	MG	BA	3172	1/1	0.86	0.14	53,53,53,53	0
57	MG	BA	3096	1/1	0.86	0.18	44,44,44,44	0
57	MG	AA	1688	1/1	0.86	0.15	77,77,77,77	0
57	MG	AA	1648	1/1	0.86	0.07	54,54,54,54	0
57	MG	AA	1635	1/1	0.86	0.19	58,58,58,58	0
57	MG	BA	3253	1/1	0.86	0.17	65,65,65,65	0
57	MG	BA	3198	1/1	0.86	0.16	60,60,60,60	0
57	MG	BA	3331	1/1	0.86	0.16	64,64,64,64	0
57	MG	AA	1669	1/1	0.86	0.07	71,71,71,71	0
57	MG	BA	3016	1/1	0.86	0.30	39,39,39,39	0
57	MG	BC	301	1/1	0.86	0.14	53,53,53,53	0
57	MG	BA	3032	1/1	0.86	0.32	38,38,38,38	0
57	MG	BE	301	1/1	0.86	0.12	67,67,67,67	0
57	MG	AA	1647	1/1	0.86	0.14	60,60,60,60	0
57	MG	AA	1652	1/1	0.87	0.17	60,60,60,60	0
57	MG	BA	3261	1/1	0.87	0.17	63,63,63,63	0
57	MG	BA	3154	1/1	0.87	0.35	43,43,43,43	0
57	MG	BA	3160	1/1	0.87	0.19	49,49,49,49	0
57	MG	AA	1675	1/1	0.87	0.11	57,57,57,57	0
57	MG	BA	3215	1/1	0.87	0.08	53,53,53,53	0
57	MG	BA	3287	1/1	0.87	0.15	83,83,83,83	0
57	MG	BA	3294	1/1	0.87	0.12	43,43,43,43	0
57	MG	BA	3295	1/1	0.87	0.19	57,57,57,57	0
57	MG	B0	102	1/1	0.87	0.14	33,33,33,33	0
57	MG	AA	1613	1/1	0.87	0.25	58,58,58,58	0
57	MG	BA	3303	1/1	0.87	0.08	56,56,56,56	0
57	MG	AA	1610	1/1	0.87	0.17	45,45,45,45	0
57	MG	BA	3356	1/1	0.87	0.17	61,61,61,61	0
57	MG	BA	3225	1/1	0.87	0.29	60,60,60,60	0
57	MG	BA	3231	1/1	0.87	0.14	56,56,56,56	0
57	MG	AA	1650	1/1	0.87	0.20	67,67,67,67	0
57	MG	BB	207	1/1	0.87	0.08	47,47,47,47	0
57	MG	BA	3313	1/1	0.87	0.22	67,67,67,67	0
57	MG	BA	3136	1/1	0.87	0.28	53,53,53,53	0
57	MG	AA	1685	1/1	0.87	0.08	64,64,64,64	0
57	MG	AA	1634	1/1	0.87	0.19	55,55,55,55	0
57	MG	BA	3247	1/1	0.87	0.19	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3144	1/1	0.88	0.12	68,68,68,68	0
57	MG	BA	3187	1/1	0.88	0.23	56,56,56,56	0
57	MG	BA	3197	1/1	0.88	0.08	38,38,38,38	0
57	MG	AA	1670	1/1	0.88	0.12	62,62,62,62	0
57	MG	AA	1654	1/1	0.88	0.23	58,58,58,58	0
57	MG	BA	3353	1/1	0.88	0.26	73,73,73,73	0
57	MG	AA	1603	1/1	0.88	0.35	42,42,42,42	0
57	MG	BA	3207	1/1	0.88	0.30	54,54,54,54	0
57	MG	BA	3157	1/1	0.88	0.26	46,46,46,46	0
57	MG	AA	1674	1/1	0.88	0.15	55,55,55,55	0
57	MG	BB	201	1/1	0.88	0.28	54,54,54,54	0
57	MG	BA	3107	1/1	0.88	0.17	36,36,36,36	0
57	MG	BA	3037	1/1	0.88	0.25	36,36,36,36	0
57	MG	BA	3048	1/1	0.88	0.29	40,40,40,40	0
57	MG	BA	3288	1/1	0.88	0.15	95,95,95,95	0
57	MG	BA	3131	1/1	0.88	0.14	40,40,40,40	0
57	MG	BA	3061	1/1	0.88	0.30	48,48,48,48	0
57	MG	BA	3296	1/1	0.88	0.17	60,60,60,60	0
57	MG	AA	1636	1/1	0.88	0.08	36,36,36,36	0
57	MG	BA	3098	1/1	0.89	0.13	47,47,47,47	0
57	MG	BA	3338	1/1	0.89	0.08	61,61,61,61	0
57	MG	AA	1663	1/1	0.89	0.15	74,74,74,74	0
57	MG	BA	3045	1/1	0.89	0.32	35,35,35,35	0
57	MG	AA	1677	1/1	0.89	0.16	57,57,57,57	0
57	MG	BA	3202	1/1	0.89	0.18	57,57,57,57	0
57	MG	BA	3304	1/1	0.89	0.19	50,50,50,50	0
57	MG	BA	3351	1/1	0.89	0.17	58,58,58,58	0
57	MG	BA	3109	1/1	0.89	0.15	38,38,38,38	0
57	MG	BA	3161	1/1	0.89	0.13	42,42,42,42	0
57	MG	AA	1666	1/1	0.89	0.17	62,62,62,62	0
57	MG	BA	3124	1/1	0.89	0.24	42,42,42,42	0
57	MG	BA	3268	1/1	0.89	0.08	52,52,52,52	0
57	MG	AA	1673	1/1	0.89	0.16	84,84,84,84	0
57	MG	BA	3274	1/1	0.89	0.24	52,52,52,52	0
57	MG	BA	3318	1/1	0.89	0.28	57,57,57,57	0
57	MG	BA	3319	1/1	0.89	0.12	68,68,68,68	0
57	MG	BA	3276	1/1	0.89	0.26	58,58,58,58	0
57	MG	BA	3068	1/1	0.89	0.24	28,28,28,28	0
57	MG	AF	201	1/1	0.89	0.17	65,65,65,65	0
57	MG	BD	302	1/1	0.89	0.27	53,53,53,53	0
57	MG	BA	3222	1/1	0.89	0.10	50,50,50,50	0
57	MG	BA	3095	1/1	0.89	0.21	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1606	1/1	0.89	0.25	45,45,45,45	0
57	MG	BA	3115	1/1	0.90	0.15	37,37,37,37	0
57	MG	AA	1625	1/1	0.90	0.09	40,40,40,40	0
57	MG	BA	3278	1/1	0.90	0.20	48,48,48,48	0
57	MG	BA	3280	1/1	0.90	0.23	73,73,73,73	0
57	MG	AA	1628	1/1	0.90	0.15	44,44,44,44	0
57	MG	AA	1692	1/1	0.90	0.14	67,67,67,67	0
57	MG	BA	3286	1/1	0.90	0.12	48,48,48,48	0
57	MG	AA	1682	1/1	0.90	0.05	76,76,76,76	0
57	MG	BA	3347	1/1	0.90	0.16	76,76,76,76	0
57	MG	BA	3134	1/1	0.90	0.24	49,49,49,49	0
57	MG	BA	3291	1/1	0.90	0.20	58,58,58,58	0
57	MG	AA	1631	1/1	0.90	0.13	60,60,60,60	0
57	MG	AA	1699	1/1	0.90	0.37	49,49,49,49	0
57	MG	BA	3186	1/1	0.90	0.13	47,47,47,47	0
57	MG	BA	3023	1/1	0.90	0.32	39,39,39,39	0
57	MG	BA	3235	1/1	0.90	0.14	64,64,64,64	0
57	MG	BA	3237	1/1	0.90	0.10	51,51,51,51	0
57	MG	BA	3238	1/1	0.90	0.14	50,50,50,50	0
57	MG	BA	3189	1/1	0.90	0.12	51,51,51,51	0
57	MG	BA	3030	1/1	0.90	0.24	38,38,38,38	0
57	MG	AA	1608	1/1	0.90	0.21	59,59,59,59	0
57	MG	BA	3153	1/1	0.90	0.18	59,59,59,59	0
57	MG	BB	206	1/1	0.90	0.09	65,65,65,65	0
57	MG	BA	3248	1/1	0.90	0.23	52,52,52,52	0
57	MG	AA	1605	1/1	0.90	0.19	38,38,38,38	0
57	MG	BA	3256	1/1	0.90	0.12	56,56,56,56	0
57	MG	BA	3203	1/1	0.90	0.18	50,50,50,50	0
57	MG	BA	3204	1/1	0.90	0.21	72,72,72,72	0
57	MG	AA	1624	1/1	0.90	0.21	51,51,51,51	0
57	MG	BA	3046	1/1	0.90	0.29	27,27,27,27	0
58	GNP	AW	602	32/32	0.90	0.10	58,71,81,83	0
57	MG	BA	3323	1/1	0.91	0.08	64,64,64,64	0
57	MG	BA	3326	1/1	0.91	0.10	42,42,42,42	0
57	MG	BA	3327	1/1	0.91	0.12	64,64,64,64	0
57	MG	BA	3138	1/1	0.91	0.25	58,58,58,58	0
57	MG	BA	3140	1/1	0.91	0.23	46,46,46,46	0
57	MG	BA	3218	1/1	0.91	0.16	50,50,50,50	0
57	MG	BA	3181	1/1	0.91	0.11	44,44,44,44	0
57	MG	AA	1616	1/1	0.91	0.14	37,37,37,37	0
57	MG	BA	3279	1/1	0.91	0.13	50,50,50,50	0
57	MG	BA	3185	1/1	0.91	0.19	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3339	1/1	0.91	0.18	76,76,76,76	0
57	MG	BA	3100	1/1	0.91	0.26	36,36,36,36	0
57	MG	BA	3345	1/1	0.91	0.24	67,67,67,67	0
57	MG	BA	3227	1/1	0.91	0.18	63,63,63,63	0
57	MG	BA	3145	1/1	0.91	0.24	55,55,55,55	0
57	MG	AA	1641	1/1	0.91	0.09	67,67,67,67	0
57	MG	BA	3233	1/1	0.91	0.15	46,46,46,46	0
57	MG	BA	3195	1/1	0.91	0.06	47,47,47,47	0
57	MG	AA	1665	1/1	0.91	0.17	56,56,56,56	0
57	MG	AL	201	1/1	0.91	0.28	54,54,54,54	0
57	MG	BA	3029	1/1	0.91	0.20	28,28,28,28	0
57	MG	AA	1643	1/1	0.91	0.14	56,56,56,56	0
57	MG	BA	3070	1/1	0.91	0.15	44,44,44,44	0
57	MG	BA	3301	1/1	0.91	0.28	64,64,64,64	0
57	MG	BA	3246	1/1	0.91	0.08	48,48,48,48	0
57	MG	AA	1678	1/1	0.91	0.17	65,65,65,65	0
57	MG	BA	3079	1/1	0.91	0.24	44,44,44,44	0
57	MG	BA	3250	1/1	0.91	0.34	66,66,66,66	0
57	MG	BA	3206	1/1	0.91	0.09	52,52,52,52	0
57	MG	BA	3254	1/1	0.91	0.15	59,59,59,59	0
57	MG	BA	3255	1/1	0.91	0.09	66,66,66,66	0
57	MG	BA	3034	1/1	0.91	0.24	36,36,36,36	0
57	MG	BA	3257	1/1	0.91	0.08	48,48,48,48	0
57	MG	AA	1655	1/1	0.91	0.17	60,60,60,60	0
57	MG	BA	3097	1/1	0.91	0.20	48,48,48,48	0
57	MG	BA	3264	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3322	1/1	0.91	0.12	62,62,62,62	0
57	MG	BA	3188	1/1	0.92	0.25	51,51,51,51	0
57	MG	AA	1612	1/1	0.92	0.20	29,29,29,29	0
57	MG	BA	3193	1/1	0.92	0.18	61,61,61,61	0
57	MG	BA	3150	1/1	0.92	0.18	53,53,53,53	0
57	MG	BA	3069	1/1	0.92	0.19	39,39,39,39	0
57	MG	BA	3336	1/1	0.92	0.07	86,86,86,86	0
57	MG	AA	1622	1/1	0.92	0.16	42,42,42,42	0
57	MG	B4	101	1/1	0.92	0.26	40,40,40,40	0
57	MG	BA	3039	1/1	0.92	0.23	31,31,31,31	0
57	MG	BA	3344	1/1	0.92	0.10	71,71,71,71	0
57	MG	BA	3158	1/1	0.92	0.13	35,35,35,35	0
57	MG	BA	3089	1/1	0.92	0.17	52,52,52,52	0
57	MG	BA	3297	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3130	1/1	0.92	0.14	41,41,41,41	0
57	MG	BA	3164	1/1	0.92	0.10	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3251	1/1	0.92	0.15	49,49,49,49	0
57	MG	AA	1676	1/1	0.92	0.13	52,52,52,52	0
57	MG	BA	3210	1/1	0.92	0.23	73,73,73,73	0
57	MG	BA	3132	1/1	0.92	0.26	52,52,52,52	0
57	MG	BA	3171	1/1	0.92	0.12	57,57,57,57	0
57	MG	AA	1660	1/1	0.92	0.09	46,46,46,46	0
57	MG	BA	3258	1/1	0.92	0.09	50,50,50,50	0
57	MG	AL	202	1/1	0.92	0.25	73,73,73,73	0
57	MG	BA	3314	1/1	0.92	0.14	56,56,56,56	0
57	MG	BA	3315	1/1	0.92	0.20	63,63,63,63	0
57	MG	BA	3137	1/1	0.92	0.19	42,42,42,42	0
57	MG	AA	1661	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3063	1/1	0.92	0.17	32,32,32,32	0
57	MG	BA	3269	1/1	0.92	0.11	51,51,51,51	0
57	MG	BA	3102	1/1	0.92	0.20	36,36,36,36	0
57	MG	BA	3143	1/1	0.92	0.08	32,32,32,32	0
57	MG	BA	3275	1/1	0.92	0.08	59,59,59,59	0
57	MG	BA	3064	1/1	0.92	0.14	24,24,24,24	0
57	MG	BA	3229	1/1	0.92	0.10	46,46,46,46	0
57	MG	BT	201	1/1	0.92	0.12	40,40,40,40	0
57	MG	BX	201	1/1	0.92	0.07	47,47,47,47	0
57	MG	AA	1617	1/1	0.92	0.15	47,47,47,47	0
57	MG	BA	3285	1/1	0.93	0.27	75,75,75,75	0
57	MG	BA	3239	1/1	0.93	0.07	71,71,71,71	0
57	MG	BA	3111	1/1	0.93	0.13	29,29,29,29	0
57	MG	BA	3199	1/1	0.93	0.18	42,42,42,42	0
57	MG	BA	3112	1/1	0.93	0.09	41,41,41,41	0
57	MG	BA	3292	1/1	0.93	0.13	54,54,54,54	0
57	MG	BA	3337	1/1	0.93	0.09	55,55,55,55	0
57	MG	BA	3076	1/1	0.93	0.21	36,36,36,36	0
57	MG	BA	3116	1/1	0.93	0.18	41,41,41,41	0
57	MG	BA	3078	1/1	0.93	0.23	32,32,32,32	0
57	MG	BA	3120	1/1	0.93	0.06	31,31,31,31	0
57	MG	BA	3122	1/1	0.93	0.11	38,38,38,38	0
57	MG	BA	3052	1/1	0.93	0.40	39,39,39,39	0
57	MG	BA	3300	1/1	0.93	0.21	69,69,69,69	0
57	MG	BA	3058	1/1	0.93	0.21	35,35,35,35	0
57	MG	BA	3129	1/1	0.93	0.14	43,43,43,43	0
57	MG	BA	3090	1/1	0.93	0.21	40,40,40,40	0
57	MG	BA	3094	1/1	0.93	0.18	47,47,47,47	0
57	MG	AA	1615	1/1	0.93	0.13	40,40,40,40	0
57	MG	BA	3307	1/1	0.93	0.08	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3308	1/1	0.93	0.12	82,82,82,82	0
57	MG	BA	3310	1/1	0.93	0.10	75,75,75,75	0
57	MG	BA	3260	1/1	0.93	0.17	50,50,50,50	0
57	MG	BA	3175	1/1	0.93	0.11	44,44,44,44	0
57	MG	BA	3062	1/1	0.93	0.14	42,42,42,42	0
57	MG	AA	1637	1/1	0.93	0.07	54,54,54,54	0
57	MG	AA	1618	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3017	1/1	0.93	0.15	30,30,30,30	0
57	MG	BA	3226	1/1	0.93	0.16	51,51,51,51	0
57	MG	AA	1627	1/1	0.93	0.17	40,40,40,40	0
57	MG	BA	3103	1/1	0.93	0.16	28,28,28,28	0
57	MG	BD	301	1/1	0.93	0.11	49,49,49,49	0
57	MG	BA	3142	1/1	0.93	0.19	50,50,50,50	0
57	MG	AA	1623	1/1	0.93	0.11	42,42,42,42	0
57	MG	AA	1629	1/1	0.93	0.17	41,41,41,41	0
57	MG	BN	201	1/1	0.93	0.16	51,51,51,51	0
57	MG	BA	3073	1/1	0.93	0.26	42,42,42,42	0
57	MG	BQ	201	1/1	0.93	0.07	44,44,44,44	0
57	MG	BA	3051	1/1	0.93	0.15	33,33,33,33	0
57	MG	BA	3328	1/1	0.93	0.10	71,71,71,71	0
57	MG	BA	3110	1/1	0.93	0.10	38,38,38,38	0
57	MG	BA	3209	1/1	0.94	0.14	42,42,42,42	0
57	MG	AA	1601	1/1	0.94	0.14	22,22,22,22	0
57	MG	AA	1684	1/1	0.94	0.24	60,60,60,60	0
57	MG	BA	3077	1/1	0.94	0.18	41,41,41,41	0
57	MG	AA	1630	1/1	0.94	0.24	48,48,48,48	0
57	MG	BA	3178	1/1	0.94	0.22	49,49,49,49	0
57	MG	BA	3302	1/1	0.94	0.17	68,68,68,68	0
57	MG	BA	3056	1/1	0.94	0.16	26,26,26,26	0
57	MG	BA	3081	1/1	0.94	0.20	35,35,35,35	0
57	MG	BA	3220	1/1	0.94	0.16	56,56,56,56	0
57	MG	AA	1690	1/1	0.94	0.09	83,83,83,83	0
57	MG	BA	3263	1/1	0.94	0.18	53,53,53,53	0
57	MG	AA	1691	1/1	0.94	0.08	63,63,63,63	0
57	MG	BA	3224	1/1	0.94	0.12	41,41,41,41	0
57	MG	BA	3092	1/1	0.94	0.31	43,43,43,43	0
57	MG	BA	3151	1/1	0.94	0.19	47,47,47,47	0
57	MG	BA	3272	1/1	0.94	0.14	55,55,55,55	0
57	MG	BA	3121	1/1	0.94	0.23	39,39,39,39	0
57	MG	AA	1702	1/1	0.94	0.19	58,58,58,58	0
57	MG	BA	3192	1/1	0.94	0.26	59,59,59,59	0
57	MG	BA	3036	1/1	0.94	0.16	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3194	1/1	0.94	0.11	49,49,49,49	0
57	MG	BA	3155	1/1	0.94	0.21	51,51,51,51	0
57	MG	BA	3156	1/1	0.94	0.13	41,41,41,41	0
57	MG	AA	1602	1/1	0.94	0.22	37,37,37,37	0
57	MG	BA	3038	1/1	0.94	0.10	21,21,21,21	0
57	MG	BA	3324	1/1	0.94	0.10	59,59,59,59	0
57	MG	BA	3325	1/1	0.94	0.22	59,59,59,59	0
57	MG	BA	3066	1/1	0.94	0.26	41,41,41,41	0
57	MG	BA	3012	1/1	0.94	0.23	18,18,18,18	0
57	MG	BA	3042	1/1	0.94	0.13	27,27,27,27	0
57	MG	BA	3329	1/1	0.94	0.13	58,58,58,58	0
57	MG	BA	3289	1/1	0.94	0.06	62,62,62,62	0
57	MG	BA	3165	1/1	0.94	0.20	52,52,52,52	0
57	MG	BA	3014	1/1	0.94	0.20	27,27,27,27	0
57	MG	AA	1693	1/1	0.94	0.13	56,56,56,56	0
57	MG	BA	3074	1/1	0.94	0.18	44,44,44,44	0
57	MG	AA	1604	1/1	0.95	0.26	42,42,42,42	0
57	MG	B0	101	1/1	0.95	0.05	23,23,23,23	0
57	MG	BA	3040	1/1	0.95	0.24	43,43,43,43	0
57	MG	BA	3041	1/1	0.95	0.10	27,27,27,27	0
57	MG	BA	3228	1/1	0.95	0.10	42,42,42,42	0
57	MG	BA	3020	1/1	0.95	0.25	29,29,29,29	0
57	MG	BA	3106	1/1	0.95	0.18	37,37,37,37	0
57	MG	BA	3071	1/1	0.95	0.24	35,35,35,35	0
57	MG	BA	3146	1/1	0.95	0.20	40,40,40,40	0
57	MG	BA	3190	1/1	0.95	0.15	43,43,43,43	0
57	MG	BA	3147	1/1	0.95	0.12	46,46,46,46	0
57	MG	BA	3044	1/1	0.95	0.27	37,37,37,37	0
57	MG	BA	3149	1/1	0.95	0.23	42,42,42,42	0
57	MG	BA	3340	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3240	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3022	1/1	0.95	0.15	28,28,28,28	0
57	MG	BA	3196	1/1	0.95	0.23	46,46,46,46	0
57	MG	AA	1619	1/1	0.95	0.11	40,40,40,40	0
57	MG	BA	3245	1/1	0.95	0.11	46,46,46,46	0
57	MG	BA	3047	1/1	0.95	0.22	51,51,51,51	0
57	MG	BA	3026	1/1	0.95	0.13	24,24,24,24	0
57	MG	BA	3027	1/1	0.95	0.30	40,40,40,40	0
57	MG	BA	3249	1/1	0.95	0.07	49,49,49,49	0
57	MG	BA	3028	1/1	0.95	0.19	26,26,26,26	0
57	MG	BA	3053	1/1	0.95	0.28	31,31,31,31	0
57	MG	BA	3088	1/1	0.95	0.14	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3054	1/1	0.95	0.23	36,36,36,36	0
57	MG	BA	3123	1/1	0.95	0.12	36,36,36,36	0
57	MG	AA	1681	1/1	0.95	0.05	38,38,38,38	0
57	MG	BA	3208	1/1	0.95	0.16	62,62,62,62	0
57	MG	BB	202	1/1	0.95	0.21	43,43,43,43	0
57	MG	BA	3091	1/1	0.95	0.29	42,42,42,42	0
57	MG	BA	3259	1/1	0.95	0.06	69,69,69,69	0
57	MG	AA	1644	1/1	0.95	0.05	49,49,49,49	0
57	MG	BA	3059	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3213	1/1	0.95	0.11	46,46,46,46	0
57	MG	BB	209	1/1	0.95	0.25	36,36,36,36	0
57	MG	AA	1695	1/1	0.95	0.09	62,62,62,62	0
57	MG	AA	1620	1/1	0.95	0.14	52,52,52,52	0
57	MG	BA	3267	1/1	0.95	0.12	52,52,52,52	0
57	MG	BA	3133	1/1	0.95	0.12	45,45,45,45	0
57	MG	BA	3320	1/1	0.95	0.13	52,52,52,52	0
57	MG	AA	1640	1/1	0.95	0.06	41,41,41,41	0
57	MG	BA	3135	1/1	0.95	0.15	45,45,45,45	0
57	MG	BA	3271	1/1	0.95	0.17	53,53,53,53	0
57	MG	BA	3176	1/1	0.95	0.12	50,50,50,50	0
57	MG	BA	3015	1/1	0.95	0.29	38,38,38,38	0
57	MG	BA	3099	1/1	0.95	0.33	44,44,44,44	0
57	MG	BA	3200	1/1	0.96	0.10	44,44,44,44	0
57	MG	BA	3033	1/1	0.96	0.19	25,25,25,25	0
57	MG	BA	3265	1/1	0.96	0.22	45,45,45,45	0
57	MG	BA	3341	1/1	0.96	0.11	57,57,57,57	0
57	MG	AA	1697	1/1	0.96	0.04	64,64,64,64	0
57	MG	BA	3234	1/1	0.96	0.11	49,49,49,49	0
57	MG	BA	3002	1/1	0.96	0.14	13,13,13,13	0
57	MG	BA	3080	1/1	0.96	0.25	43,43,43,43	0
57	MG	BA	3127	1/1	0.96	0.15	38,38,38,38	0
57	MG	BA	3309	1/1	0.96	0.04	62,62,62,62	0
57	MG	BA	3050	1/1	0.96	0.19	33,33,33,33	0
57	MG	BA	3273	1/1	0.96	0.13	72,72,72,72	0
57	MG	BA	3083	1/1	0.96	0.30	47,47,47,47	0
57	MG	BA	3180	1/1	0.96	0.05	45,45,45,45	0
57	MG	BA	3087	1/1	0.96	0.18	42,42,42,42	0
57	MG	BA	3277	1/1	0.96	0.08	42,42,42,42	0
57	MG	BA	3183	1/1	0.96	0.05	48,48,48,48	0
57	MG	BA	3010	1/1	0.96	0.14	33,33,33,33	0
57	MG	BA	3108	1/1	0.96	0.18	42,42,42,42	0
57	MG	BA	3024	1/1	0.96	0.27	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3282	1/1	0.96	0.14	55,55,55,55	0
57	MG	AA	1698	1/1	0.96	0.05	51,51,51,51	0
57	MG	BB	204	1/1	0.96	0.24	53,53,53,53	0
57	MG	AA	1611	1/1	0.96	0.21	44,44,44,44	0
57	MG	BA	3217	1/1	0.96	0.12	56,56,56,56	0
57	MG	AA	1614	1/1	0.96	0.18	42,42,42,42	0
57	MG	BA	3252	1/1	0.96	0.19	49,49,49,49	0
57	MG	BA	3114	1/1	0.96	0.16	32,32,32,32	0
57	MG	BA	3290	1/1	0.96	0.06	56,56,56,56	0
57	MG	BA	3191	1/1	0.96	0.07	57,57,57,57	0
57	MG	BA	3139	1/1	0.96	0.16	43,43,43,43	0
57	MG	BA	3293	1/1	0.96	0.09	53,53,53,53	0
57	MG	BD	304	1/1	0.96	0.21	28,28,28,28	0
57	MG	BA	3072	1/1	0.96	0.18	36,36,36,36	0
57	MG	B2	101	1/1	0.96	0.04	49,49,49,49	0
57	MG	BA	3166	1/1	0.96	0.06	50,50,50,50	0
57	MG	BA	3167	1/1	0.96	0.28	48,48,48,48	0
57	MG	BR	201	1/1	0.96	0.13	69,69,69,69	0
57	MG	BR	202	1/1	0.96	0.10	51,51,51,51	0
57	MG	AA	1653	1/1	0.96	0.13	41,41,41,41	0
57	MG	BA	3060	1/1	0.96	0.27	27,27,27,27	0
57	MG	BA	3019	1/1	0.96	0.15	15,15,15,15	0
57	MG	BA	3035	1/1	0.97	0.19	26,26,26,26	0
57	MG	BA	3212	1/1	0.97	0.24	45,45,45,45	0
57	MG	BA	3084	1/1	0.97	0.20	21,21,21,21	0
57	MG	BA	3086	1/1	0.97	0.24	43,43,43,43	0
57	MG	BA	3067	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3021	1/1	0.97	0.14	18,18,18,18	0
57	MG	BA	3283	1/1	0.97	0.22	25,25,25,25	0
57	MG	BA	3008	1/1	0.97	0.14	22,22,22,22	0
57	MG	BA	3009	1/1	0.97	0.18	14,14,14,14	0
57	MG	AH	201	1/1	0.97	0.12	50,50,50,50	0
57	MG	BA	3162	1/1	0.97	0.07	56,56,56,56	0
57	MG	BA	3221	1/1	0.97	0.23	43,43,43,43	0
57	MG	BA	3011	1/1	0.97	0.30	23,23,23,23	0
57	MG	BA	3113	1/1	0.97	0.17	34,34,34,34	0
57	MG	BA	3093	1/1	0.97	0.15	42,42,42,42	0
57	MG	BA	3057	1/1	0.97	0.22	33,33,33,33	0
57	MG	BA	3168	1/1	0.97	0.03	32,32,32,32	0
57	MG	AA	1609	1/1	0.97	0.28	40,40,40,40	0
57	MG	AA	1607	1/1	0.97	0.20	33,33,33,33	0
57	MG	BA	3118	1/1	0.97	0.23	40,40,40,40	0

Continued on next page...

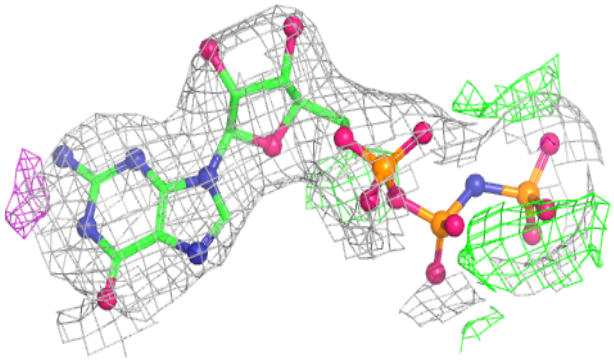
Continued from previous page...

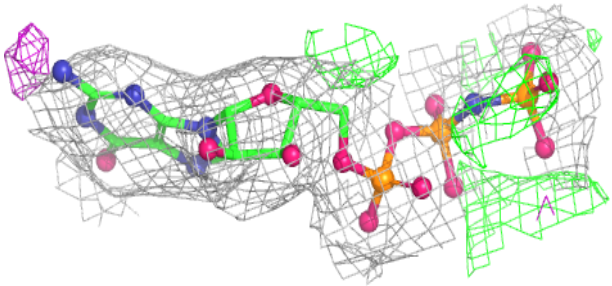
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3230	1/1	0.97	0.09	46,46,46,46	0
57	MG	BA	3119	1/1	0.97	0.11	29,29,29,29	0
57	MG	BA	3173	1/1	0.97	0.06	36,36,36,36	0
57	MG	BA	3266	1/1	0.97	0.05	56,56,56,56	0
57	MG	BA	3043	1/1	0.97	0.23	26,26,26,26	0
57	MG	BA	3003	1/1	0.97	0.25	18,18,18,18	0
57	MG	BD	305	1/1	0.97	0.08	16,16,16,16	0
57	MG	BA	3004	1/1	0.97	0.18	21,21,21,21	0
57	MG	BA	3236	1/1	0.97	0.07	46,46,46,46	0
57	MG	BA	3005	1/1	0.97	0.11	20,20,20,20	0
57	MG	BA	3101	1/1	0.97	0.10	43,43,43,43	0
57	MG	BA	3006	1/1	0.97	0.18	22,22,22,22	0
57	MG	BA	3342	1/1	0.97	0.09	54,54,54,54	0
57	MG	BA	3007	1/1	0.97	0.18	17,17,17,17	0
57	MG	BA	3128	1/1	0.97	0.10	33,33,33,33	0
57	MG	BA	3182	1/1	0.97	0.19	48,48,48,48	0
57	MG	BA	3013	1/1	0.98	0.18	20,20,20,20	0
57	MG	BA	3085	1/1	0.98	0.15	40,40,40,40	0
57	MG	BA	3163	1/1	0.98	0.14	49,49,49,49	0
57	MG	BA	3241	1/1	0.98	0.08	57,57,57,57	0
57	MG	BA	3126	1/1	0.98	0.14	31,31,31,31	0
57	MG	BA	3018	1/1	0.98	0.16	16,16,16,16	0
57	MG	BA	3049	1/1	0.98	0.14	31,31,31,31	0
57	MG	AA	1626	1/1	0.98	0.25	45,45,45,45	0
57	MG	BA	3025	1/1	0.98	0.17	32,32,32,32	0
57	MG	AA	1664	1/1	0.98	0.05	41,41,41,41	0
57	MG	BA	3159	1/1	0.98	0.17	49,49,49,49	0
57	MG	AA	1642	1/1	0.98	0.08	53,53,53,53	0
57	MG	BA	3082	1/1	0.99	0.27	36,36,36,36	0
57	MG	BA	3031	1/1	0.99	0.18	25,25,25,25	0
57	MG	BA	3055	1/1	0.99	0.19	24,24,24,24	0

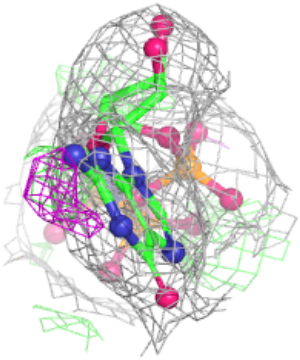
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.