wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 10:37 am BST

PDB ID	:	4V9H
Title	:	Crystal structure of the ribosome bound to elongation factor G in the guanosine triphosphatase state
Authors	:	Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2013-03-25
Resolution	:	2.86 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 following versions of software and data (see references (1)) were used in the production of this report:

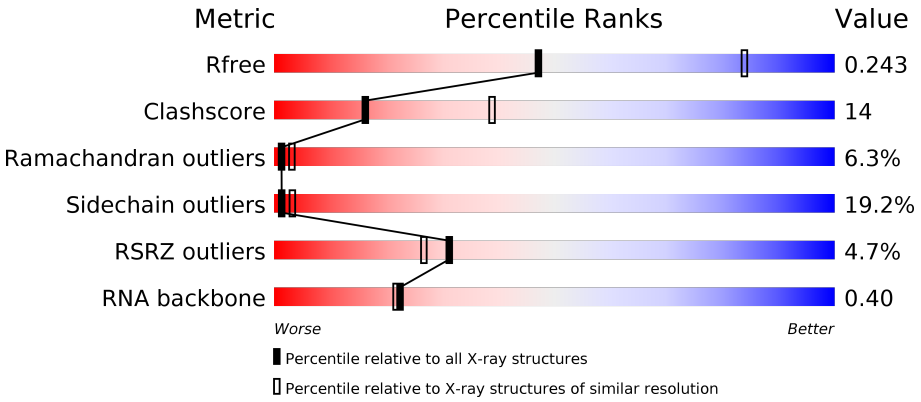
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1516	3% 51% 36% 10% •
2	AV	76	% 42% 26% 24% 5% •
3	AX	25	4% 16% 8% 76%
4	AJ	98	3% 58% 28% 14%

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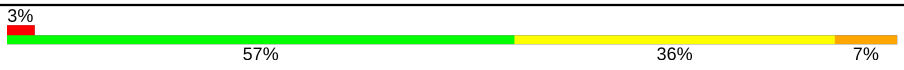
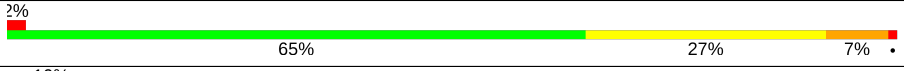
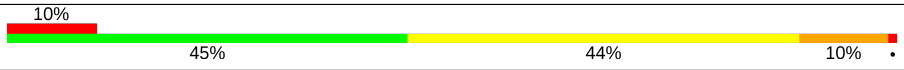
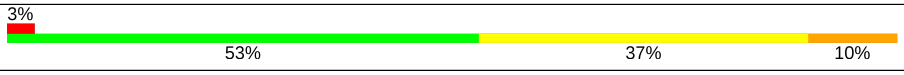
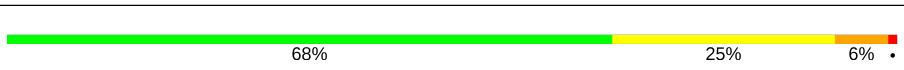
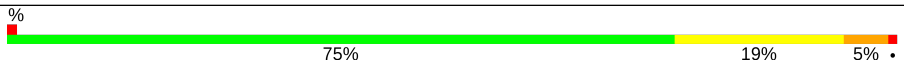
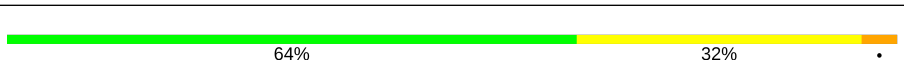
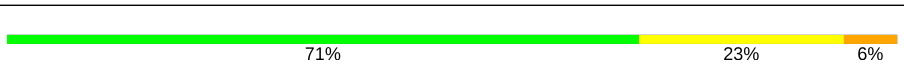
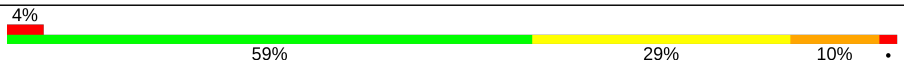
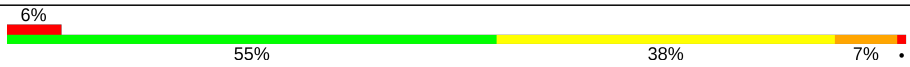
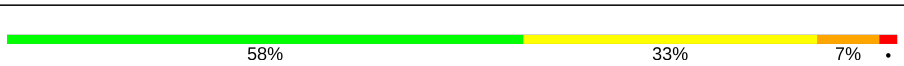
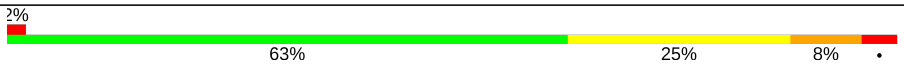
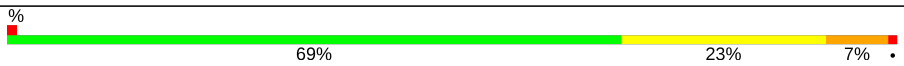
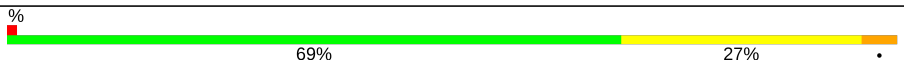
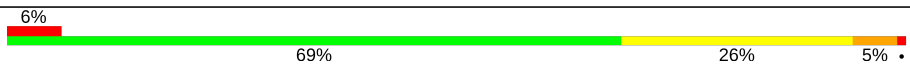
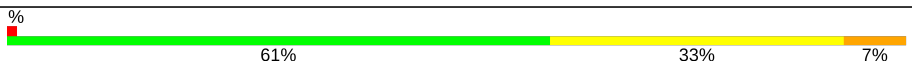
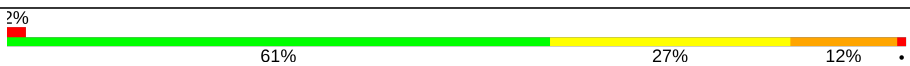
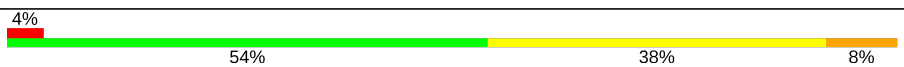
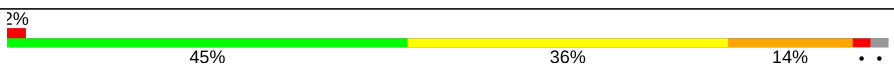
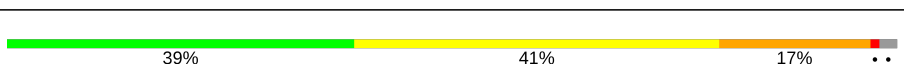
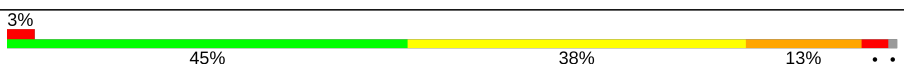
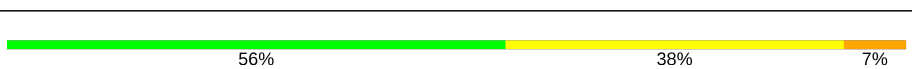
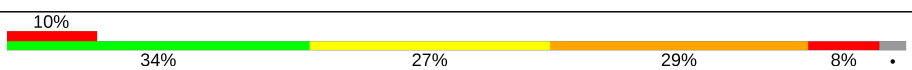
Mol	Chain	Length	Quality of chain
5	AK	119	
6	AL	124	
7	AM	124	
8	AN	60	
9	AO	88	
10	AP	83	
11	AQ	99	
12	AR	70	
13	AS	78	
14	AT	99	
15	AB	234	
16	AC	206	
17	AD	208	
18	AE	150	
19	AF	101	
20	AG	155	
21	AH	138	
22	AI	127	
23	AY	680	
24	AU	24	
25	BA	2915	
26	BB	122	
27	BN	140	
28	BO	122	
29	BP	150	

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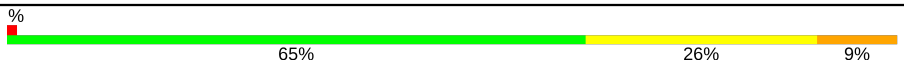
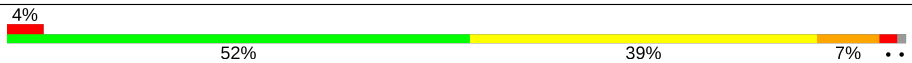
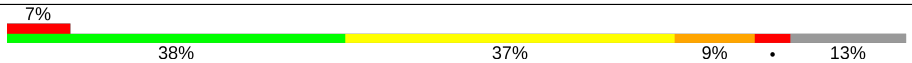
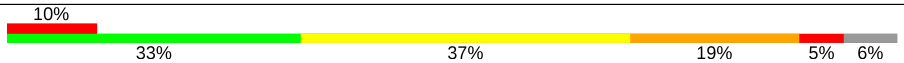
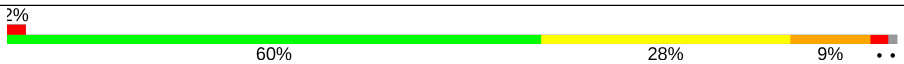
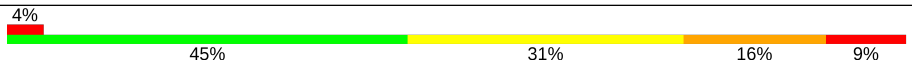
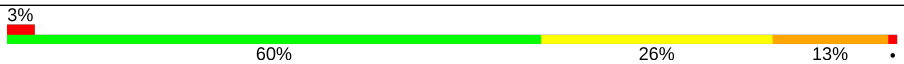
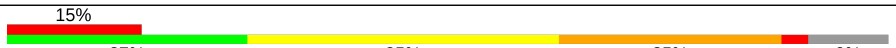
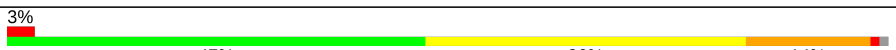
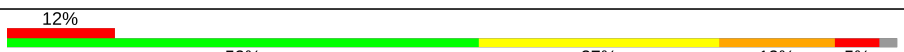
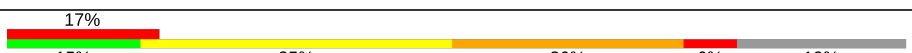
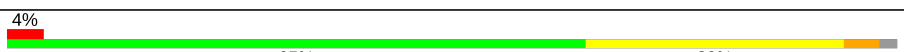
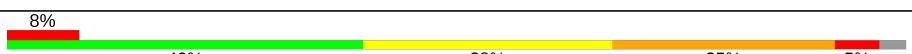
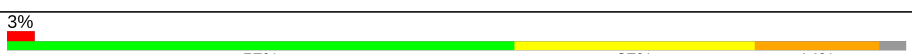
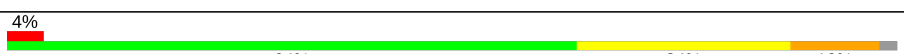
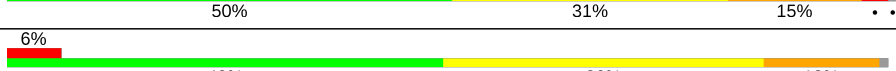
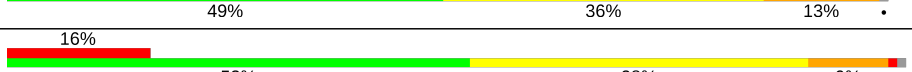
Mol	Chain	Length	Quality of chain
30	BQ	141	
31	BR	118	
32	BS	112	
33	BT	146	
34	BU	118	
35	BV	101	
36	BW	113	
37	BX	96	
38	BY	110	
39	BZ	206	
40	B0	85	
41	B1	98	
42	B2	72	
43	BD	276	
44	B3	60	
45	B4	71	
46	B5	60	
47	B6	54	
48	B7	49	
49	B8	65	
50	B9	37	
51	BC	229	
52	BE	206	
53	BF	210	
54	BG	182	

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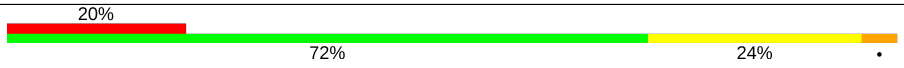
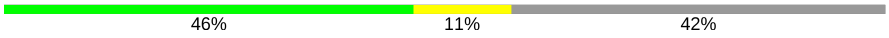
Mol	Chain	Length	Quality of chain
55	BH	180	
56	BK	147	
57	BJ	130	
58	BL	125	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151831 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1514	32529	14480	6018	10518	1513	0	0	0

- Molecule 2 is a RNA chain called PE hybrid state tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AV	74	1579	705	285	516	73	0	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AX	6	125	56	19	44	6	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AJ	98	795	499	156	139	1	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S11.

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

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AL	124	971	611	195	164	1	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 8 is a protein called 30S ribosomal protein S14 TYPE Z.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 12 is a protein called 30S ribosomal protein S18.

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

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 14 is a protein called 30S ribosomal protein S20.

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

- Molecule 15 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 17 is a protein called 30S ribosomal protein S4.

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

- Molecule 18 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

- Molecule 19 is a protein called 30S ribosomal protein S6.

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

- Molecule 20 is a protein called 30S ribosomal protein S7.

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

- Molecule 21 is a protein called 30S ribosomal protein S8.

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

- Molecule 22 is a protein called 30S ribosomal protein S9.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	622	Total	C	N	O	S	0	0	0
			4877	3097	837	924	19			

- Molecule 24 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2859	Total	C	N	O	P	0	0	0
			61580	27407	11519	19796	2858			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L13.

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

- Molecule 28 is a protein called 50S ribosomal protein L14.

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

- Molecule 29 is a protein called 50S ribosomal protein L15.

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

- Molecule 30 is a protein called 50S ribosomal protein L16.

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

- Molecule 31 is a protein called 50S ribosomal protein L17.

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

- Molecule 32 is a protein called 50S ribosomal protein L18.

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

- Molecule 33 is a protein called 50S ribosomal protein L19.

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

- Molecule 34 is a protein called 50S ribosomal protein L20.

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

- Molecule 35 is a protein called 50S ribosomal protein L21.

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

- Molecule 36 is a protein called 50S ribosomal protein L22.

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

- Molecule 37 is a protein called 50S ribosomal protein L23.

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

- Molecule 38 is a protein called 50S ribosomal protein L24.

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

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BZ	198	Total	C	N	O	S	0	0	0
			1508	960	274	272	2			

- Molecule 40 is a protein called 50S ribosomal protein L27.

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

- Molecule 41 is a protein called 50S ribosomal protein L28.

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

- Molecule 42 is a protein called 50S ribosomal protein L29.

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

- Molecule 43 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 44 is a protein called 50S ribosomal protein L30.

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

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 46 is a protein called 50S ribosomal protein L32.

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

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 48 is a protein called 50S ribosomal protein L34.

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

- Molecule 49 is a protein called 50S ribosomal protein L35.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BC	225	Total	C	N	O	S	0	0	0
			1718	1085	315	316	2			

- Molecule 52 is a protein called 50S ribosomal protein L3.

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

- Molecule 53 is a protein called 50S ribosomal protein L4.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BH	173	Total	C	N	O	S	0	0	0
			1303	824	244	234	1			

- Molecule 56 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	127	Total	C	N	O	S	0	0	0
			936	598	161	172	5			

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

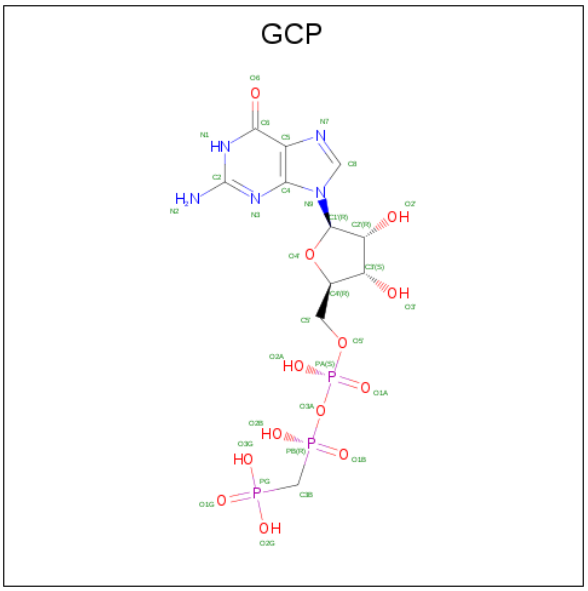
- Molecule 58 is a protein called 50S ribosomal protein L12 CTD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BL	72	Total	C	N	O	0	0	1
			356	213	72	71			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	88	Total	Mg	0	0
			88	88		
59	BD	1	Total	Mg	0	0
			1	1		
59	BF	1	Total	Mg	0	0
			1	1		
59	B8	1	Total	Mg	0	0
			1	1		
59	BE	1	Total	Mg	0	0
			1	1		
59	AA	45	Total	Mg	0	0
			45	45		
59	AY	1	Total	Mg	0	0
			1	1		

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 61 is water.

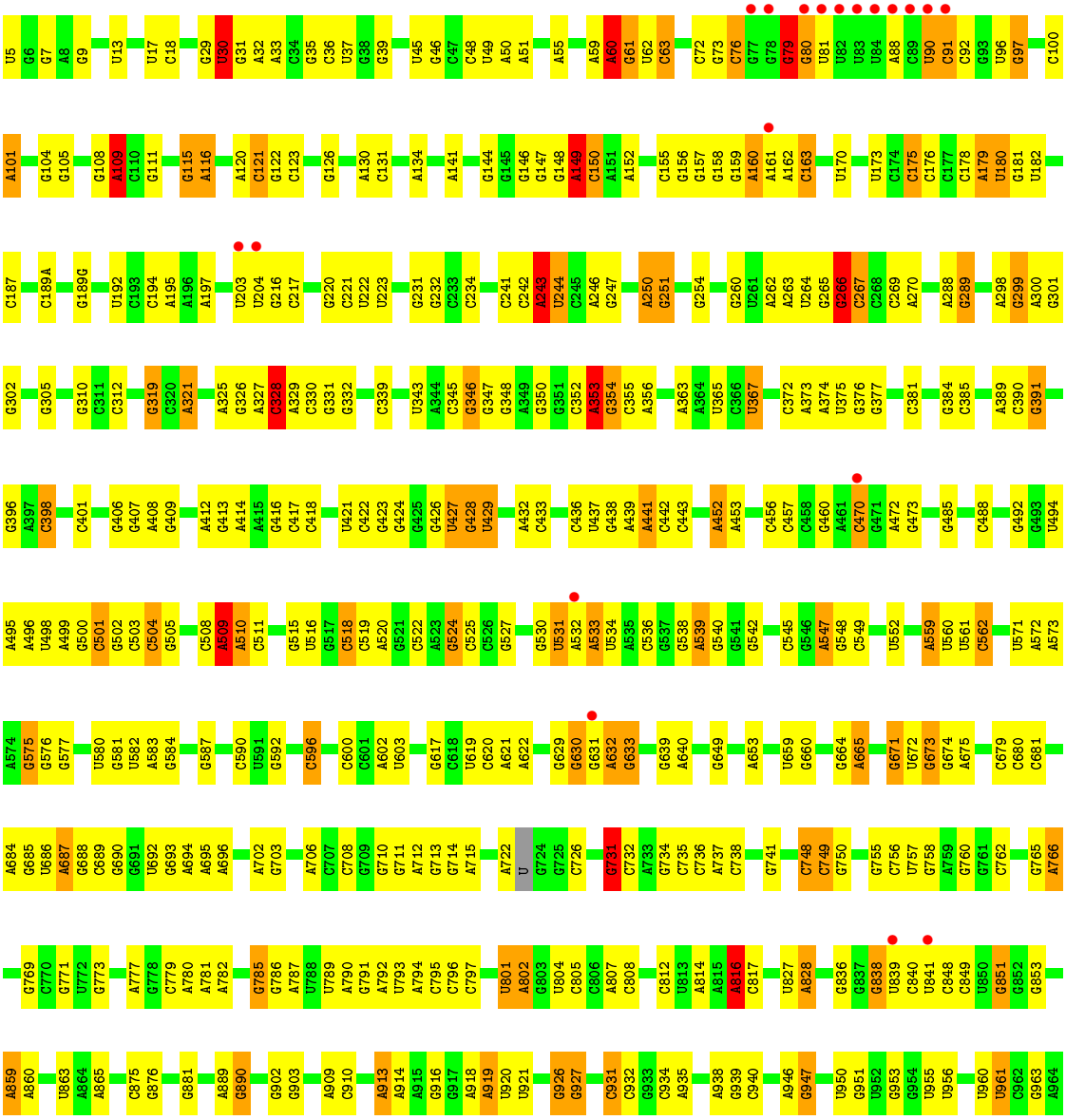
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	4	Total	O	0	0
			4	4		

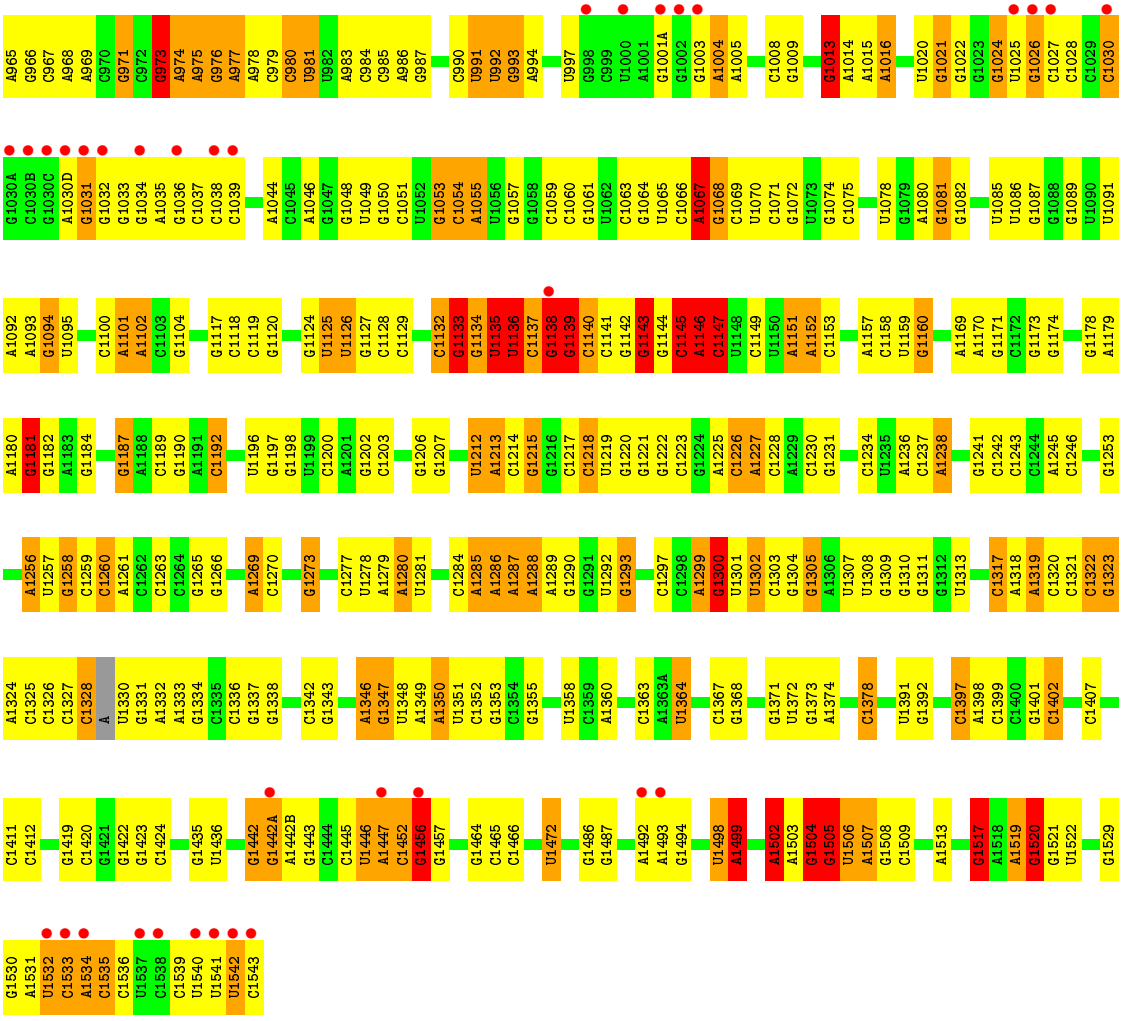
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

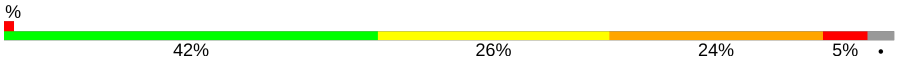
Chain AA:

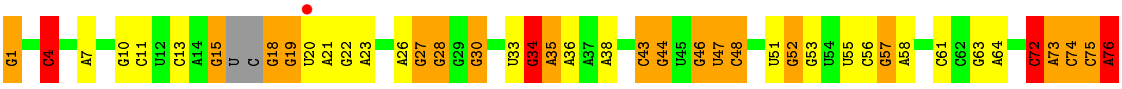




• Molecule 2: PE hybrid state tRNA Phe

Chain AV:



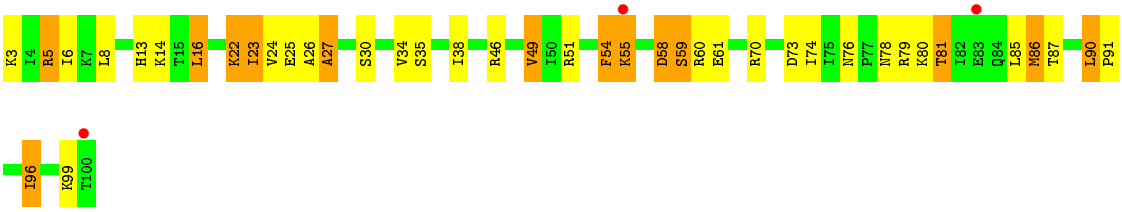


• Molecule 3: mRNA

Chain AX:

• Molecule 4: 30S ribosomal protein S10

Chain AJ:

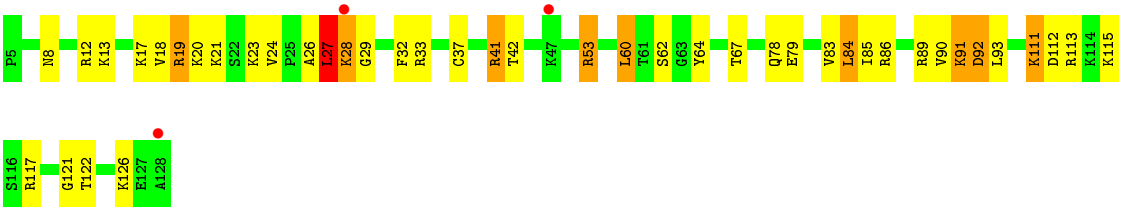


- Molecule 5: 30S ribosomal protein S11

Chain AK:

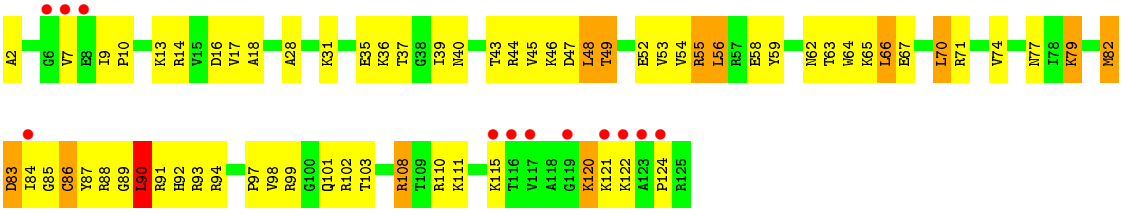
- Molecule 6: 30S ribosomal protein S12

Chain AL:



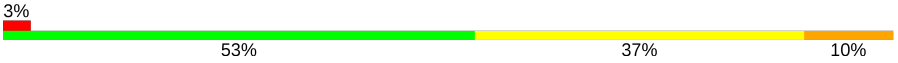
- Molecule 7: 30S ribosomal protein S13

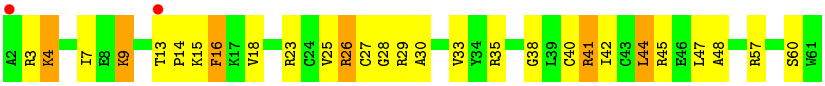
Chain AM:



- Molecule 8: 30S ribosomal protein S14 TYPE Z

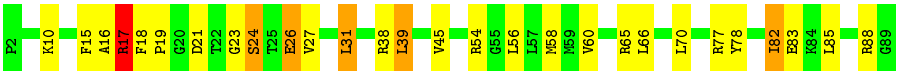
Chain AN:





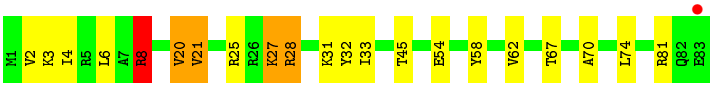
- Molecule 9: 30S ribosomal protein S15

Chain AO:



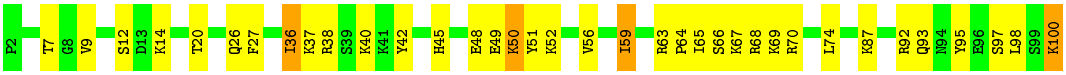
• Molecule 10: 30S ribosomal protein S16

Chain AP:



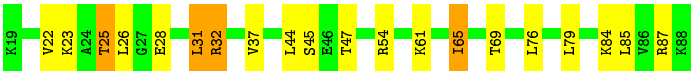
• Molecule 11: 30S ribosomal protein S17

Chain AQ:



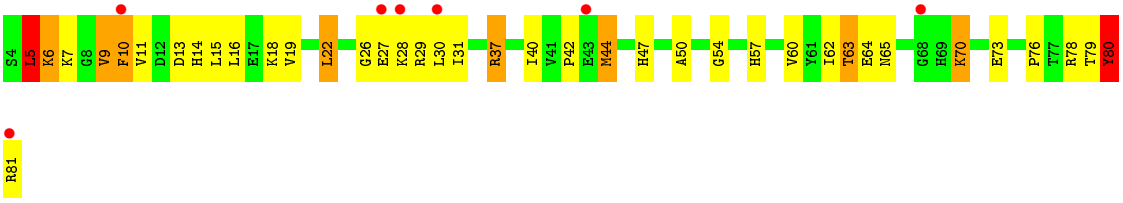
• Molecule 12: 30S ribosomal protein S18

Chain AR:



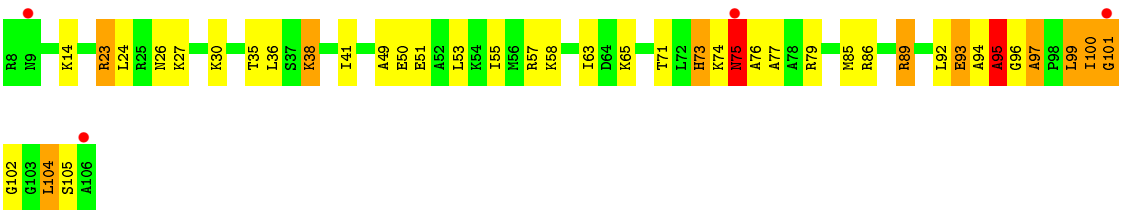
• Molecule 13: 30S ribosomal protein S19

Chain AS:



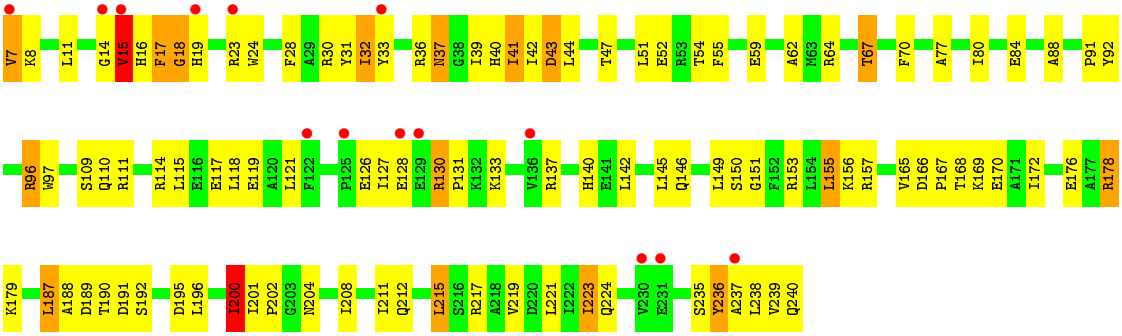
• Molecule 14: 30S ribosomal protein S20

Chain AT:



• Molecule 15: 30S ribosomal protein S2

Chain AB:

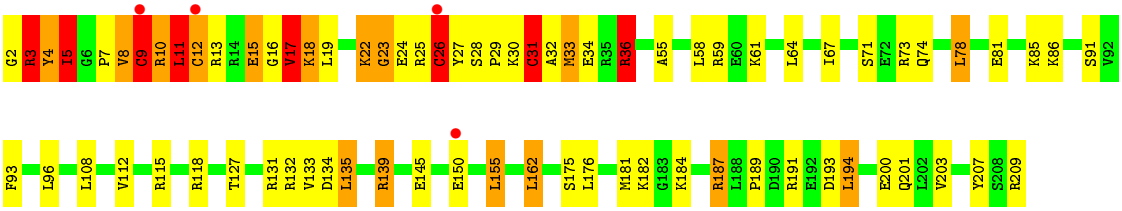


- Molecule 16: 30S ribosomal protein S3

Chain AC:

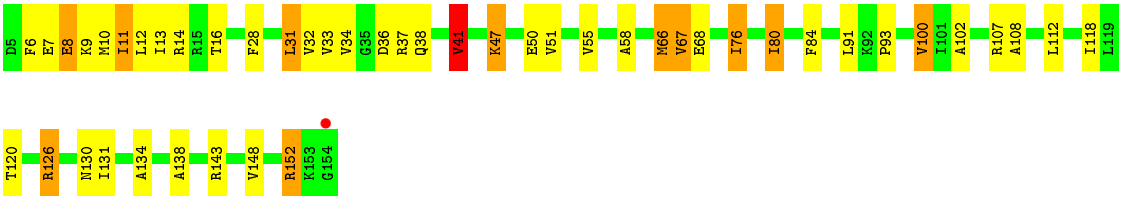
- Molecule 17: 30S ribosomal protein S4

Chain AD:



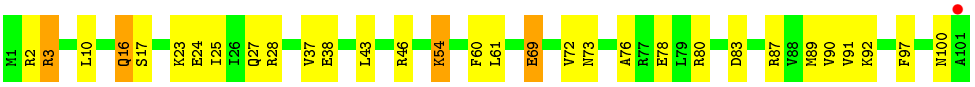
- Molecule 18: 30S ribosomal protein S5

Chain AE:

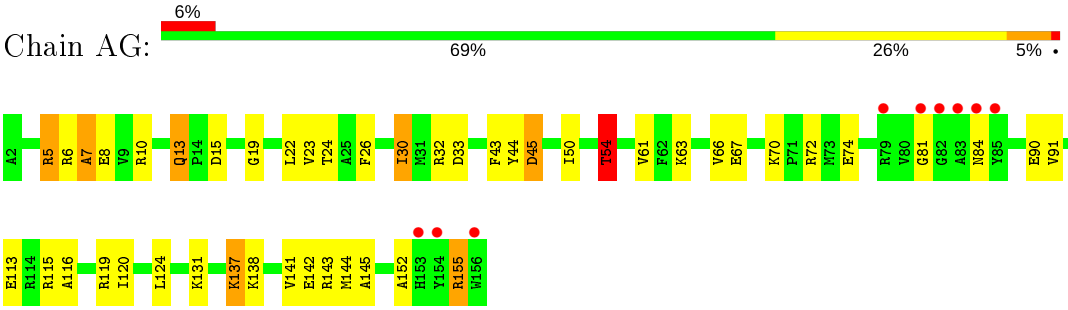


- Molecule 19: 30S ribosomal protein S6

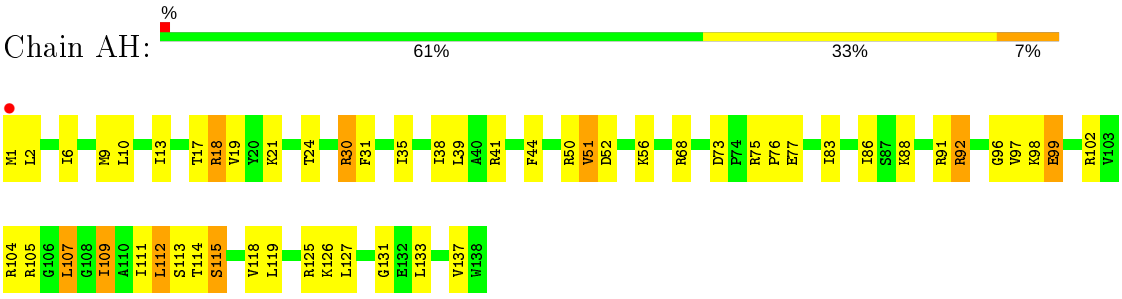
Chain AF:



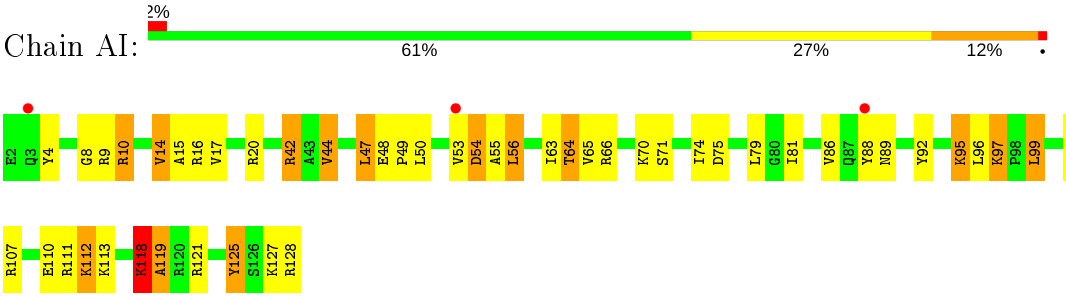
• Molecule 20: 30S ribosomal protein S7



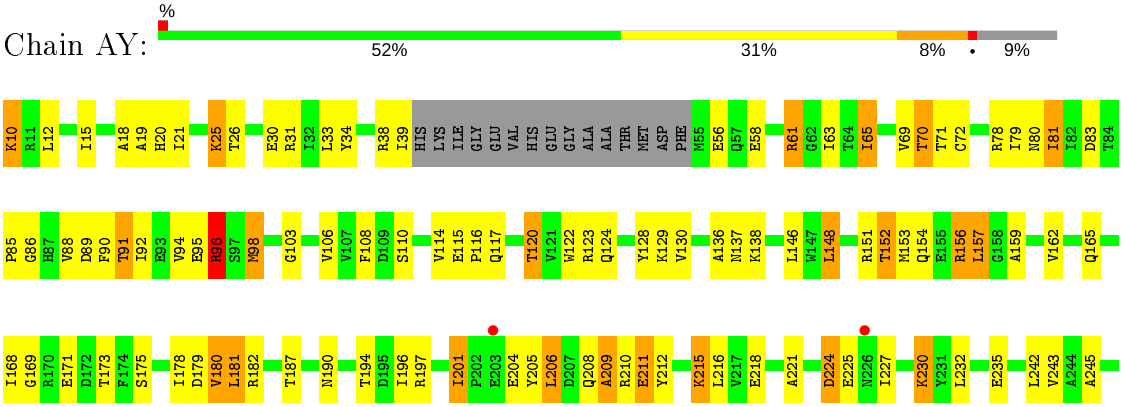
• Molecule 21: 30S ribosomal protein S8

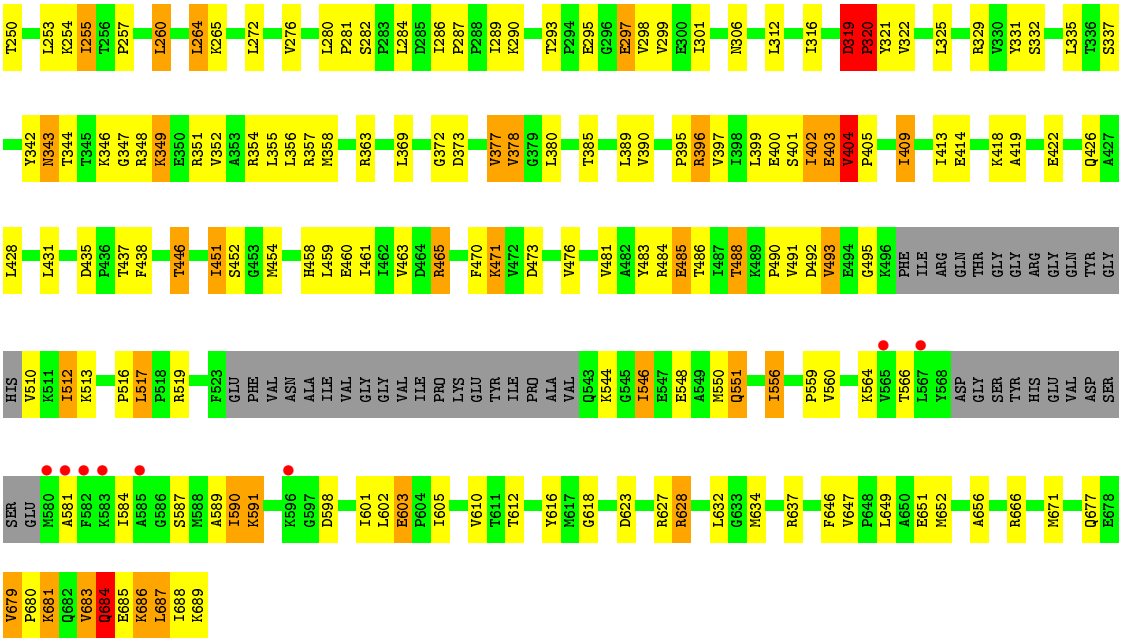


• Molecule 22: 30S ribosomal protein S9



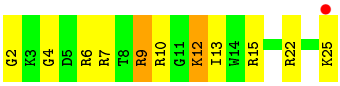
• Molecule 23: Elongation factor G





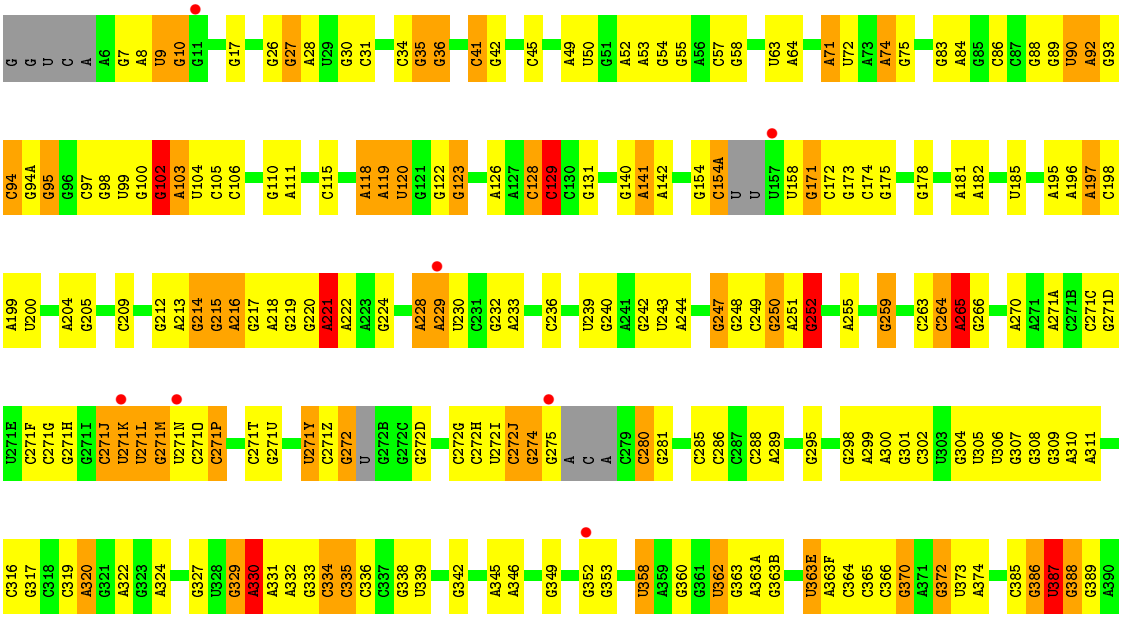
- Molecule 24: 30S ribosomal protein THX

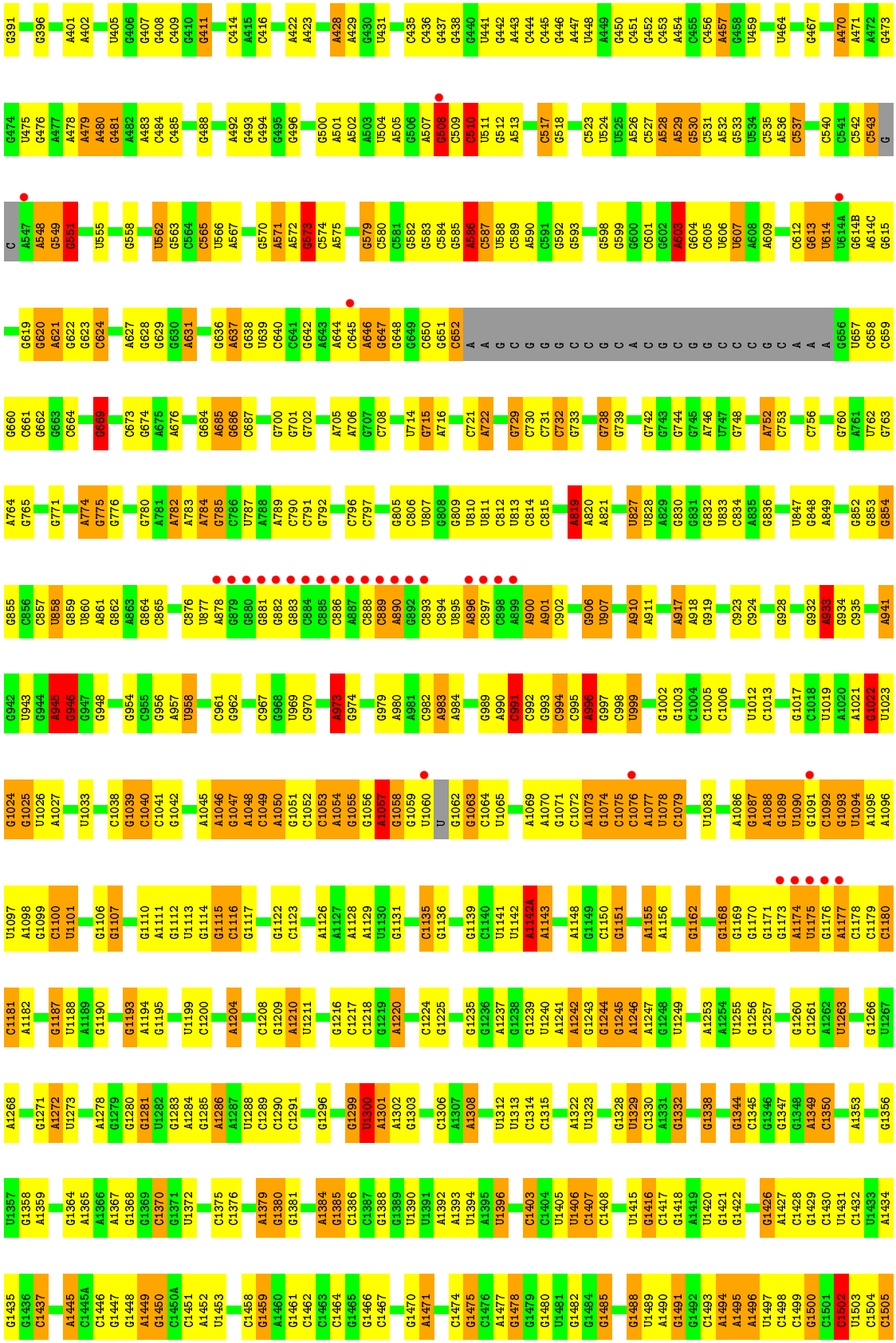
Chain AU:



- Molecule 25: 23S ribosomal RNA

Chain BA:

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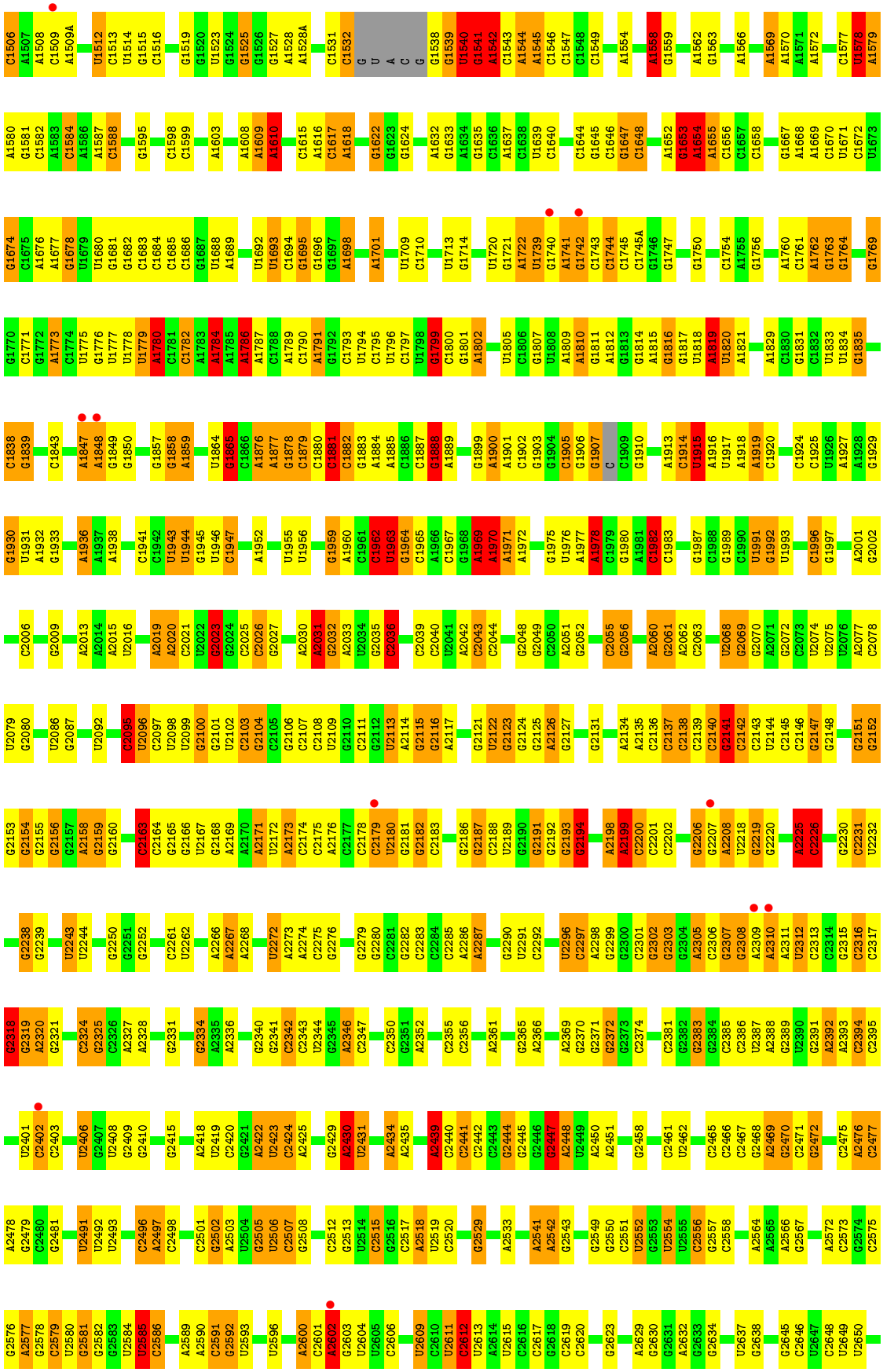
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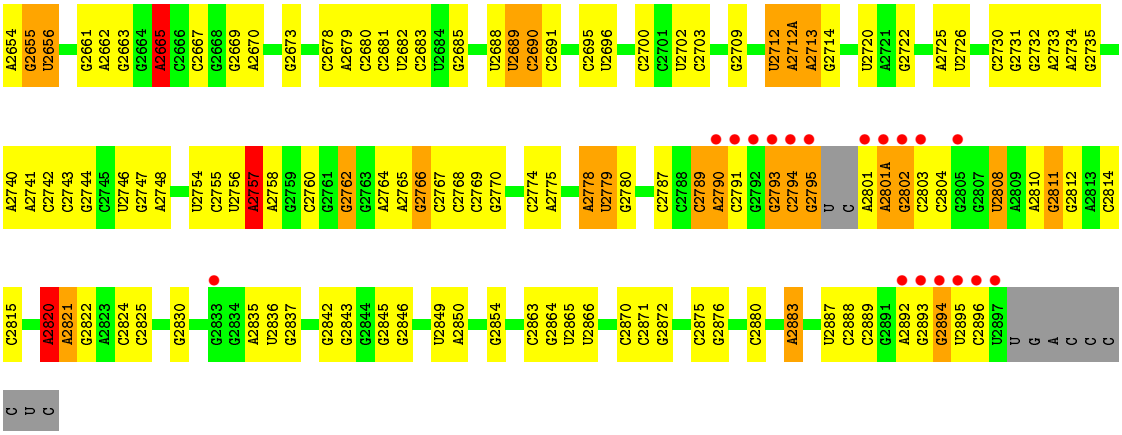
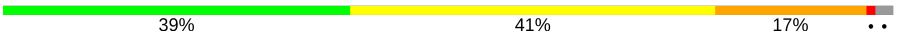
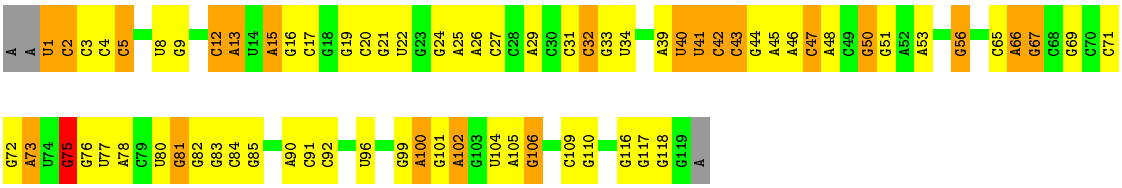


- Molecule 26: 5S ribosomal RNA

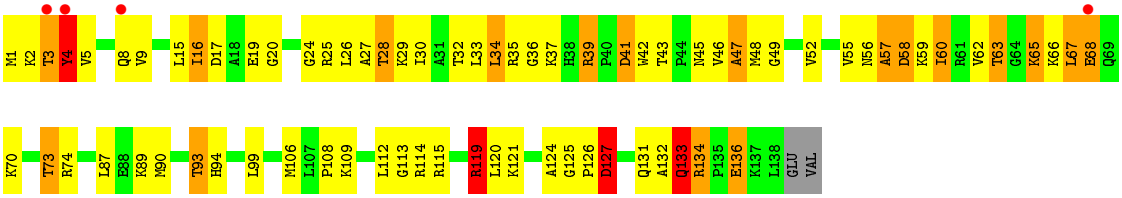
Chain BB:





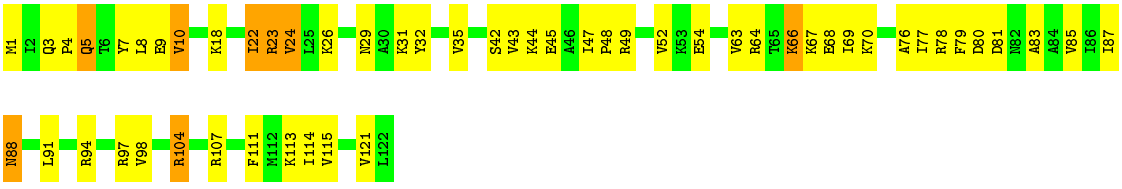
- Molecule 27: 50S ribosomal protein L13

Chain BN:



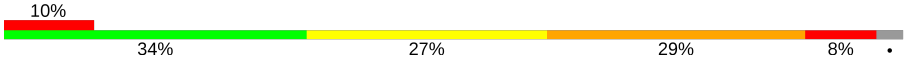
- Molecule 28: 50S ribosomal protein L14

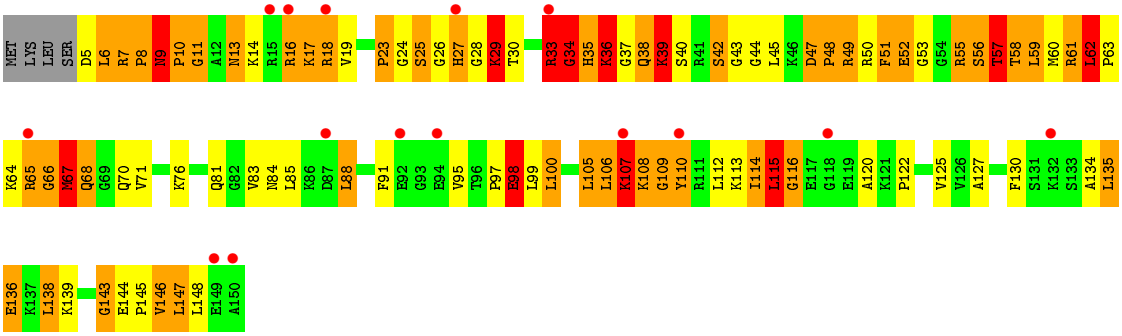
Chain BO:



- Molecule 29: 50S ribosomal protein L15

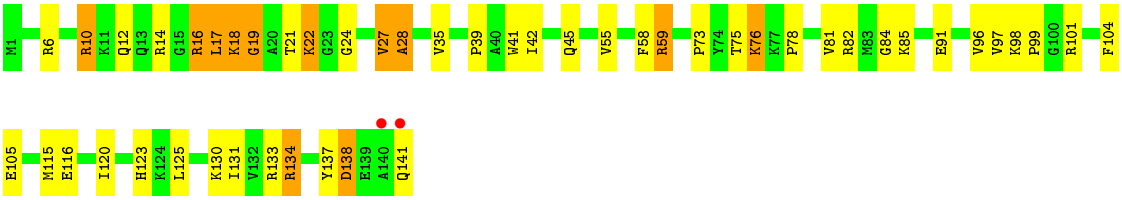
Chain BP:





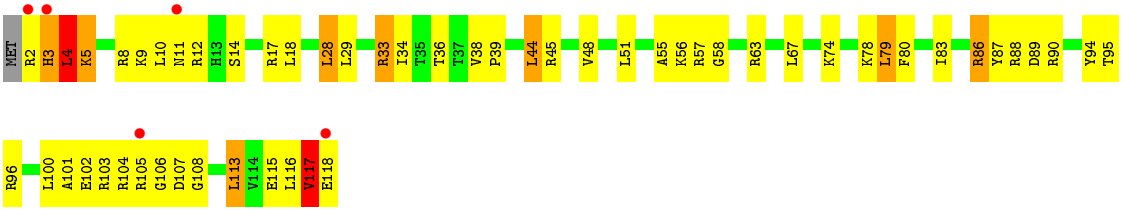
• Molecule 30: 50S ribosomal protein L16

Chain BQ:



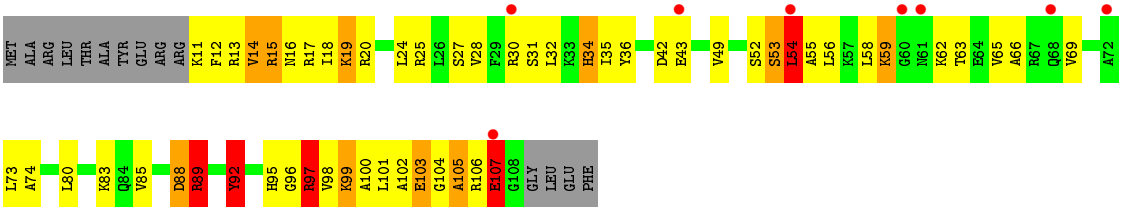
• Molecule 31: 50S ribosomal protein L17

Chain BR:



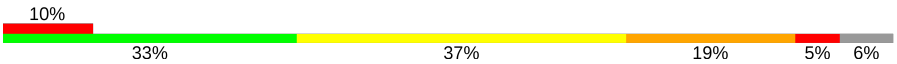
• Molecule 32: 50S ribosomal protein L18

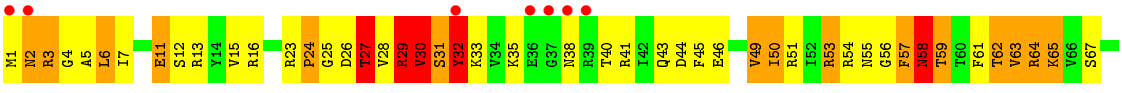
Chain BS:

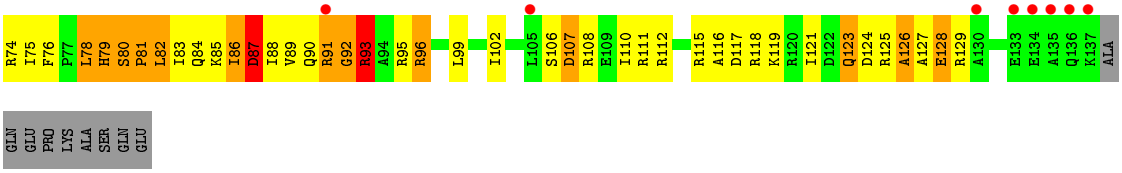


• Molecule 33: 50S ribosomal protein L19

Chain BT:

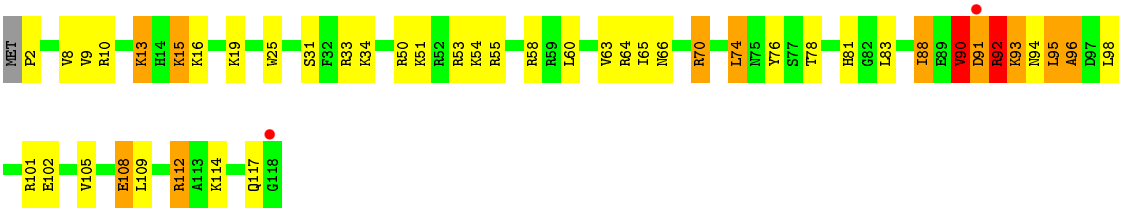






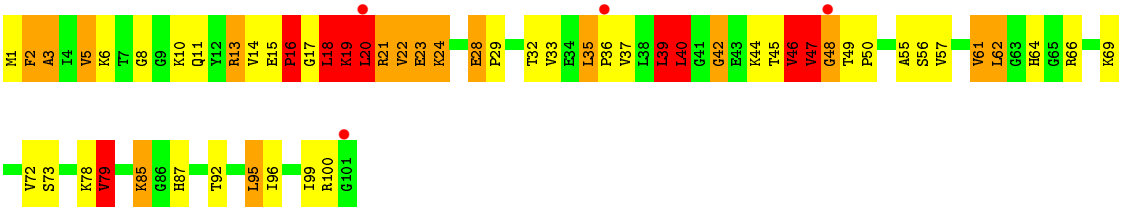
• Molecule 34: 50S ribosomal protein L20

Chain BU:



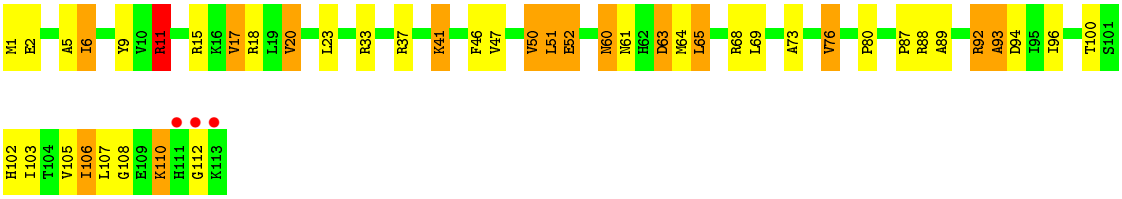
• Molecule 35: 50S ribosomal protein L21

Chain BV:



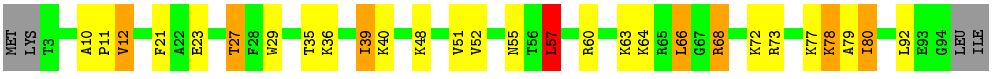
• Molecule 36: 50S ribosomal protein L22

Chain BW:



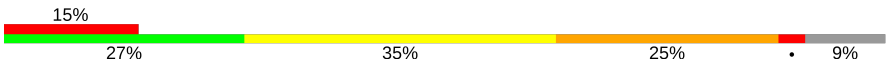
• Molecule 37: 50S ribosomal protein L23

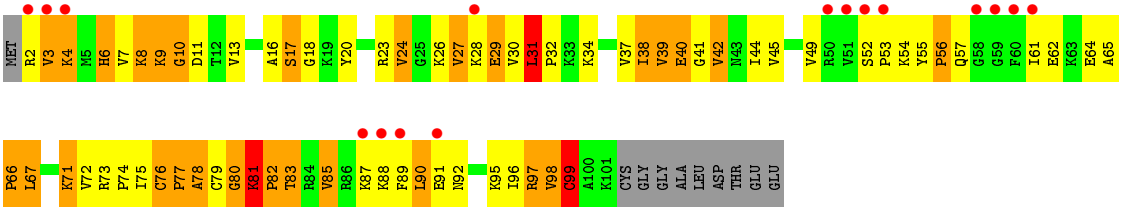
Chain BX:



• Molecule 38: 50S ribosomal protein L24

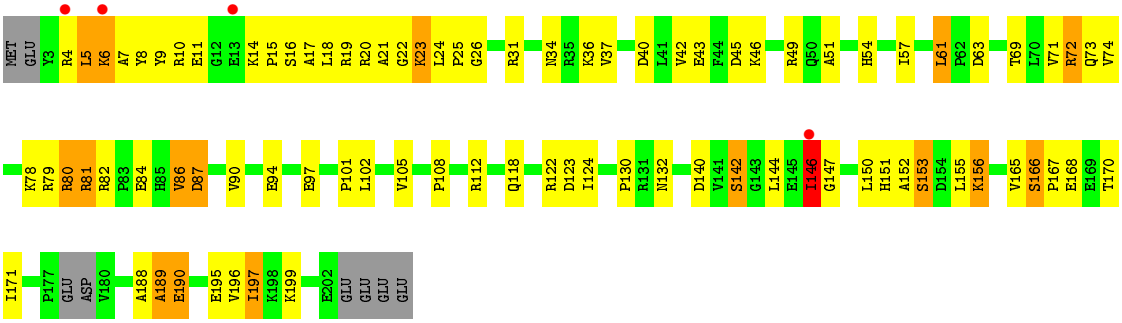
Chain BY:





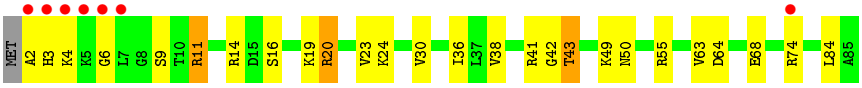
• Molecule 39: 50S ribosomal protein L25

Chain BZ:



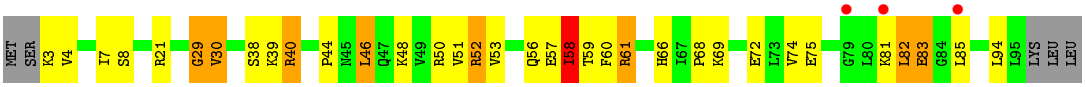
• Molecule 40: 50S ribosomal protein L27

Chain B0:



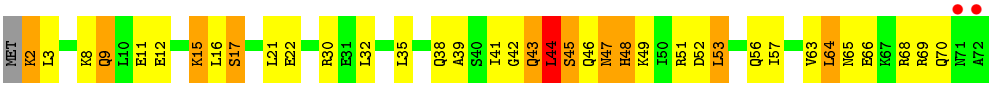
• Molecule 41: 50S ribosomal protein L28

Chain B1:



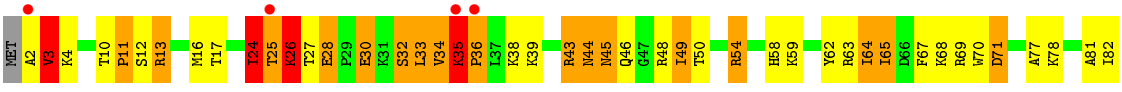
• Molecule 42: 50S ribosomal protein L29

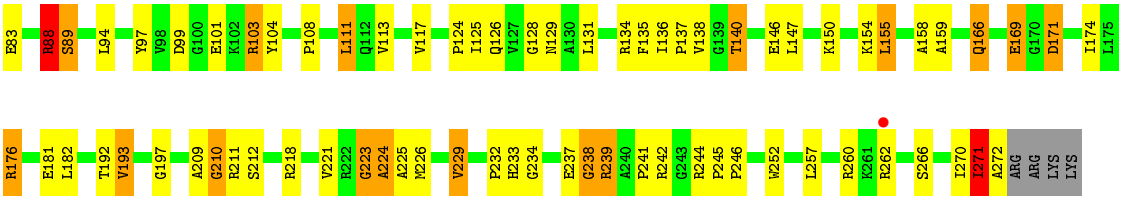
Chain B2:



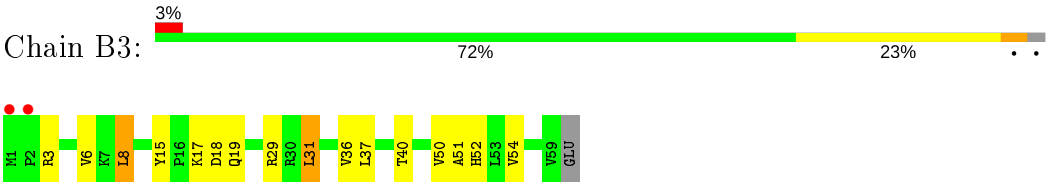
• Molecule 43: 50S ribosomal protein L2

Chain BD:

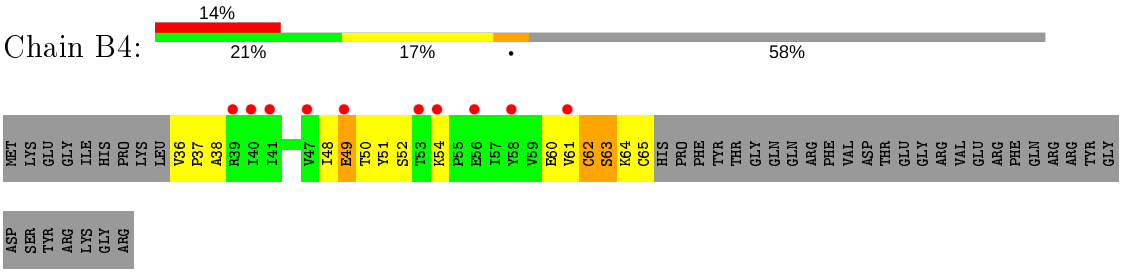




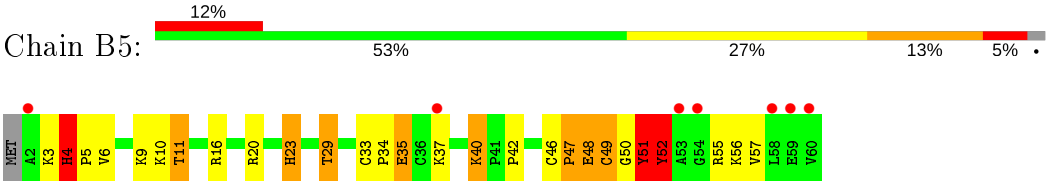
- Molecule 44: 50S ribosomal protein L30



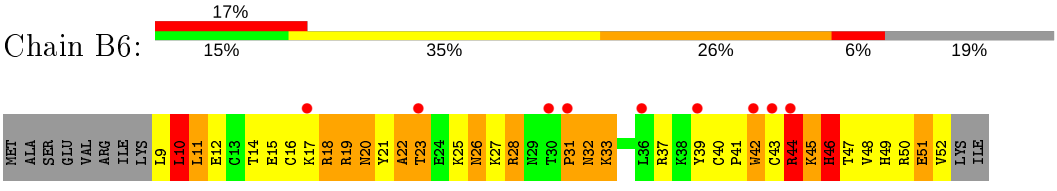
- Molecule 45: 50S ribosomal protein L31



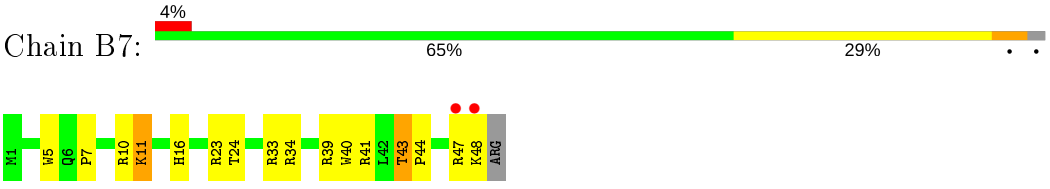
- Molecule 46: 50S ribosomal protein L32



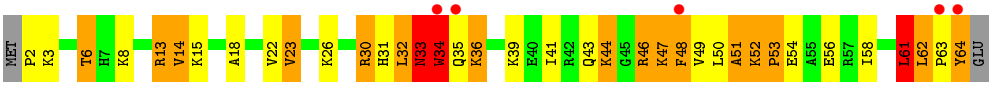
- Molecule 47: 50S ribosomal protein L33



- Molecule 48: 50S ribosomal protein L34

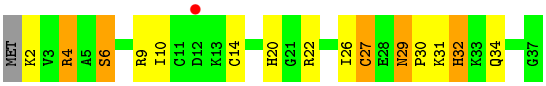


- Molecule 49: 50S ribosomal protein L35



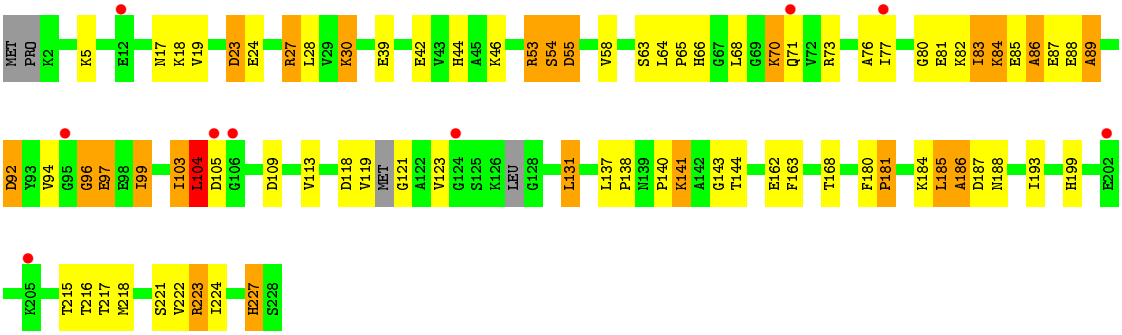
- Molecule 50: 50S ribosomal protein L36

Chain B9:



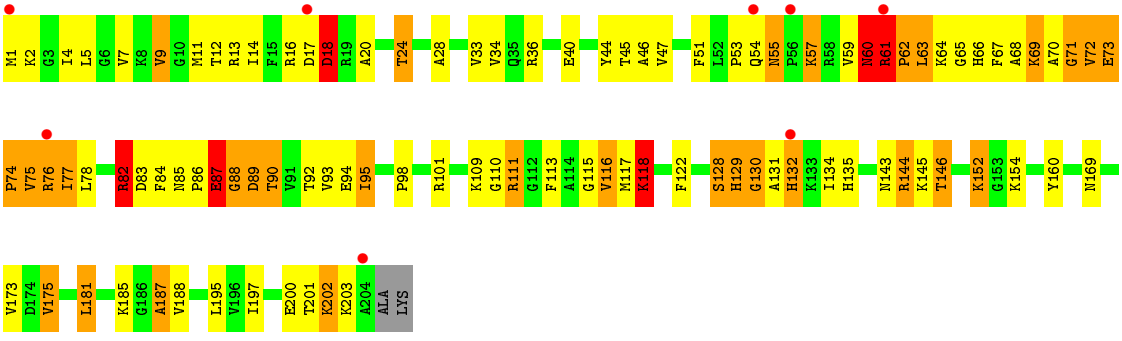
- Molecule 51: 50S ribosomal protein L1

Chain BC:



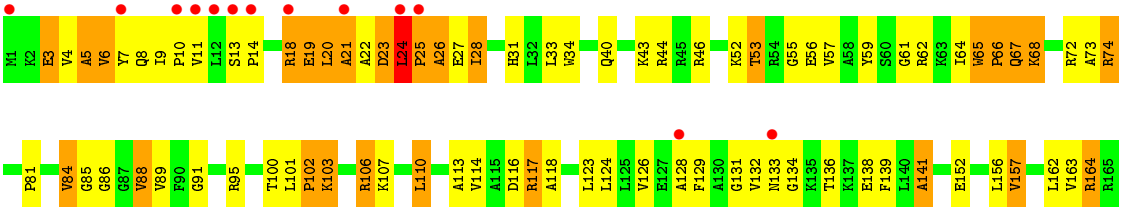
- Molecule 52: 50S ribosomal protein L3

Chain BE:



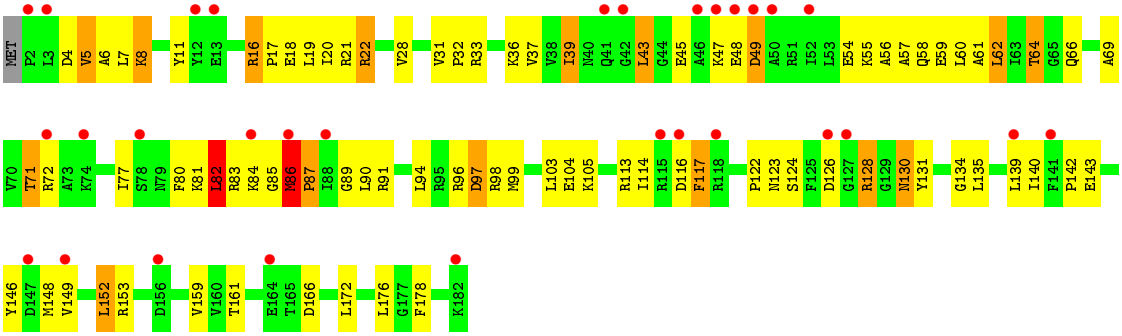
- Molecule 53: 50S ribosomal protein L4

Chain BF:



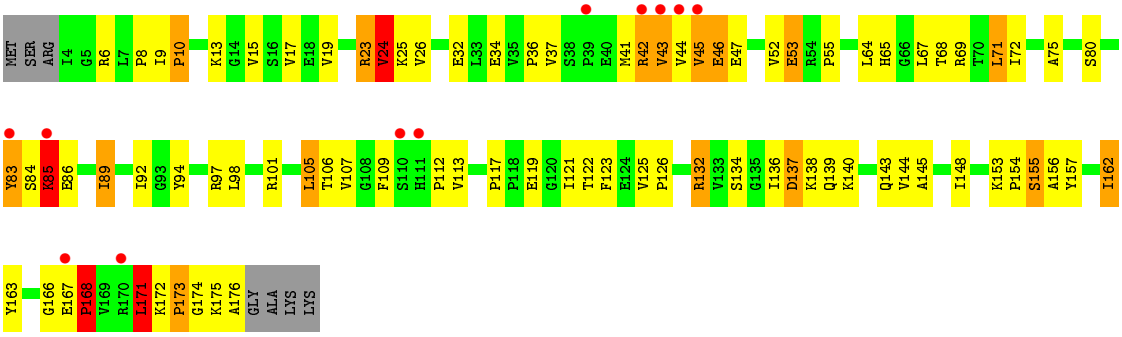
- Molecule 54: 50S ribosomal protein L5

Chain BG:



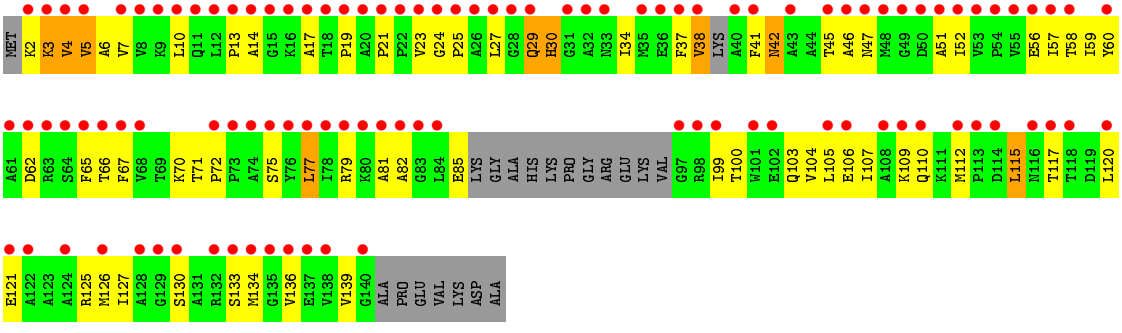
- Molecule 55: 50S ribosomal protein L6

Chain BH:



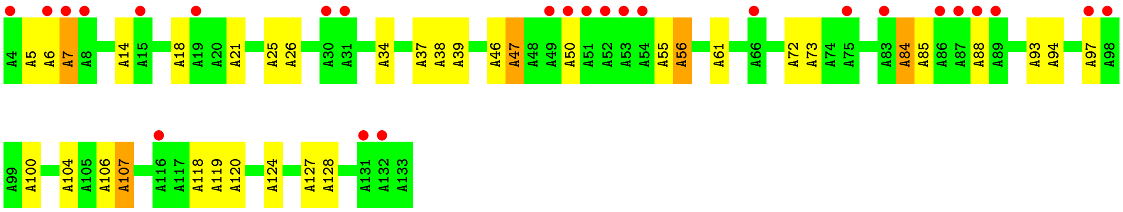
- Molecule 56: 50S ribosomal protein L11

Chain BK:



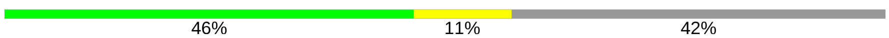
- Molecule 57: 50S ribosomal protein L10

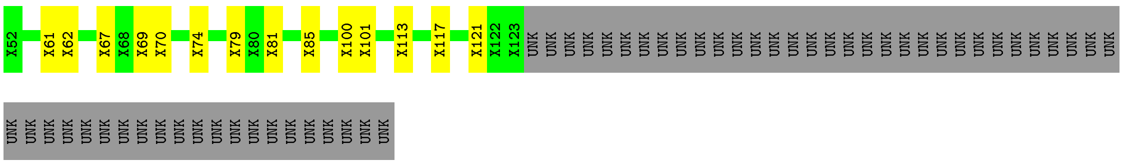
Chain BJ:



- Molecule 58: 50S ribosomal protein L12 CTD

Chain BL:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	201.58Å 241.65Å 305.80Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	39.60 – 2.86 39.59 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-2.86) 98.5 (39.59-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.250 0.201 , 0.243	Depositor DCC
R_{free} test set	32790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	151831	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, MG

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	0.54	8/36408 (0.0%)	0.90	98/56818 (0.2%)
2	AV	0.49	1/1764 (0.1%)	0.96	11/2747 (0.4%)
3	AX	0.50	0/138	0.79	0/212
4	AJ	0.66	0/808	0.96	0/1085
5	AK	0.59	0/900	0.86	0/1213
6	AL	0.67	0/987	1.03	1/1320 (0.1%)
7	AM	0.54	0/999	0.89	0/1336
8	AN	0.61	0/501	1.08	2/664 (0.3%)
9	AO	0.61	0/745	0.94	1/992 (0.1%)
10	AP	0.59	0/717	0.92	2/963 (0.2%)
11	AQ	0.68	0/837	0.89	1/1117 (0.1%)
12	AR	0.60	0/579	0.84	0/768
13	AS	0.58	0/643	0.91	1/865 (0.1%)
14	AT	0.61	0/765	0.90	0/1007
15	AB	0.56	0/1936	0.83	1/2609 (0.0%)
16	AC	0.64	0/1637	0.93	3/2205 (0.1%)
17	AD	0.63	2/1733 (0.1%)	0.97	8/2318 (0.3%)
18	AE	0.71	0/1163	0.93	3/1564 (0.2%)
19	AF	0.55	0/856	0.78	0/1154
20	AG	0.54	0/1276	0.82	0/1709
21	AH	0.64	0/1136	0.95	1/1527 (0.1%)
22	AI	0.57	0/1029	0.92	0/1378
23	AY	0.53	0/4961	0.81	3/6710 (0.0%)
24	AU	0.58	0/213	0.92	0/277
25	BA	0.61	43/68964 (0.1%)	0.95	224/107644 (0.2%)
26	BB	0.40	0/2853	0.84	4/4451 (0.1%)
27	BN	0.74	1/1131 (0.1%)	1.07	5/1525 (0.3%)
28	BO	0.67	0/943	0.98	2/1269 (0.2%)
29	BP	0.86	0/1131	1.29	8/1504 (0.5%)
30	BQ	0.64	0/1143	0.92	0/1527
31	BR	0.70	0/974	1.01	1/1302 (0.1%)
32	BS	0.55	0/778	0.87	0/1036

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BT	0.70	0/1155	1.15	5/1542 (0.3%)
34	BU	0.75	0/975	1.02	1/1297 (0.1%)
35	BV	0.69	0/790	0.99	1/1057 (0.1%)
36	BW	0.67	0/907	1.02	3/1216 (0.2%)
37	BX	0.69	0/739	0.90	1/993 (0.1%)
38	BY	0.81	0/788	1.08	1/1051 (0.1%)
39	BZ	0.56	0/1539	0.87	0/2093
40	B0	0.57	0/671	0.86	0/892
41	B1	0.69	0/738	0.95	0/981
42	B2	0.57	0/600	0.86	0/793
43	BD	0.87	3/2154 (0.1%)	1.08	5/2905 (0.2%)
44	B3	0.55	0/472	0.80	0/634
45	B4	0.54	0/228	0.71	0/309
46	B5	0.85	0/473	1.22	5/639 (0.8%)
47	B6	0.94	0/387	1.36	3/518 (0.6%)
48	B7	0.74	0/426	0.85	0/561
49	B8	0.79	0/515	1.22	3/679 (0.4%)
50	B9	0.69	0/302	1.05	1/397 (0.3%)
51	BC	0.56	1/1747 (0.1%)	1.01	4/2351 (0.2%)
52	BE	0.75	0/1596	1.01	3/2153 (0.1%)
53	BF	0.69	0/1658	0.93	2/2244 (0.1%)
54	BG	0.48	0/1499	0.78	2/2016 (0.1%)
55	BH	0.59	0/1327	0.93	2/1794 (0.1%)
56	BK	0.41	0/951	0.60	0/1290
57	BJ	0.51	0/650	0.62	0/907
All	All	0.61	59/163935 (0.0%)	0.93	422/244128 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	AJ	0	1
6	AL	0	1
8	AN	0	1
14	AT	0	2
17	AD	0	2
23	AY	0	4
27	BN	0	2
29	BP	0	15
30	BQ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BR	0	2
32	BS	0	1
33	BT	0	6
34	BU	0	3
35	BV	0	3
38	BY	0	6
41	B1	0	2
43	BD	0	4
46	B5	0	2
47	B6	0	3
51	BC	0	2
52	BE	0	5
53	BF	0	1
55	BH	0	1
58	BL	0	1
All	All	0	72

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2506	U	O3'-P	12.63	1.76	1.61
25	BA	1695	G	O3'-P	-9.03	1.50	1.61
27	BN	127	ASP	CB-CG	8.59	1.69	1.51
25	BA	1299	G	O3'-P	-7.33	1.52	1.61
25	BA	1300	U	O3'-P	-6.92	1.52	1.61

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	BC	27	ARG	NE-CZ-NH2	-24.39	108.10	120.30
25	BA	996	A	O5'-P-OP1	-17.66	89.51	110.70
1	AA	1499	A	O5'-P-OP1	-14.95	92.25	105.70
25	BA	946	G	O5'-P-OP1	-14.17	92.95	105.70
25	BA	2502	G	O5'-P-OP1	-13.94	93.15	105.70

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AJ	54	PHE	Peptide
6	AL	28	LYS	Peptide

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Mol	Chain	Res	Type	Group
8	AN	13	THR	Peptide
14	AT	73	HIS	Peptide
14	AT	95	ALA	Peptide

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	32529	0	16426	525	0
2	AV	1579	0	802	43	0
3	AX	125	0	64	2	0
4	AJ	795	0	840	29	0
5	AK	885	0	904	28	0
6	AL	971	0	1057	26	0
7	AM	988	0	1059	43	0
8	AN	492	0	529	21	0
9	AO	734	0	771	16	0
10	AP	701	0	720	14	0
11	AQ	824	0	891	19	0
12	AR	574	0	644	10	0
13	AS	630	0	652	25	0
14	AT	763	0	861	30	0
15	AB	1901	0	1951	86	0
16	AC	1613	0	1677	49	0
17	AD	1703	0	1763	64	0
18	AE	1147	0	1207	33	0
19	AF	843	0	857	19	0
20	AG	1257	0	1296	25	0
21	AH	1116	0	1177	27	0
22	AI	1011	0	1043	35	0
23	AY	4877	0	4964	166	0
24	AU	209	0	221	8	0
25	BA	61580	0	31049	1148	0
26	BB	2551	0	1295	55	0
27	BN	1104	0	1180	63	0
28	BO	933	0	996	35	0
29	BP	1114	0	1187	142	0
30	BQ	1122	0	1179	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BR	960	0	1021	39	0
32	BS	770	0	832	42	0
33	BT	1141	0	1202	114	0
34	BU	958	0	1015	51	0
35	BV	779	0	852	50	0
36	BW	896	0	953	27	0
37	BX	725	0	778	15	0
38	BY	775	0	870	71	0
39	BZ	1508	0	1486	56	0
40	B0	662	0	688	22	0
41	B1	731	0	808	33	0
42	B2	598	0	653	31	0
43	BD	2104	0	2182	101	0
44	B3	467	0	523	5	0
45	B4	225	0	229	10	0
46	B5	459	0	477	31	0
47	B6	380	0	390	55	0
48	B7	418	0	467	12	0
49	B8	507	0	576	58	0
50	B9	299	0	323	10	0
51	BC	1718	0	1766	54	0
52	BE	1563	0	1629	81	0
53	BF	1623	0	1677	83	0
54	BG	1474	0	1535	56	0
55	BH	1303	0	1348	55	0
56	BK	936	0	970	60	0
57	BJ	651	0	649	17	0
58	BL	356	0	75	7	0
59	AA	45	0	0	0	0
59	AY	1	0	0	0	0
59	B8	1	0	0	0	0
59	BA	88	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
60	AY	32	0	14	5	0
61	AY	4	0	0	1	0
All	All	151831	0	105250	3647	0

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 14.

The worst 5 of 3647 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)
25:BA:2111:C:N3	25:BA:2147:G:N2	1.74	1.36
25:BA:1332:G:N2	25:BA:1609:A:O2'	1.62	1.26
47:B6:40:CYS:SG	47:B6:45:LYS:NZ	1.02	1.24
25:BA:90:U:O2'	25:BA:92:A:OP2	1.54	1.24
25:BA:1332:G:N2	25:BA:1609:A:HO2'	1.30	1.23

There are no symmetry-related clashes.

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
4	AJ	96/98 (98%)	80 (83%)	10 (10%)	6 (6%)	1 3
5	AK	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	5 17
6	AL	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3 9
7	AM	122/124 (98%)	82 (67%)	32 (26%)	8 (7%)	1 3
8	AN	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3 12
9	AO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13 35
10	AP	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
11	AQ	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15 40
12	AR	68/70 (97%)	60 (88%)	5 (7%)	3 (4%)	2 8
13	AS	76/78 (97%)	60 (79%)	8 (10%)	8 (10%)	0 1
14	AT	97/99 (98%)	86 (89%)	5 (5%)	6 (6%)	1 3
15	AB	232/234 (99%)	191 (82%)	32 (14%)	9 (4%)	3 10
16	AC	204/206 (99%)	173 (85%)	22 (11%)	9 (4%)	2 8
17	AD	206/208 (99%)	171 (83%)	25 (12%)	10 (5%)	2 6
18	AE	148/150 (99%)	141 (95%)	5 (3%)	2 (1%)	11 31
19	AF	99/101 (98%)	91 (92%)	8 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	AG	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	5 17
21	AH	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	6 21
22	AI	125/127 (98%)	99 (79%)	17 (14%)	9 (7%)	1 2
23	AY	612/680 (90%)	520 (85%)	72 (12%)	20 (3%)	4 13
24	AU	22/24 (92%)	17 (77%)	5 (23%)	0	100 100
27	BN	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	2 8
28	BO	120/122 (98%)	113 (94%)	3 (2%)	4 (3%)	4 13
29	BP	144/150 (96%)	90 (62%)	21 (15%)	33 (23%)	0 0
30	BQ	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3 11
31	BR	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	2 8
32	BS	96/112 (86%)	61 (64%)	20 (21%)	15 (16%)	0 0
33	BT	135/146 (92%)	96 (71%)	24 (18%)	15 (11%)	0 1
34	BU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3 12
35	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0 0
36	BW	111/113 (98%)	101 (91%)	4 (4%)	6 (5%)	2 5
37	BX	90/96 (94%)	83 (92%)	7 (8%)	0	100 100
38	BY	98/110 (89%)	58 (59%)	18 (18%)	22 (22%)	0 0
39	BZ	194/206 (94%)	146 (75%)	32 (16%)	16 (8%)	1 1
40	B0	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	3 11
41	B1	91/98 (93%)	76 (84%)	12 (13%)	3 (3%)	4 13
42	B2	69/72 (96%)	58 (84%)	4 (6%)	7 (10%)	0 1
43	BD	269/276 (98%)	231 (86%)	24 (9%)	14 (5%)	2 5
44	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8 25
45	B4	28/71 (39%)	21 (75%)	4 (14%)	3 (11%)	0 1
46	B5	57/60 (95%)	47 (82%)	4 (7%)	6 (10%)	0 1
47	B6	42/54 (78%)	20 (48%)	15 (36%)	7 (17%)	0 0
48	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6 21
49	B8	61/65 (94%)	45 (74%)	11 (18%)	5 (8%)	1 1
50	B9	34/37 (92%)	32 (94%)	2 (6%)	0	100 100
51	BC	219/229 (96%)	166 (76%)	35 (16%)	18 (8%)	1 1
52	BE	202/206 (98%)	145 (72%)	30 (15%)	27 (13%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	BF	205/210 (98%)	165 (80%)	24 (12%)	16 (8%)	1 2
54	BG	179/182 (98%)	123 (69%)	44 (25%)	12 (7%)	1 2
55	BH	171/180 (95%)	128 (75%)	26 (15%)	17 (10%)	0 1
56	BK	121/147 (82%)	84 (69%)	30 (25%)	7 (6%)	1 4
57	BJ	128/130 (98%)	84 (66%)	31 (24%)	13 (10%)	0 1
All	All	6610/6949 (95%)	5383 (81%)	812 (12%)	415 (6%)	1 3

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AJ	23	ILE
4	AJ	59	SER
4	AJ	86	MET
5	AK	117	ASN
5	AK	128	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
4	AJ	88/88 (100%)	70 (80%)	18 (20%)	1 2
5	AK	90/90 (100%)	68 (76%)	22 (24%)	0 1
6	AL	104/104 (100%)	85 (82%)	19 (18%)	1 4
7	AM	99/99 (100%)	83 (84%)	16 (16%)	2 6
8	AN	49/49 (100%)	38 (78%)	11 (22%)	1 2
9	AO	79/79 (100%)	67 (85%)	12 (15%)	3 7
10	AP	72/72 (100%)	61 (85%)	11 (15%)	2 7
11	AQ	94/94 (100%)	79 (84%)	15 (16%)	2 6
12	AR	61/61 (100%)	52 (85%)	9 (15%)	3 8
13	AS	69/69 (100%)	52 (75%)	17 (25%)	0 1
14	AT	76/76 (100%)	61 (80%)	15 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	AB	202/202 (100%)	172 (85%)	30 (15%)	3 8
16	AC	160/160 (100%)	125 (78%)	35 (22%)	1 2
17	AD	180/180 (100%)	144 (80%)	36 (20%)	1 3
18	AE	115/115 (100%)	104 (90%)	11 (10%)	8 22
19	AF	90/90 (100%)	76 (84%)	14 (16%)	2 6
20	AG	126/126 (100%)	110 (87%)	16 (13%)	4 11
21	AH	119/119 (100%)	96 (81%)	23 (19%)	1 3
22	AI	98/98 (100%)	76 (78%)	22 (22%)	1 2
23	AY	528/573 (92%)	420 (80%)	108 (20%)	1 2
24	AU	19/19 (100%)	14 (74%)	5 (26%)	0 1
27	BN	117/119 (98%)	84 (72%)	33 (28%)	0 1
28	BO	100/100 (100%)	84 (84%)	16 (16%)	2 6
29	BP	112/116 (97%)	82 (73%)	30 (27%)	0 1
30	BQ	111/111 (100%)	96 (86%)	15 (14%)	4 9
31	BR	100/101 (99%)	80 (80%)	20 (20%)	1 3
32	BS	77/88 (88%)	62 (80%)	15 (20%)	1 3
33	BT	120/127 (94%)	91 (76%)	29 (24%)	0 1
34	BU	92/94 (98%)	76 (83%)	16 (17%)	2 5
35	BV	82/82 (100%)	56 (68%)	26 (32%)	0 0
36	BW	91/92 (99%)	75 (82%)	16 (18%)	2 4
37	BX	74/78 (95%)	59 (80%)	15 (20%)	1 3
38	BY	84/91 (92%)	65 (77%)	19 (23%)	1 2
39	BZ	154/179 (86%)	127 (82%)	27 (18%)	2 4
40	B0	66/67 (98%)	56 (85%)	10 (15%)	3 7
41	B1	78/83 (94%)	63 (81%)	15 (19%)	1 3
42	B2	66/67 (98%)	51 (77%)	15 (23%)	1 2
43	BD	213/218 (98%)	170 (80%)	43 (20%)	1 3
44	B3	51/52 (98%)	41 (80%)	10 (20%)	1 3
45	B4	27/63 (43%)	23 (85%)	4 (15%)	3 8
46	B5	51/52 (98%)	42 (82%)	9 (18%)	2 4
47	B6	43/52 (83%)	31 (72%)	12 (28%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	B7	41/42 (98%)	35 (85%)	6 (15%)	3 8
49	B8	53/55 (96%)	33 (62%)	20 (38%)	0 0
50	B9	33/34 (97%)	23 (70%)	10 (30%)	0 0
51	BC	177/181 (98%)	159 (90%)	18 (10%)	7 20
52	BE	165/166 (99%)	131 (79%)	34 (21%)	1 2
53	BF	165/166 (99%)	134 (81%)	31 (19%)	1 3
54	BG	155/156 (99%)	128 (83%)	27 (17%)	2 5
55	BH	136/148 (92%)	107 (79%)	29 (21%)	1 2
56	BK	96/111 (86%)	85 (88%)	11 (12%)	5 15
All	All	5448/5654 (96%)	4402 (81%)	1046 (19%)	1 3

5 of 1046 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	BN	33	LEU
32	BS	49	VAL
53	BF	102	PRO
27	BN	73	THR
29	BP	88	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
31	BR	23	ASN
36	BW	102	HIS
53	BF	31	HIS
33	BT	90	GLN
39	BZ	34	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1512/1516 (99%)	315 (20%)	65 (4%)
2	AV	73/76 (96%)	28 (38%)	9 (12%)
25	BA	2849/2915 (97%)	756 (26%)	130 (4%)
26	BB	119/122 (97%)	34 (28%)	4 (3%)
3	AX	5/25 (20%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4558/4654 (97%)	1133 (24%)	208 (4%)

5 of 1133 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	U
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	405	U
25	BA	974	G
25	BA	2497	A
25	BA	542	C
25	BA	746	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 139 ligands modelled in this entry, 138 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	$\#\|Z\|>2$
60	GCP	AY	702	59	26,34,34	3.84	11 (42%)	31,54,54	2.05	11 (35%)

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
60	GCP	AY	702	59	-	6/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AY	702	GCP	C4-N9	-11.39	1.32	1.47
60	AY	702	GCP	C5-C6	-11.09	1.33	1.52
60	AY	702	GCP	C6-N1	5.10	1.41	1.33
60	AY	702	GCP	PB-O2B	-4.23	1.46	1.56
60	AY	702	GCP	C2'-C3'	-3.97	1.42	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	AY	702	GCP	O4'-C4'-C5'	-4.73	93.80	109.37
60	AY	702	GCP	C4-C5-N7	3.85	107.56	102.46
60	AY	702	GCP	O1G-PG-C3B	-3.81	103.03	111.24
60	AY	702	GCP	C2'-C3'-C4'	-3.66	95.53	102.64
60	AY	702	GCP	O4'-C1'-N9	3.62	114.43	109.04

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

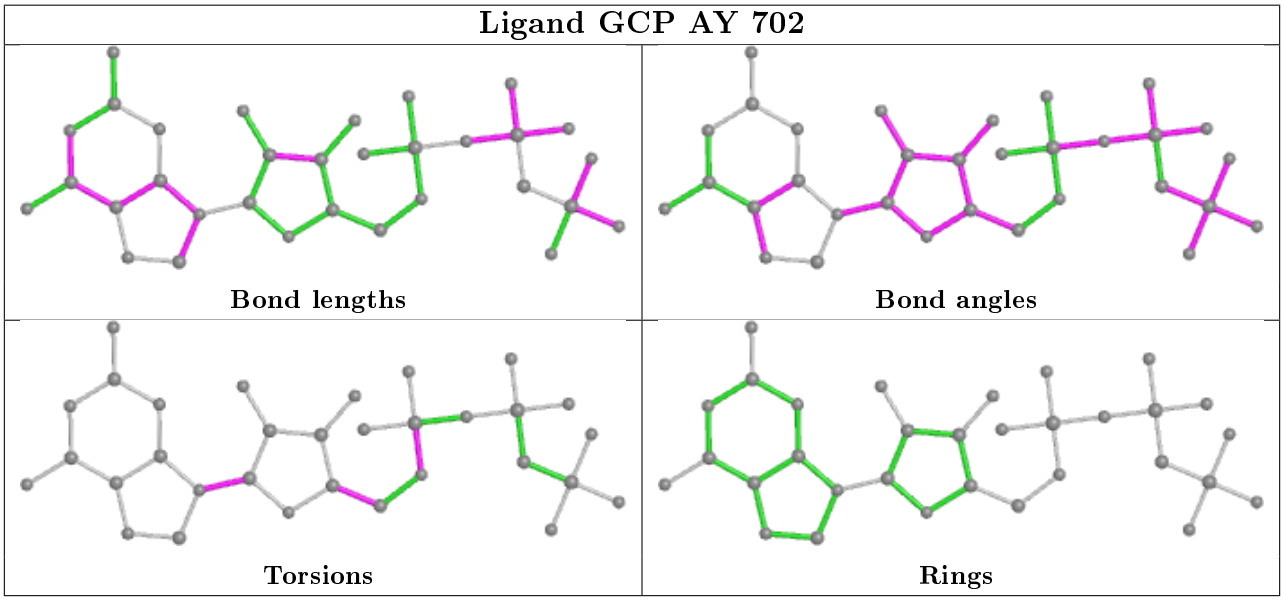
Mol	Chain	Res	Type	Atoms
60	AY	702	GCP	C5'-O5'-PA-O1A
60	AY	702	GCP	O4'-C1'-N9-C4
60	AY	702	GCP	C2'-C1'-N9-C8
60	AY	702	GCP	C2'-C1'-N9-C4
60	AY	702	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AY	702	GCP	5	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.



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
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2506:U	O3'	2507:C	P	1.76

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	1514/1516 (99%)	-0.25	53 (3%) 44 38	9, 32, 113, 247	0
2	AV	74/76 (97%)	0.03	1 (1%) 75 74	23, 54, 91, 134	0
3	AX	6/25 (24%)	0.11	1 (16%) 1 1	18, 22, 53, 75	0
4	AJ	98/98 (100%)	0.20	3 (3%) 49 44	22, 49, 98, 108	0
5	AK	119/119 (100%)	-0.10	4 (3%) 45 39	18, 41, 65, 104	0
6	AL	124/124 (100%)	-0.19	3 (2%) 59 56	16, 32, 64, 107	0
7	AM	124/124 (100%)	0.74	12 (9%) 7 5	31, 69, 118, 161	0
8	AN	60/60 (100%)	-0.19	2 (3%) 46 41	21, 33, 69, 83	0
9	AO	88/88 (100%)	-0.25	0 100 100	24, 41, 67, 73	0
10	AP	83/83 (100%)	-0.28	1 (1%) 79 78	29, 40, 60, 112	0
11	AQ	99/99 (100%)	-0.46	0 100 100	20, 34, 53, 59	0
12	AR	70/70 (100%)	-0.26	0 100 100	23, 41, 75, 92	0
13	AS	78/78 (100%)	0.52	7 (8%) 9 6	39, 69, 107, 121	0
14	AT	99/99 (100%)	-0.16	4 (4%) 38 32	24, 39, 78, 90	0
15	AB	234/234 (100%)	0.04	14 (5%) 21 17	21, 55, 117, 134	0
16	AC	206/206 (100%)	-0.37	0 100 100	22, 41, 67, 103	0
17	AD	208/208 (100%)	-0.11	4 (1%) 66 64	26, 49, 75, 90	0
18	AE	150/150 (100%)	-0.41	1 (0%) 87 87	19, 30, 54, 81	0
19	AF	101/101 (100%)	-0.14	1 (0%) 82 81	28, 52, 75, 87	0
20	AG	155/155 (100%)	-0.02	9 (5%) 23 18	31, 53, 104, 148	0
21	AH	138/138 (100%)	-0.46	1 (0%) 87 87	19, 32, 55, 84	0
22	AI	127/127 (100%)	-0.09	3 (2%) 59 56	21, 51, 82, 108	0
23	AY	622/680 (91%)	-0.11	10 (1%) 72 70	30, 55, 97, 131	0
24	AU	24/24 (100%)	0.29	1 (4%) 36 31	33, 48, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	BA	2859/2915 (98%)	-0.30	67 (2%) 60 57	7, 27, 90, 267	0
26	BB	119/122 (97%)	-0.00	0 100 100	26, 63, 95, 134	0
27	BN	138/140 (98%)	-0.21	4 (2%) 51 47	18, 35, 66, 80	0
28	BO	122/122 (100%)	-0.56	0 100 100	18, 31, 49, 60	0
29	BP	146/150 (97%)	0.56	15 (10%) 6 4	18, 55, 94, 127	0
30	BQ	141/141 (100%)	-0.26	2 (1%) 75 74	23, 35, 64, 112	0
31	BR	117/118 (99%)	-0.27	5 (4%) 35 30	15, 33, 58, 75	0
32	BS	98/112 (87%)	0.72	8 (8%) 11 8	50, 80, 106, 125	0
33	BT	137/146 (93%)	0.43	15 (10%) 5 4	23, 50, 135, 151	0
34	BU	117/118 (99%)	-0.29	2 (1%) 70 68	16, 29, 58, 85	0
35	BV	101/101 (100%)	0.05	4 (3%) 38 32	15, 49, 77, 97	0
36	BW	113/113 (100%)	-0.21	3 (2%) 54 50	18, 29, 67, 122	0
37	BX	92/96 (95%)	-0.34	0 100 100	20, 34, 54, 61	0
38	BY	100/110 (90%)	0.92	16 (16%) 1 1	29, 56, 122, 168	0
39	BZ	198/206 (96%)	0.03	4 (2%) 65 62	33, 59, 92, 103	0
40	B0	84/85 (98%)	0.33	7 (8%) 11 8	26, 41, 96, 133	0
41	B1	93/98 (94%)	0.08	3 (3%) 47 42	18, 33, 72, 121	0
42	B2	71/72 (98%)	0.01	2 (2%) 53 48	30, 49, 82, 100	0
43	BD	271/276 (98%)	-0.41	5 (1%) 68 66	9, 20, 46, 89	0
44	B3	59/60 (98%)	0.06	2 (3%) 45 39	24, 40, 76, 137	0
45	B4	30/71 (42%)	1.63	10 (33%) 0 0	102, 130, 156, 174	0
46	B5	59/60 (98%)	0.37	7 (11%) 4 3	10, 35, 98, 134	0
47	B6	44/54 (81%)	1.08	9 (20%) 1 0	34, 59, 99, 109	0
48	B7	48/49 (97%)	-0.34	2 (4%) 36 31	10, 19, 59, 101	0
49	B8	63/65 (96%)	0.16	5 (7%) 12 9	22, 37, 61, 118	0
50	B9	36/37 (97%)	0.13	1 (2%) 53 48	26, 44, 69, 77	0
51	BC	225/229 (98%)	0.03	9 (4%) 38 32	36, 64, 111, 132	0
52	BE	204/206 (99%)	-0.16	8 (3%) 39 34	14, 32, 85, 109	0
53	BF	207/210 (98%)	0.02	13 (6%) 20 15	15, 37, 103, 187	0
54	BG	181/182 (99%)	1.01	30 (16%) 1 1	67, 101, 130, 147	0
55	BH	173/180 (96%)	0.33	11 (6%) 19 15	35, 60, 95, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	BK	127/147 (86%)	4.70	105 (82%) 0 0	127, 181, 237, 263	0
57	BJ	130/130 (100%)	1.18	26 (20%) 1 0	74, 106, 140, 195	0
58	BL	0/125	-	-	-	-
All	All	11304/11728 (96%)	-0.04	535 (4%) 31 27	7, 40, 108, 267	0

The worst 5 of 535 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	BH	44	VAL	18.6
7	AM	123	ALA	17.7
56	BK	136	VAL	14.8
56	BK	83	GLY	13.4
53	BF	11	VAL	12.9

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3012	1/1	0.86	0.12	10,10,10,10	0
59	MG	BA	3004	1/1	0.87	0.15	46,46,46,46	0
59	MG	BA	3059	1/1	0.87	0.21	9,9,9,9	0
59	MG	BA	3013	1/1	0.88	0.20	26,26,26,26	0
59	MG	AA	1636	1/1	0.88	0.11	24,24,24,24	0
59	MG	AA	1644	1/1	0.89	0.36	33,33,33,33	0
59	MG	AA	1635	1/1	0.89	0.22	24,24,24,24	0
59	MG	AA	1629	1/1	0.89	0.14	38,38,38,38	0
59	MG	BA	3065	1/1	0.90	0.30	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3067	1/1	0.90	0.19	16,16,16,16	0
59	MG	BA	3072	1/1	0.90	0.25	19,19,19,19	0
59	MG	BA	3039	1/1	0.90	0.19	24,24,24,24	0
59	MG	AA	1633	1/1	0.91	0.12	27,27,27,27	0
59	MG	BA	3029	1/1	0.91	0.24	28,28,28,28	0
59	MG	BA	3027	1/1	0.91	0.34	30,30,30,30	0
59	MG	AA	1603	1/1	0.91	0.22	23,23,23,23	0
59	MG	BA	3081	1/1	0.91	0.15	17,17,17,17	0
59	MG	BA	3070	1/1	0.91	0.29	24,24,24,24	0
59	MG	BA	3073	1/1	0.91	0.26	14,14,14,14	0
59	MG	BA	3071	1/1	0.92	0.32	29,29,29,29	0
59	MG	AA	1615	1/1	0.92	0.17	24,24,24,24	0
59	MG	B8	101	1/1	0.92	0.12	15,15,15,15	0
59	MG	BA	3001	1/1	0.92	0.33	32,32,32,32	0
59	MG	AA	1621	1/1	0.93	0.17	14,14,14,14	0
59	MG	AA	1641	1/1	0.93	0.13	25,25,25,25	0
59	MG	BA	3047	1/1	0.93	0.35	27,27,27,27	0
59	MG	AA	1637	1/1	0.93	0.12	34,34,34,34	0
59	MG	AA	1606	1/1	0.93	0.24	15,15,15,15	0
59	MG	AA	1643	1/1	0.93	0.14	31,31,31,31	0
59	MG	BA	3035	1/1	0.93	0.38	18,18,18,18	0
59	MG	AA	1602	1/1	0.94	0.31	16,16,16,16	0
59	MG	AA	1639	1/1	0.94	0.17	20,20,20,20	0
59	MG	BF	301	1/1	0.94	0.16	27,27,27,27	0
59	MG	BA	3080	1/1	0.94	0.23	16,16,16,16	0
59	MG	BA	3087	1/1	0.94	0.24	26,26,26,26	0
59	MG	BA	3083	1/1	0.94	0.11	37,37,37,37	0
59	MG	BA	3041	1/1	0.94	0.33	11,11,11,11	0
59	MG	BA	3051	1/1	0.94	0.29	24,24,24,24	0
59	MG	AA	1619	1/1	0.94	0.22	27,27,27,27	0
59	MG	BA	3088	1/1	0.95	0.30	26,26,26,26	0
59	MG	BA	3064	1/1	0.95	0.17	22,22,22,22	0
59	MG	BA	3074	1/1	0.95	0.15	16,16,16,16	0
59	MG	BA	3009	1/1	0.95	0.30	31,31,31,31	0
59	MG	BA	3010	1/1	0.95	0.30	14,14,14,14	0
59	MG	BA	3026	1/1	0.95	0.18	19,19,19,19	0
59	MG	AA	1626	1/1	0.95	0.18	19,19,19,19	0
59	MG	BE	301	1/1	0.95	0.27	16,16,16,16	0
59	MG	BA	3063	1/1	0.95	0.17	22,22,22,22	0
59	MG	BA	3018	1/1	0.95	0.23	12,12,12,12	0
59	MG	BA	3020	1/1	0.95	0.32	6,6,6,6	0
59	MG	BA	3045	1/1	0.95	0.21	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1623	1/1	0.95	0.23	15,15,15,15	0
59	MG	BA	3002	1/1	0.95	0.17	17,17,17,17	0
59	MG	AA	1604	1/1	0.95	0.09	3,3,3,3	0
59	MG	AA	1645	1/1	0.95	0.39	35,35,35,35	0
59	MG	BA	3025	1/1	0.95	0.21	16,16,16,16	0
59	MG	AA	1642	1/1	0.95	0.23	30,30,30,30	0
59	MG	BA	3084	1/1	0.95	0.19	22,22,22,22	0
59	MG	AY	701	1/1	0.95	0.12	41,41,41,41	0
59	MG	BA	3066	1/1	0.95	0.27	15,15,15,15	0
59	MG	BA	3014	1/1	0.95	0.28	27,27,27,27	0
59	MG	BA	3052	1/1	0.95	0.23	19,19,19,19	0
59	MG	AA	1622	1/1	0.96	0.23	25,25,25,25	0
59	MG	AA	1609	1/1	0.96	0.24	16,16,16,16	0
59	MG	BA	3085	1/1	0.96	0.27	18,18,18,18	0
59	MG	BA	3030	1/1	0.96	0.32	12,12,12,12	0
59	MG	BA	3032	1/1	0.96	0.27	21,21,21,21	0
59	MG	BA	3078	1/1	0.96	0.17	15,15,15,15	0
59	MG	BA	3076	1/1	0.96	0.23	8,8,8,8	0
59	MG	BA	3068	1/1	0.96	0.26	7,7,7,7	0
59	MG	BA	3082	1/1	0.96	0.26	21,21,21,21	0
59	MG	BA	3060	1/1	0.96	0.30	22,22,22,22	0
59	MG	AA	1607	1/1	0.96	0.14	24,24,24,24	0
59	MG	AA	1613	1/1	0.96	0.17	6,6,6,6	0
59	MG	BA	3021	1/1	0.96	0.20	25,25,25,25	0
59	MG	BA	3043	1/1	0.96	0.30	7,7,7,7	0
59	MG	AA	1640	1/1	0.96	0.16	21,21,21,21	0
59	MG	AA	1611	1/1	0.96	0.24	7,7,7,7	0
59	MG	BA	3086	1/1	0.96	0.24	26,26,26,26	0
59	MG	AA	1630	1/1	0.96	0.29	29,29,29,29	0
59	MG	BA	3038	1/1	0.97	0.36	19,19,19,19	0
59	MG	AA	1638	1/1	0.97	0.16	22,22,22,22	0
59	MG	BA	3033	1/1	0.97	0.26	12,12,12,12	0
59	MG	AA	1616	1/1	0.97	0.18	5,5,5,5	0
59	MG	BA	3023	1/1	0.97	0.25	9,9,9,9	0
59	MG	BA	3055	1/1	0.97	0.21	5,5,5,5	0
59	MG	BA	3077	1/1	0.97	0.14	17,17,17,17	0
59	MG	AA	1612	1/1	0.97	0.15	14,14,14,14	0
59	MG	BA	3075	1/1	0.97	0.19	12,12,12,12	0
59	MG	BA	3008	1/1	0.97	0.27	13,13,13,13	0
59	MG	BA	3056	1/1	0.97	0.15	18,18,18,18	0
59	MG	BA	3011	1/1	0.97	0.24	30,30,30,30	0
59	MG	AA	1625	1/1	0.97	0.34	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3015	1/1	0.97	0.22	10,10,10,10	0
59	MG	BA	3040	1/1	0.97	0.25	10,10,10,10	0
59	MG	AA	1605	1/1	0.97	0.10	25,25,25,25	0
59	MG	BA	3017	1/1	0.97	0.20	16,16,16,16	0
59	MG	BA	3046	1/1	0.97	0.18	14,14,14,14	0
59	MG	BA	3058	1/1	0.97	0.17	3,3,3,3	0
59	MG	BA	3036	1/1	0.97	0.27	20,20,20,20	0
59	MG	AA	1618	1/1	0.97	0.20	22,22,22,22	0
59	MG	BA	3062	1/1	0.97	0.23	18,18,18,18	0
59	MG	AA	1632	1/1	0.97	0.21	22,22,22,22	0
59	MG	BA	3034	1/1	0.97	0.28	5,5,5,5	0
59	MG	BA	3042	1/1	0.97	0.33	11,11,11,11	0
59	MG	BA	3028	1/1	0.97	0.20	23,23,23,23	0
59	MG	BA	3057	1/1	0.97	0.22	8,8,8,8	0
59	MG	BA	3037	1/1	0.98	0.20	7,7,7,7	0
59	MG	BA	3006	1/1	0.98	0.30	13,13,13,13	0
59	MG	AA	1601	1/1	0.98	0.24	13,13,13,13	0
59	MG	BA	3061	1/1	0.98	0.30	8,8,8,8	0
59	MG	BA	3048	1/1	0.98	0.25	9,9,9,9	0
59	MG	AA	1624	1/1	0.98	0.19	14,14,14,14	0
59	MG	BA	3007	1/1	0.98	0.30	4,4,4,4	0
59	MG	BA	3022	1/1	0.98	0.33	13,13,13,13	0
59	MG	BA	3016	1/1	0.98	0.07	15,15,15,15	0
59	MG	BA	3024	1/1	0.98	0.28	2,2,2,2	0
59	MG	BA	3049	1/1	0.98	0.30	2,2,2,2	0
59	MG	BA	3031	1/1	0.98	0.29	16,16,16,16	0
59	MG	AA	1631	1/1	0.98	0.19	13,13,13,13	0
59	MG	AA	1627	1/1	0.98	0.23	15,15,15,15	0
59	MG	BA	3069	1/1	0.98	0.34	14,14,14,14	0
59	MG	AA	1610	1/1	0.98	0.23	14,14,14,14	0
59	MG	BA	3019	1/1	0.98	0.27	16,16,16,16	0
59	MG	AA	1620	1/1	0.98	0.37	18,18,18,18	0
59	MG	BA	3079	1/1	0.98	0.23	14,14,14,14	0
59	MG	BD	301	1/1	0.98	0.26	7,7,7,7	0
59	MG	AA	1614	1/1	0.98	0.24	11,11,11,11	0
59	MG	AA	1617	1/1	0.98	0.32	21,21,21,21	0
59	MG	AA	1608	1/1	0.98	0.42	23,23,23,23	0
60	GCP	AY	702	32/32	0.98	0.12	27,42,47,49	0
59	MG	BA	3053	1/1	0.99	0.22	7,7,7,7	0
59	MG	BA	3003	1/1	0.99	0.36	2,2,2,2	0
59	MG	BA	3044	1/1	0.99	0.17	15,15,15,15	0
59	MG	AA	1634	1/1	0.99	0.07	6,6,6,6	0

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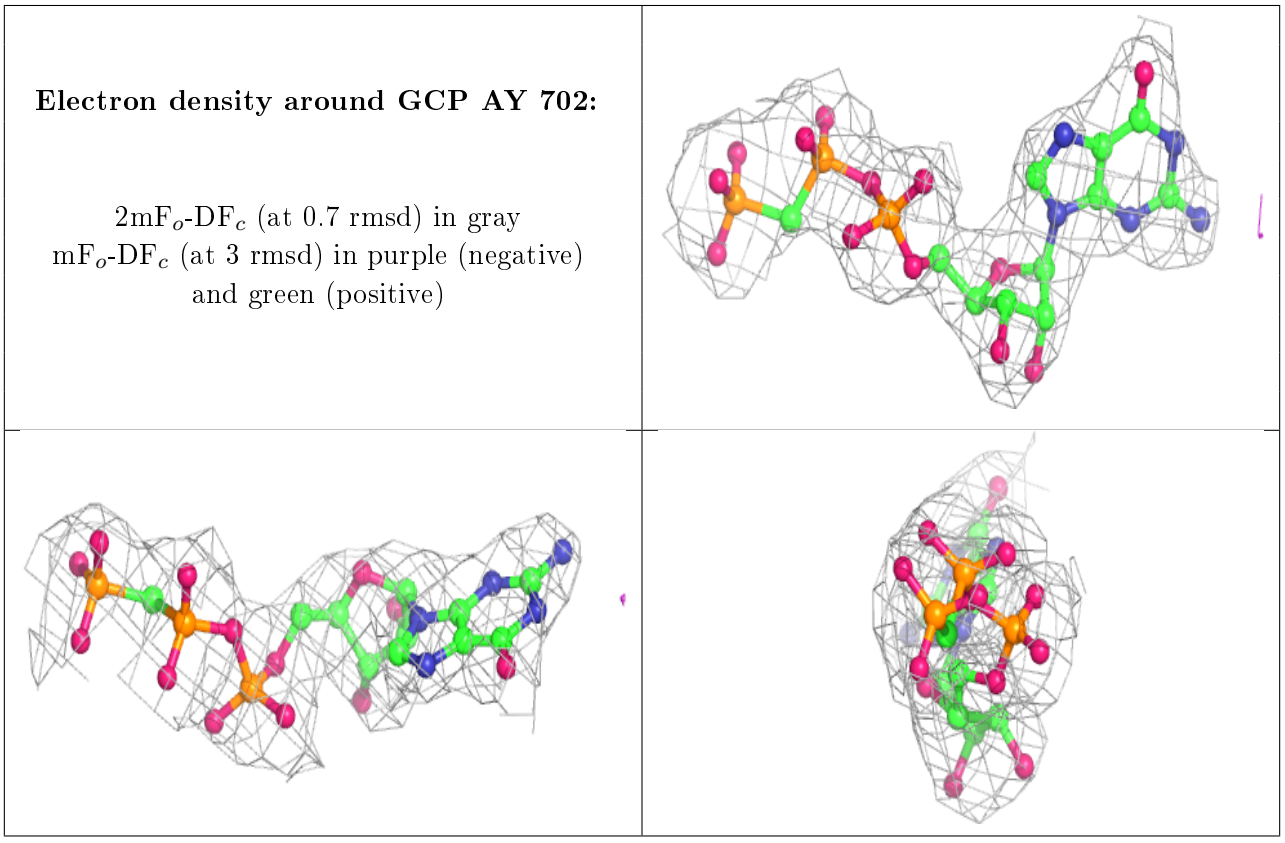
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3005	1/1	0.99	0.32	12,12,12,12	0
59	MG	BA	3054	1/1	0.99	0.27	9,9,9,9	0
59	MG	AA	1628	1/1	0.99	0.07	18,18,18,18	0
59	MG	BA	3050	1/1	1.00	0.27	10,10,10,10	0

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

Electron density around GCP AY 702:

$2mF_o$-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.