



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 12:03 pm BST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

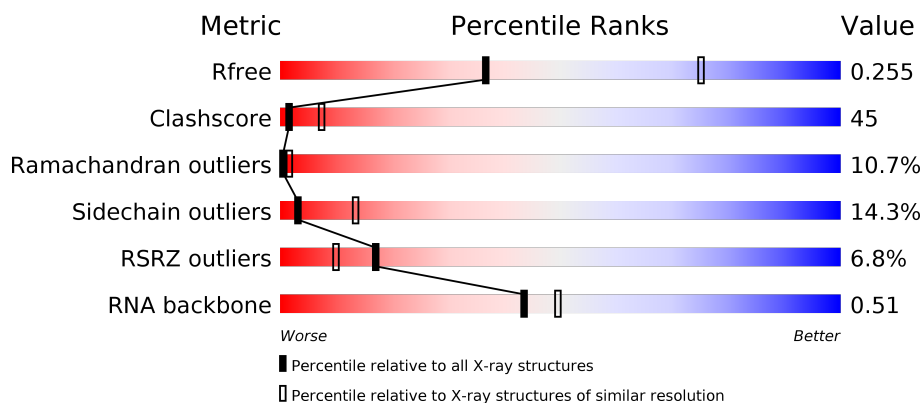
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1519	<div> <div>3%</div> <div> <div>33%</div> <div>47%</div> <div>19%</div> <div>•</div> </div> </div>
2	AB	256	<div> <div>8%</div> <div> <div>21%</div> <div>49%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
3	AC	239	<div> <div>4%</div> <div> <div>23%</div> <div>44%</div> <div>18%</div> <div>•</div> <div>13%</div> </div> </div>
4	AD	209	<div> <div>2%</div> <div> <div>45%</div> <div>45%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	132	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
23	AX	9	
24	AY	691	
25	B0	84	
26	B1	97	
27	B2	71	
28	B3	60	
29	B4	71	

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1606	-	-	-	X
59	MG	AA	1628	-	-	-	X
59	MG	AA	1636	-	-	-	X
59	MG	AA	1637	-	-	-	X
59	MG	AA	1647	-	-	-	X
59	MG	AA	1666	-	-	-	X
59	MG	AA	1674	-	-	-	X
59	MG	AA	1703	-	-	-	X
59	MG	AA	1714	-	-	-	X
59	MG	AA	1724	-	-	-	X
59	MG	AA	1740	-	-	-	X
59	MG	AA	1741	-	-	-	X
59	MG	AA	1753	-	-	-	X
59	MG	AA	1754	-	-	-	X
59	MG	AA	1760	-	-	-	X
59	MG	AA	1762	-	-	-	X
59	MG	AA	1773	-	-	-	X
59	MG	AA	1779	-	-	-	X
59	MG	BA	3009	-	-	-	X
59	MG	BA	3012	-	-	-	X
59	MG	BA	3016	-	-	-	X
59	MG	BA	3019	-	-	-	X
59	MG	BA	3028	-	-	-	X
59	MG	BA	3030	-	-	-	X
59	MG	BA	3040	-	-	-	X
59	MG	BA	3147	-	-	-	X
59	MG	BA	3174	-	-	-	X
59	MG	BA	3179	-	-	-	X
59	MG	BA	3197	-	-	-	X
59	MG	BA	3201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3209	-	-	-	X
59	MG	BA	3215	-	-	-	X
59	MG	BA	3242	-	-	-	X
59	MG	BA	3252	-	-	-	X
59	MG	BA	3260	-	-	-	X
59	MG	BA	3264	-	-	-	X
59	MG	BA	3265	-	-	-	X
59	MG	BA	3276	-	-	-	X
59	MG	BA	3279	-	-	-	X
59	MG	BA	3281	-	-	-	X
59	MG	BA	3284	-	-	-	X
61	GCP	AY	701	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

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

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	88	Total	C	N	O	S	0	0	1
			692	440	128	122	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			

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

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

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

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

- Molecule 24 is a protein called ELONGATION FACTOR G.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 37 is a protein called RIBOSOMAL PROTEIN L1.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 43 is a protein called CHAIN J.

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

- Molecule 44 is a protein called CHAIN K.

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

- Molecule 45 is a protein called CHAIN L.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

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

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

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

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

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

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

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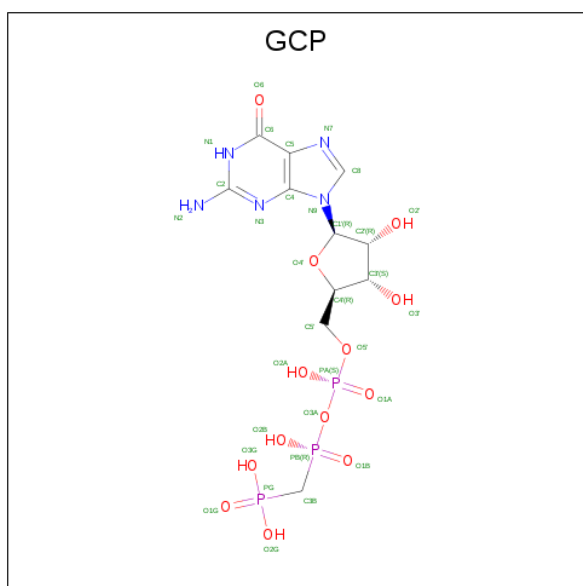
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	198	Total	Mg	0	0
			198	198		
59	B0	1	Total	Mg	0	0
			1	1		
59	AY	1	Total	Mg	0	0
			1	1		
59	BC	1	Total	Mg	0	0
			1	1		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

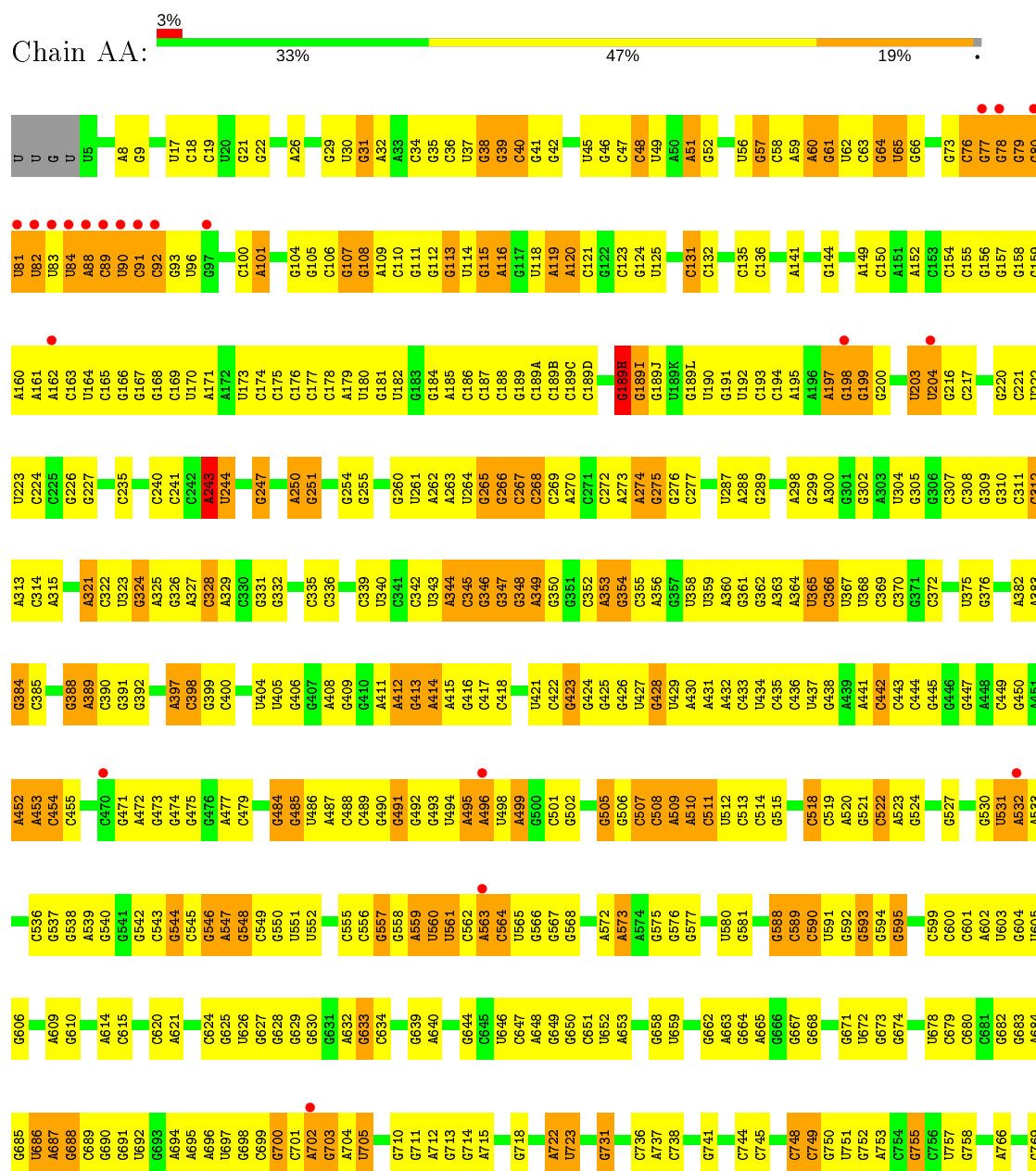


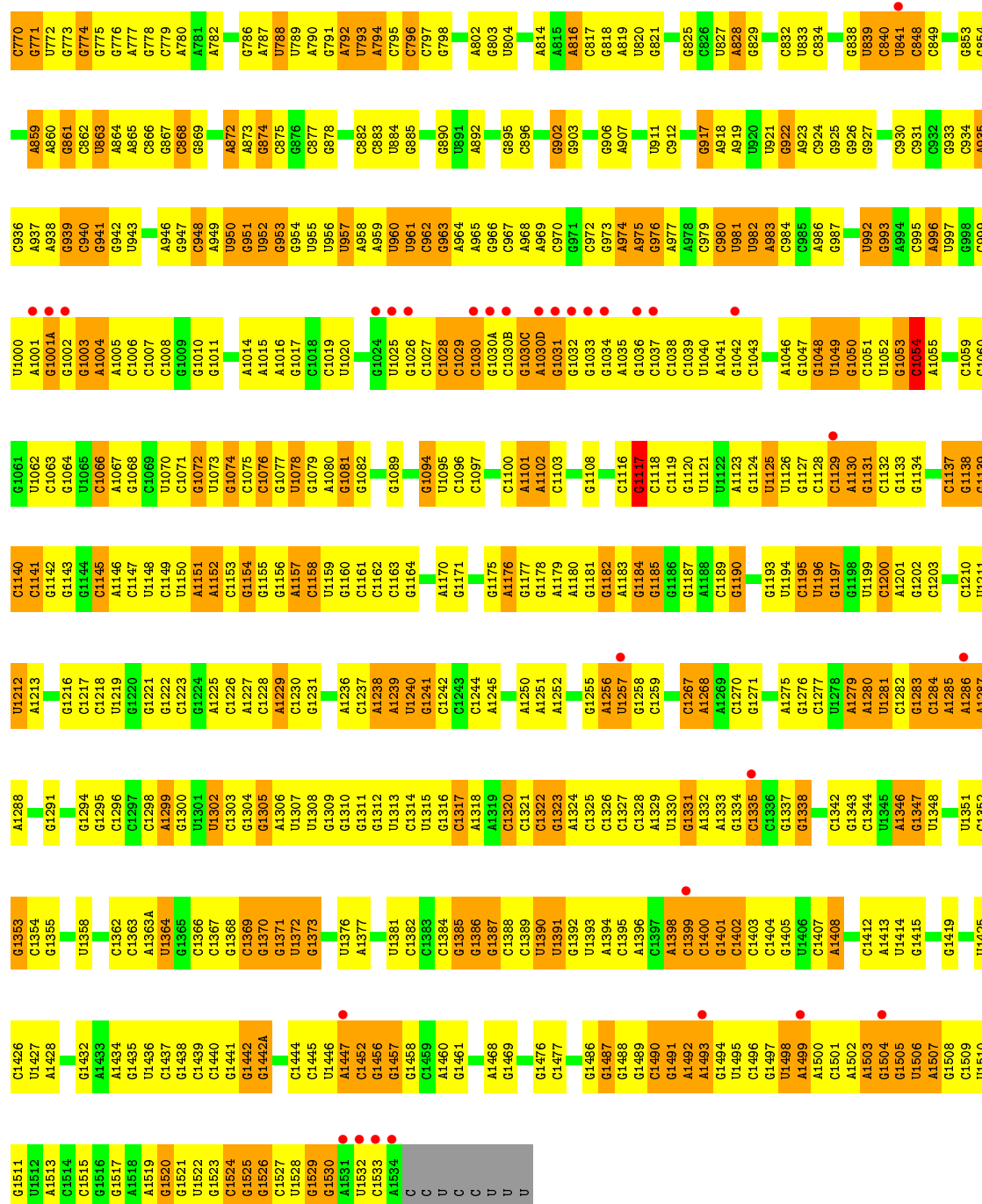
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

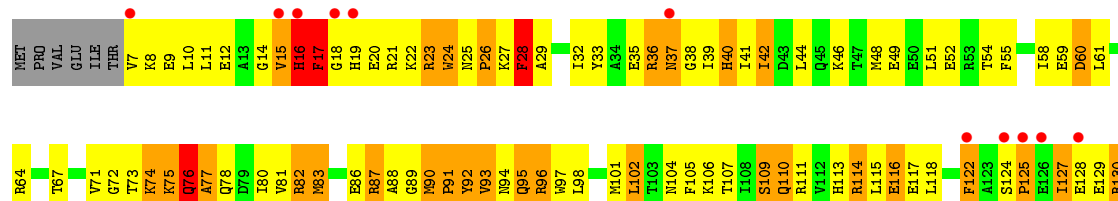
• Molecule 1: 16S RIBOSOMAL RNA

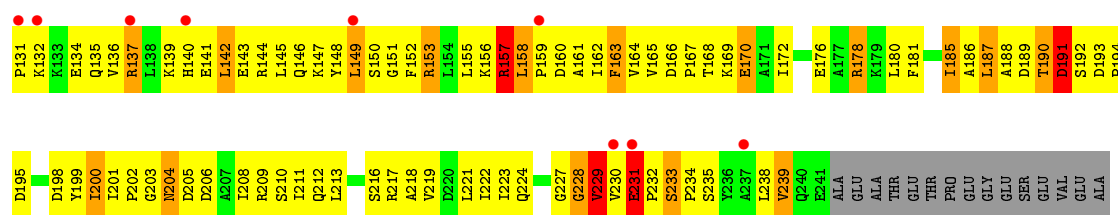




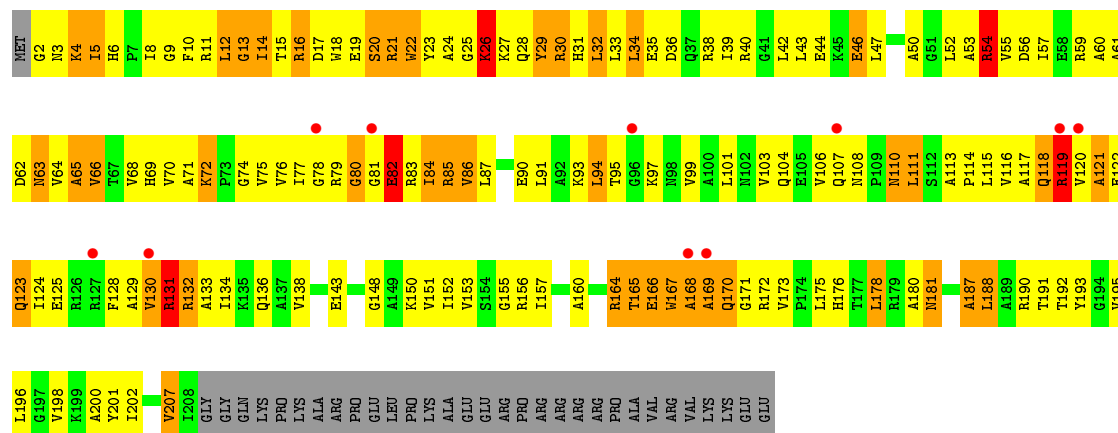
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB: 8% 21% 49% 18% 8%

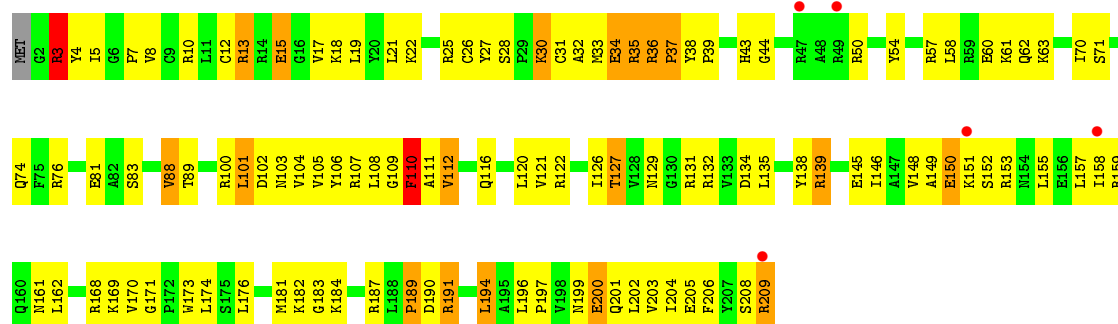




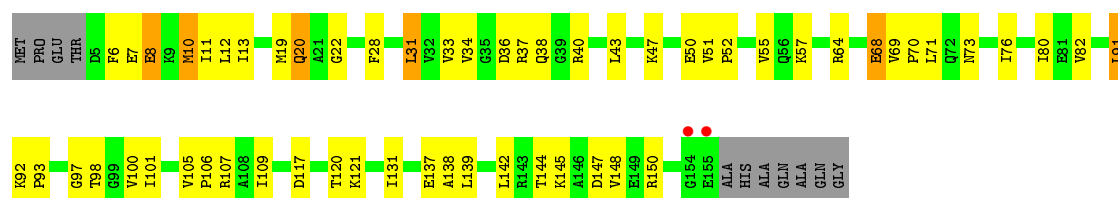
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



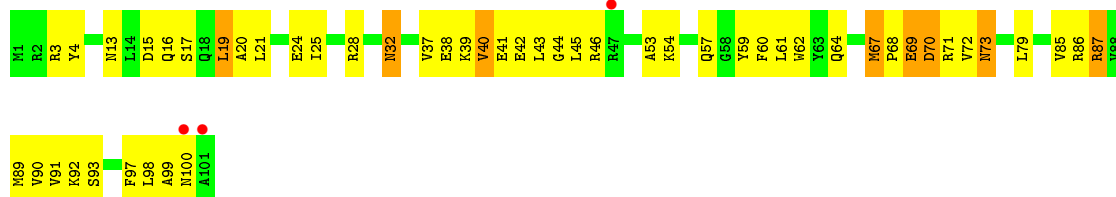
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



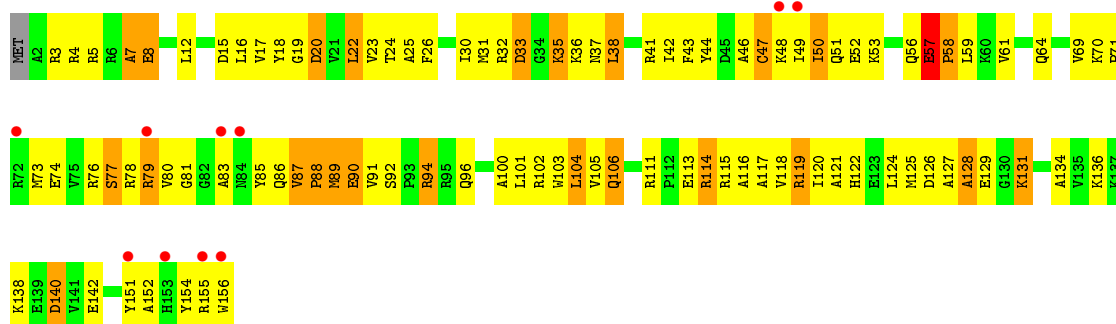
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



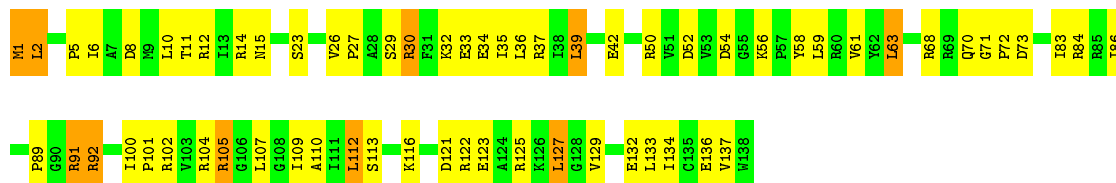
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



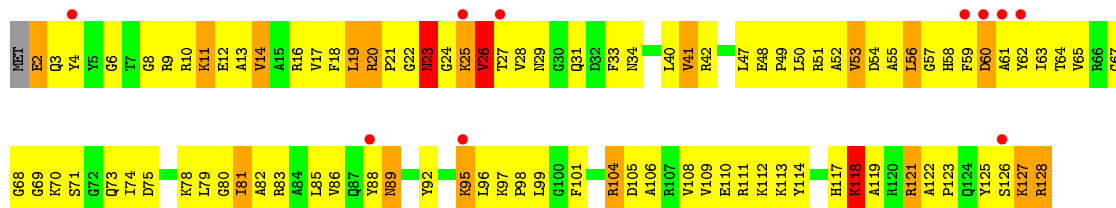
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

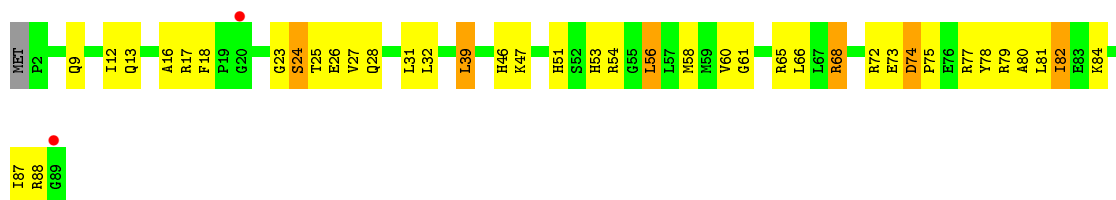


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

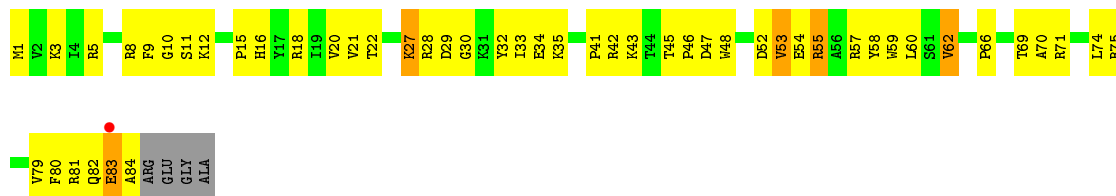


- Molecule 10: 30S RIBOSOMAL PROTEIN S10

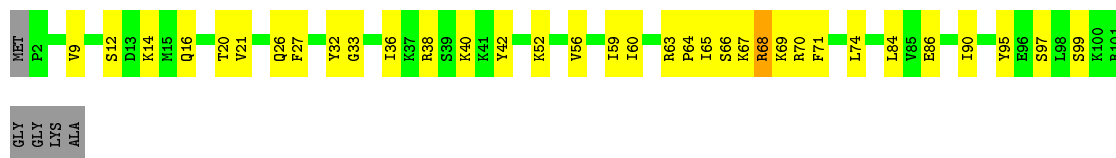




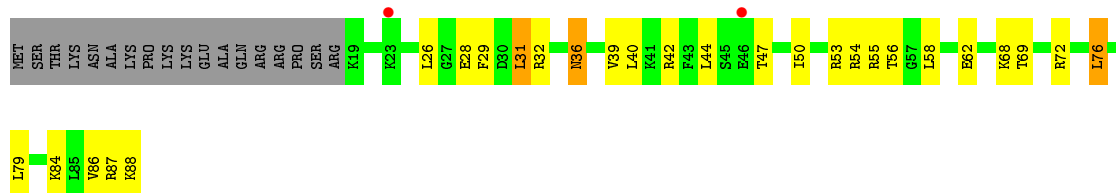
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



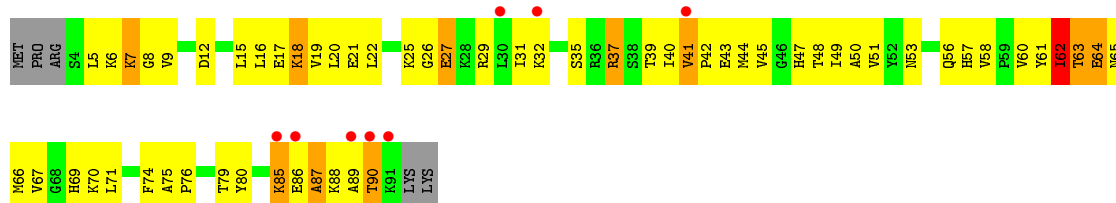
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



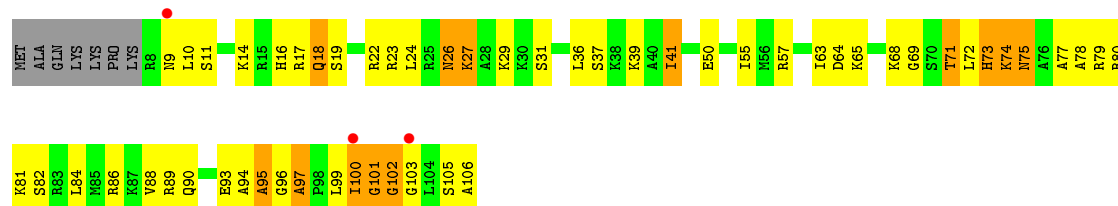
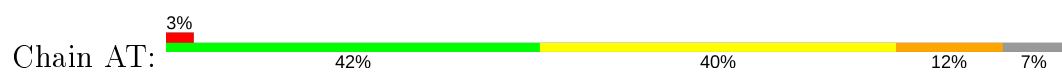
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



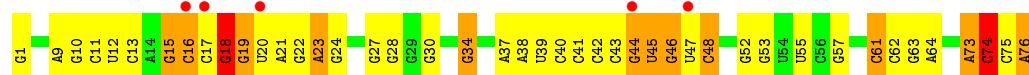
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



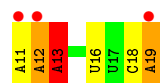
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



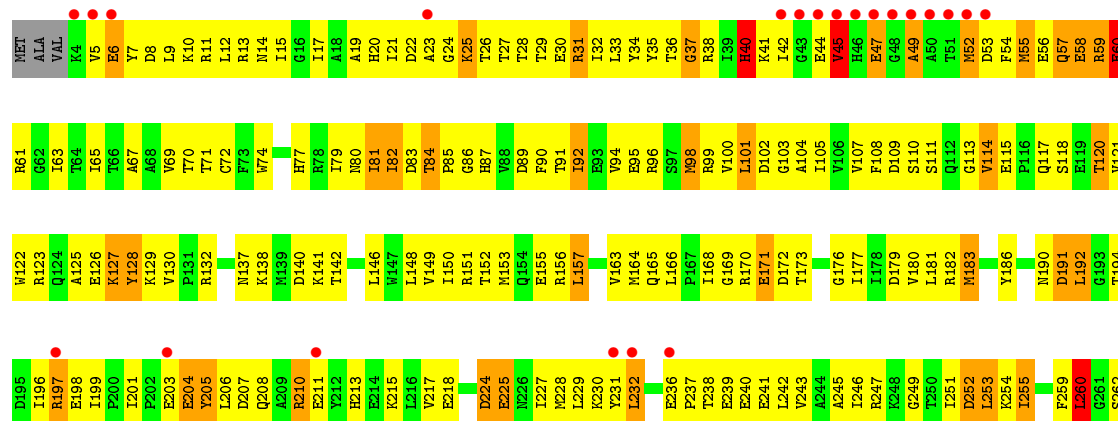
- Molecule 22: RNA (77-MER)

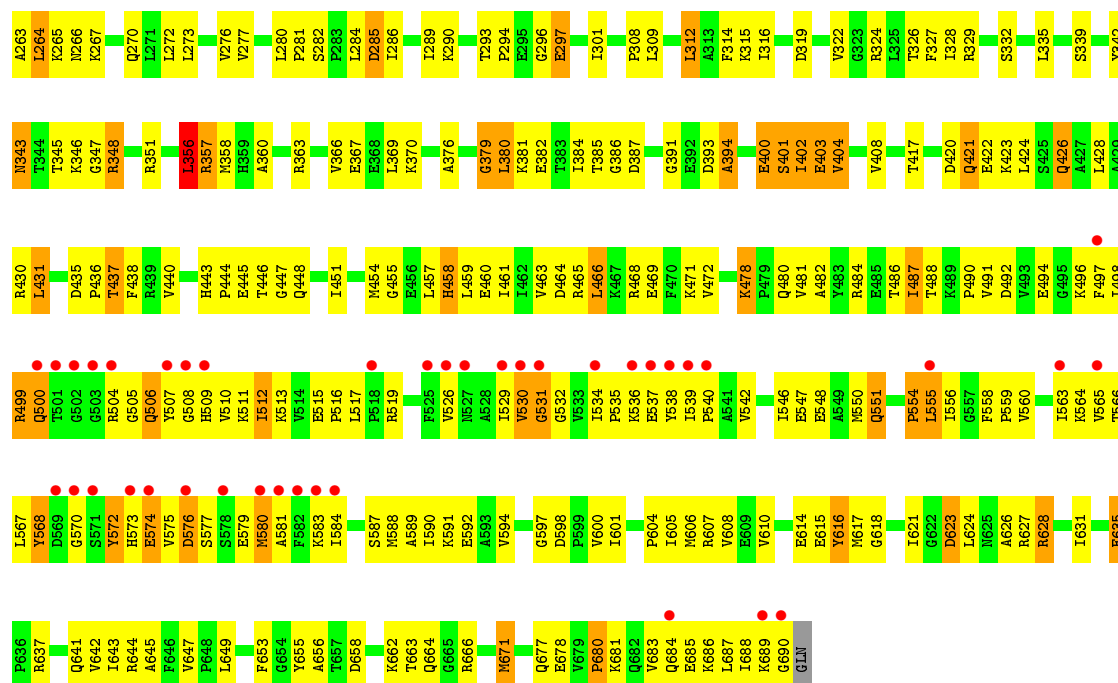


- Molecule 23: 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

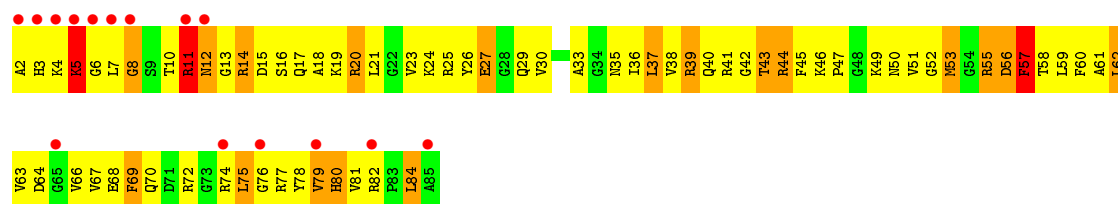
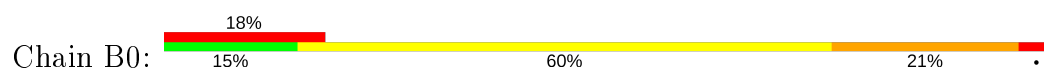


- Molecule 24: ELONGATION FACTOR G

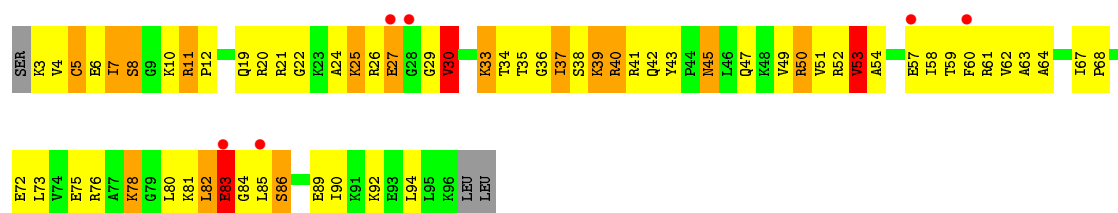




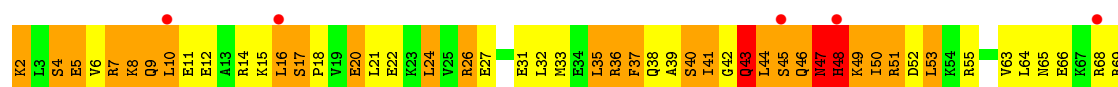
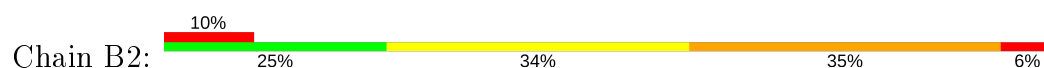
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

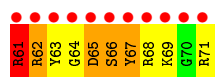
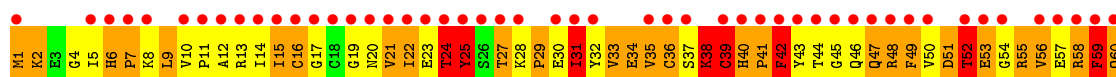
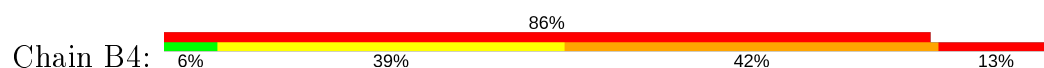




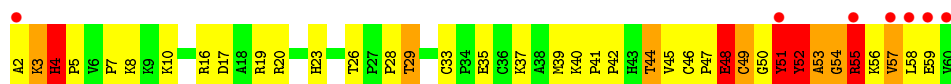
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



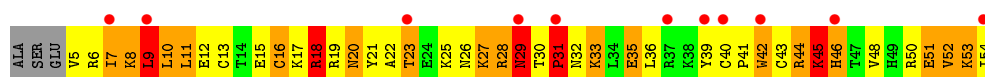
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



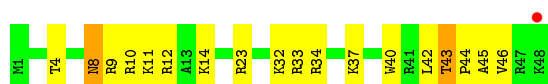
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



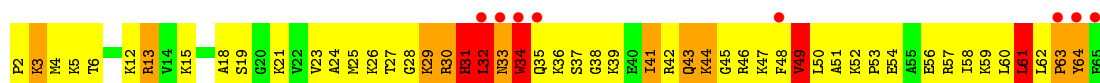
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 32: 50S RIBOSOMAL PROTEIN L34



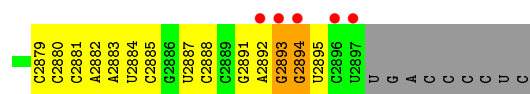
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



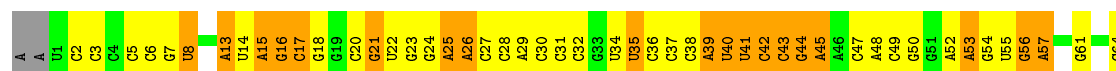
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

G1748	C1658	A1570	G1487	G1332	C1257	U1188	C1119	G1055	G974	G936	C840	G770
A1749	U1659	A1571	G1488	C1333	C1258	A1189	G1120	G1056	C975	U907	G843	G771
G1750	C1660	A1572	U1489	G1422	G1260	G1190	C1121	A1057	C976	C908	C844	G772
C1751	G1661	C1577	A1490	A1336	G1263	G1191	C1122	G1058	A983	U909	C845	U773
G1754	C1662	C1578	G1425	G1337	U1263	G1192	C1123	U1060	G889	A910	U847	A774
C1663	A1494	A1579	G1426	G1344	G1264	G1193	C1124	U1061	C992	A911	C848	G775
A1669	A1495	A1580	A1427	C1345	A1265	A1126	G1125	U1062	C993	C914	C849	G776
C1670	U1496	G1428	G1429	G1346	G1266	G1197	A1127	G1063	G994	C915	A849	A777
C1674	U1497	G1429	U1431	G1348	U1267	U1198	U1130	C1064	G995	C916	C850	G778
G1675	C1501	U1432	U1433	A1349	A1268	C1200	G1131	U1065	C996	C917	U851	U779
A1676	U1502	U1434	U1435	C1351	A1269	C1201	A1132	U1066	A996	A918	U852	G780
C1677	U1503	U1436	U1437	U1352	C1270	G1202	U1133	A1067	G997	C921	A781	A782
G1678	C1504	A1434	A1435	A1353	G1271	G1203	C1135	G1068	C998	U922	A783	A783
C1681	C1505	G1436	G1437	A1358	A1272	A1204	G1136	A1069	U999	C923	A784	A784
G1682	C1506	U1438	A1439	G1358	A1274	U1205	G1137	A1070	A1000	C924	U786	U786
G1683	C1509	G1441	G1442	A1359	A1278	C1208	G1138	G1072	C1006	C925	U787	C787
C1684	A1509A	U1443	U1444	A1360	G1279	A1210	C1140	A1073	A1009	A926	A788	A788
A1685	G1509B	G1445	G1446	G1361	G1280	U1211	U1141	G1074	A1010	U930	A789	A789
C1686	G1510	A1447	G1448	G1362	G1281	G1212	U1142	C1075	G1011	U931	C790	C790
U1687	C1511	C1448	A1449	C1363	U1282	A1213	A1143	G1076	U1012	G932	C865	G791
C1598	C1516	C1449	A1450	A1364	G1283	A1214	G1144	U1078	C1013	A933	C866	A793
C1599	G1517	C1450	G1451	A1365	A1284	G1215	C1145	G934	U1014	G934	C867	G794
A1600	U1518	G1452	G1453	G1366	G1285	G1216	C1146	C935	G1015	C935	U888	C795
G1601	G1519	G1454	G1455	G1368	A1286	C1217	C1147	A1084	G1016	C936	C796	C796
U1602	C1520	G1455	G1456	G1374	A1287	U1217	A1148	A1085	A1019	G940	A870	C797
C1607	A1528	G1456	G1457	C1375	U1288	A1220	C1149	A1086	A1020	U941	A871	A802
U1608	A1528A	A1457	A1458	C1376	U1289	C1221	C1150	G1087	A1021	U942	A872	A803
A1609	G1529	A1458	A1459	G1377	C1290	U1221A	G1151	A1088	U1022	U943	U804	A804
C1610	C1531	U1459	G1460	A1378	C1291	C1222	C1152	G1089	G1023	U944	G805	G805
A1616	U1534	G1461	A1462	A1379	U1292	G1223	C1153	C1091	G1024	A945	U807	U807
C1617	A1535	G1462	A1463	G1380	C1293	C1224	A1154	C1092	U1025	G946	G808	G808
A1618	C1536	G1463	G1464	G1381	U1294	G1225	C1155	G1093	G1026	G947	G809	G809
C1625	G1539	A1471	G1465	A1382	G1295	A1226	U1159	U1094	A1027	G948	U810	U810
G1626	U1540	U1472	G1466	G1383	G1296	G1227	G1160	A1095	A1028	G952	U811	U811
C1636	G1541	C1473	C1467	A1384	C1297	U1228	C1161	U1097	A1029	A953	C812	C812
A1637	A1542	C1474	C1468	G1385	U1300	G1229	U1165	A1098	A1032	G954	C813	U813
C1638	A1543	C1475	C1469	C1386	A1301	G1230	C1166	G1099	U1033	C955	C814	C814
U1639	A1544	C1476	C1470	C1387	A1302	G1231	U1167	G1100	G1034	G956	C815	C815
C1640	A1545	A1477	C1471	U1396	G1303	U1234	G1168	U1101	U1035	A957	C816	C816
A1641	C1547	U1478	C1472	C1403	U1313	G1235	G1169	C1102	G1036	U958	A819	A819
G1642	C1548	C1479	C1473	C1404	C1314	G1239	G1170	A1103	U1037	A959	U824	A824
C1643	C1549	C1479	C1474	U1405	G1315	U1240	G1171	C1104	C1038	C961	C825	C825
C1644	C1554	C1479	C1475	U1406	U1316	U1241	A1173	G1105	G1039	C962	U826	U826
G1645	A1554	C1479	C1476	C1407	A1317	A1242	A1174	G1106	C1040	U963	U827	U827
C1646	C1555	C1479	C1477	C1408	G1318	A1243	U1175	G1107	G1041	C964	U828	U828
A1647	U1554	C1479	C1478	C1409	G1319	G1244	G1176	U1108	A1045	C965	U829	U829
C1648	A1558	C1479	C1477	A1411	C1320	G1244	A1177	A1109	A1046	C966	A829	A829
G1649	G1559	C1479	C1478	A1412	A1321	G1248	C1178	G1110	G1047	C967	G830	G830
C1650	C1564	C1479	C1478	G1413	U1326	U1249	C1180	G1112	A1048	U968	G831	G831
G1651	C1565	C1479	C1478	G1414	U1327	U1252	C1181	G1113	C1049	A901	G832	G832
A1652	C1568	C1479	C1478	G1415	G1328	A1253	A1182	G1114	A1050	C970	U833	U833
G1654	G1569	C1479	C1478	G1416	U1329	G1256	G1183	C1115	G1051	C971	C834	C834
C1745A	C1746	C1747	C1748	G1417	C1330	G1256	G1187	A1054	A1054	A973	U905	U905
G1747A	C1747A	C1748A	C1749A	G1418	C1331	G1256	G1187	A1054	A1054	A973	U905	U905
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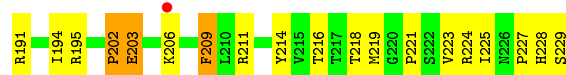
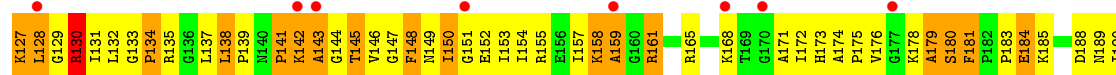
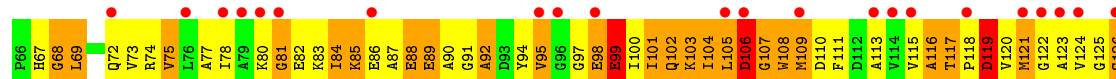
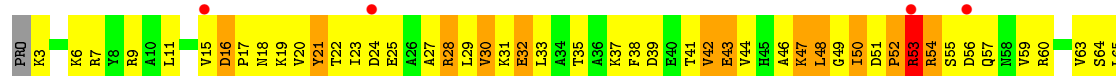




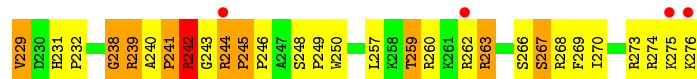
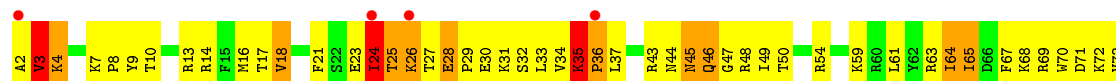
• Molecule 36: 5S RIBOSOMAL RNA



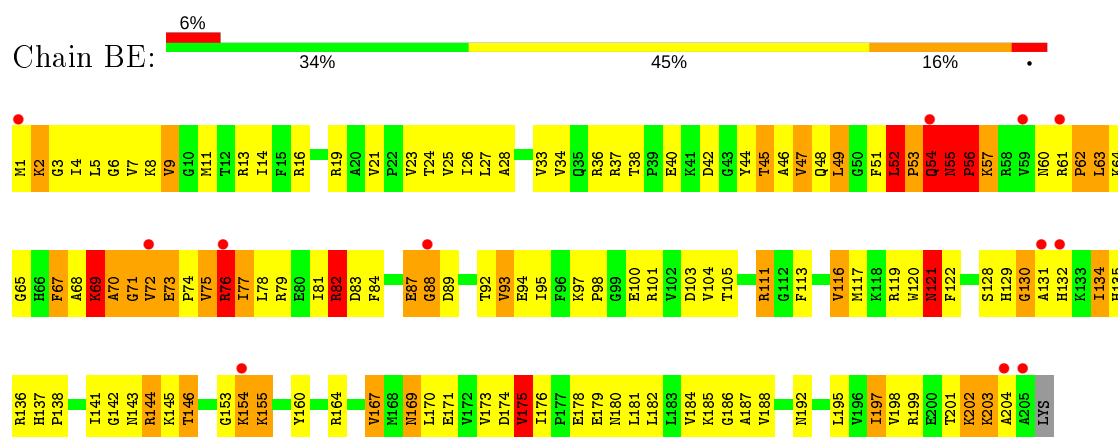
• Molecule 37: RIBOSOMAL PROTEIN L1



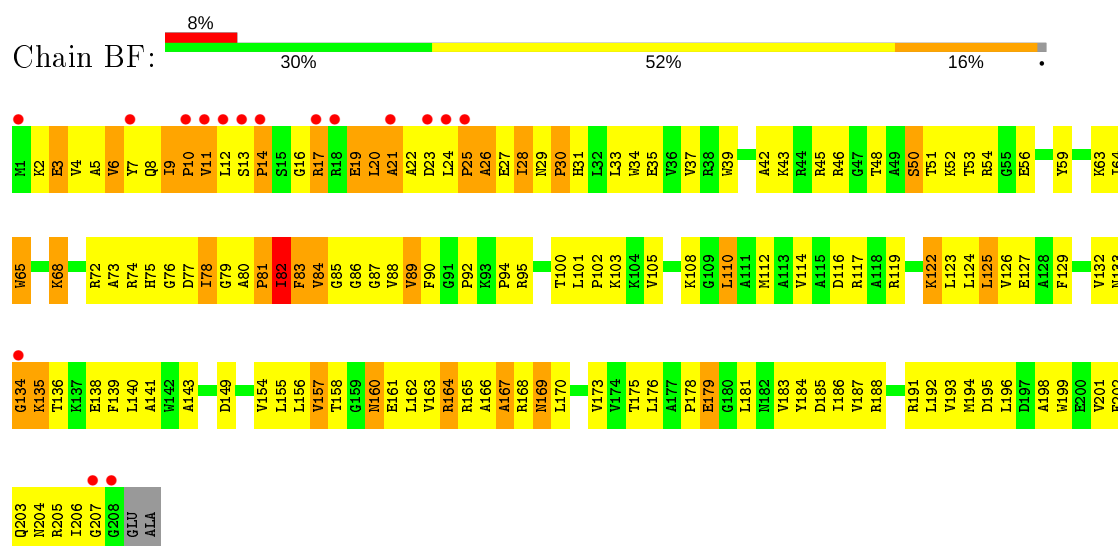
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



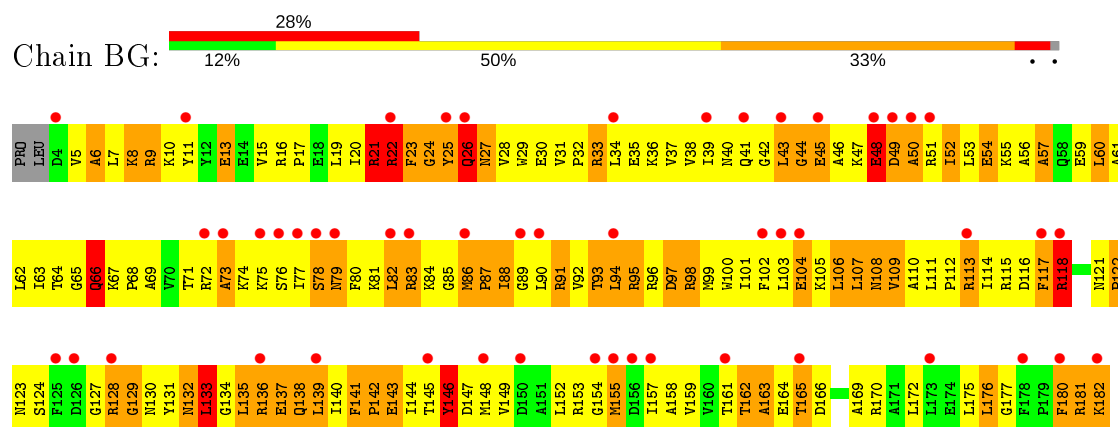
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L4

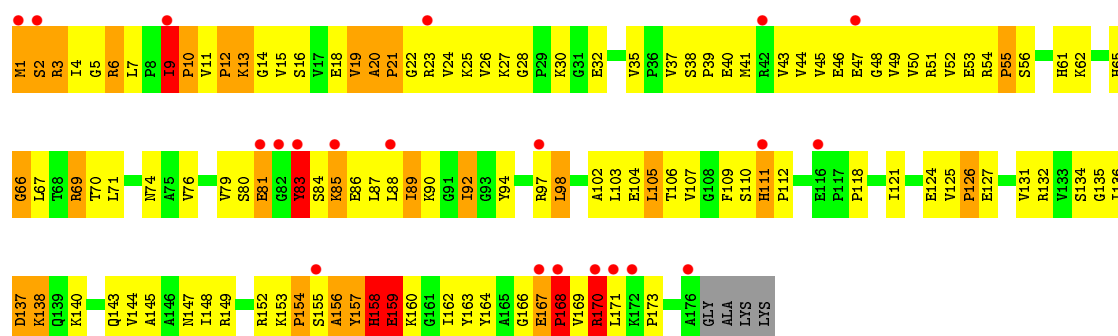


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

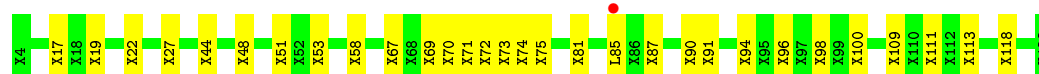
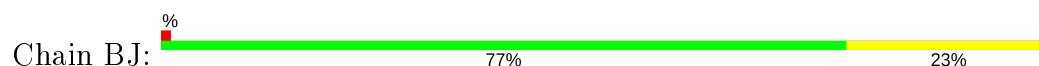


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

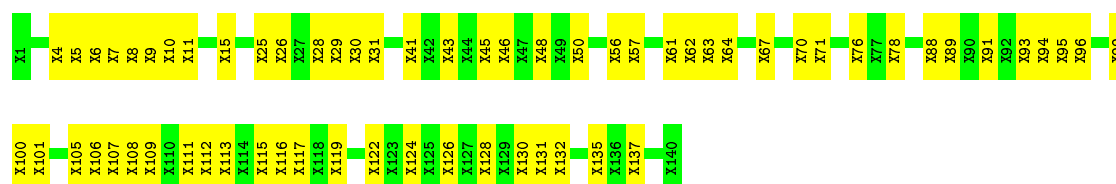




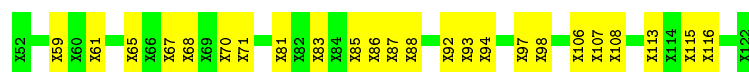
• Molecule 43: CHAIN J



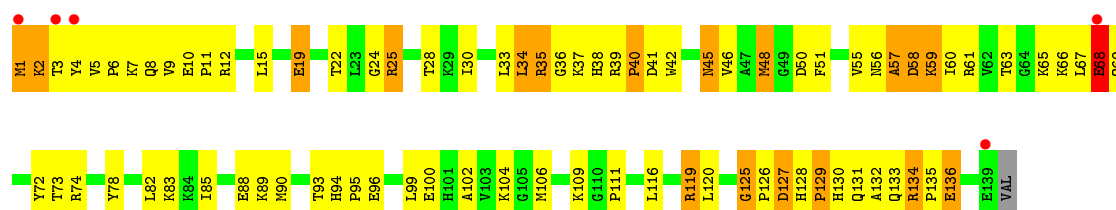
• Molecule 44: CHAIN K



• Molecule 45: CHAIN L

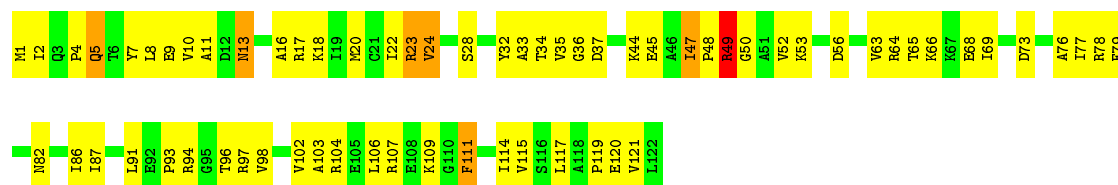


• Molecule 46: 50S RIBOSOMAL PROTEIN L13

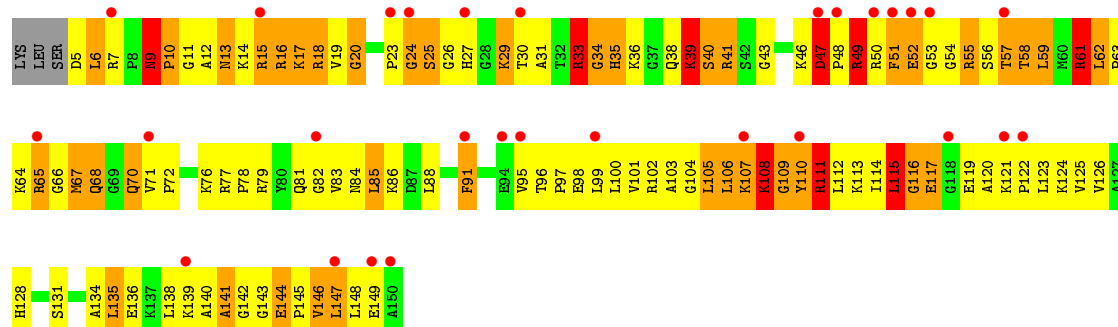
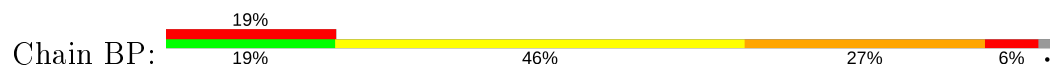


• Molecule 47: 50S RIBOSOMAL PROTEIN L14

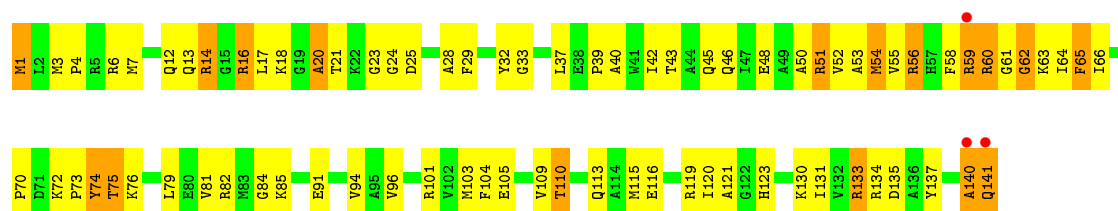




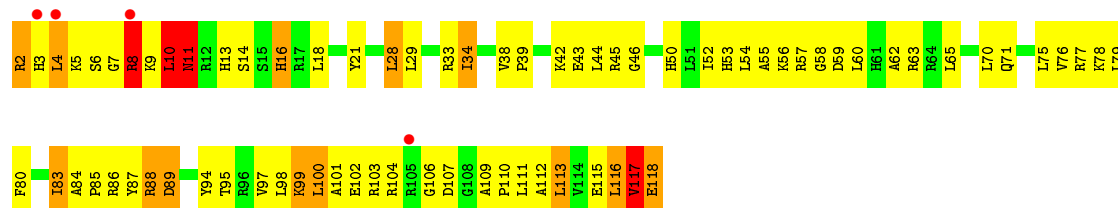
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



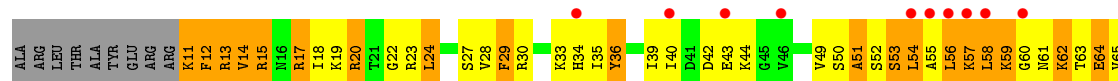
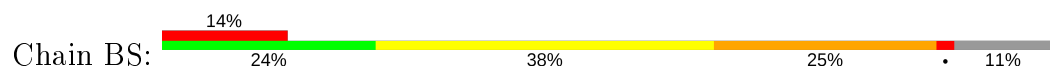
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

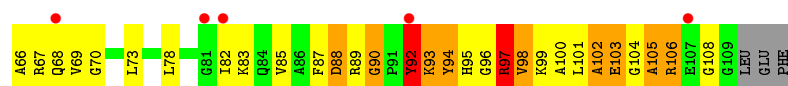


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

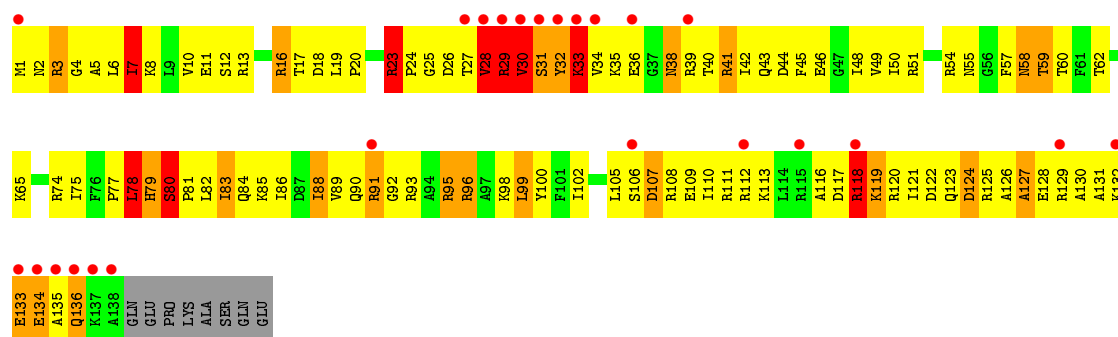


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

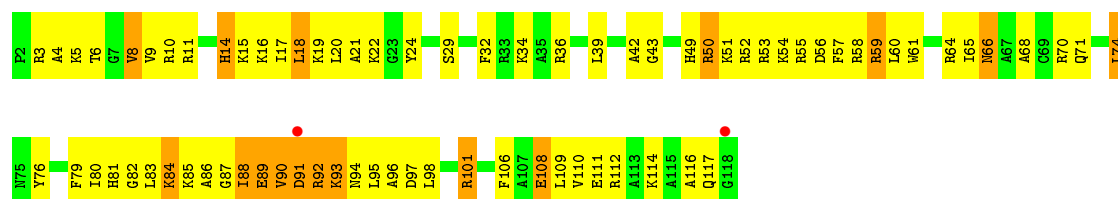




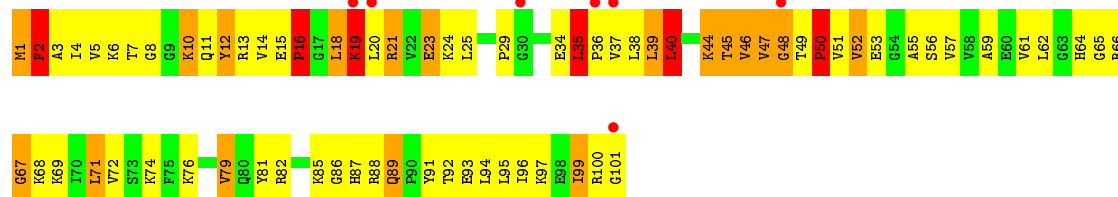
● Molecule 52: 50S RIBOSOMAL PROTEIN L19



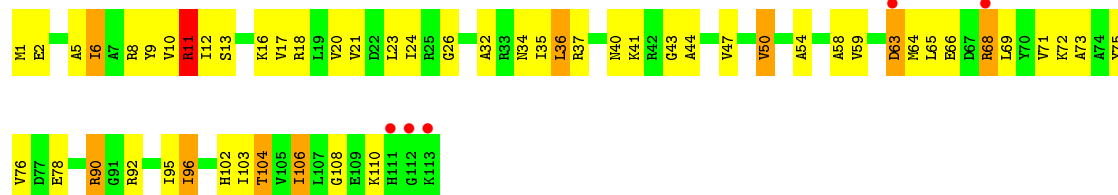
● Molecule 53: 50S RIBOSOMAL PROTEIN L20



● Molecule 54: 50S RIBOSOMAL PROTEIN L21

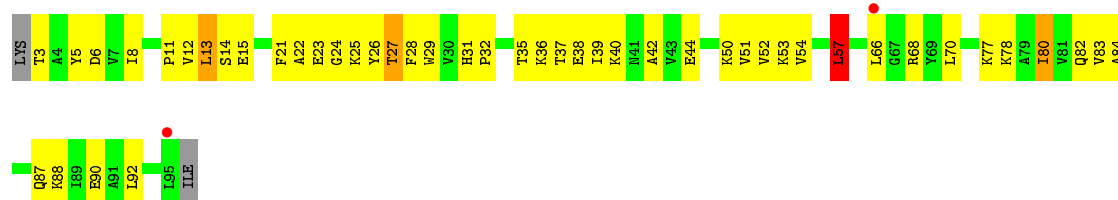


● Molecule 55: 50S RIBOSOMAL PROTEIN L22




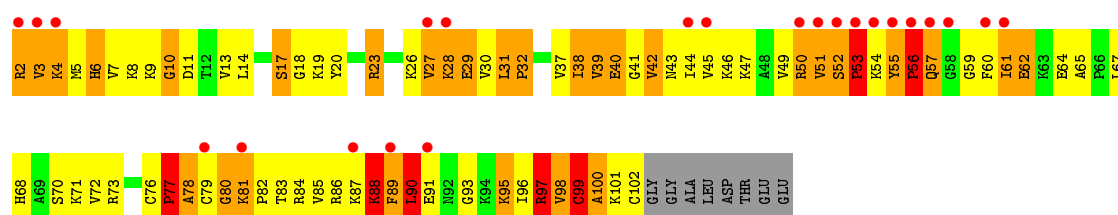
● Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX: 



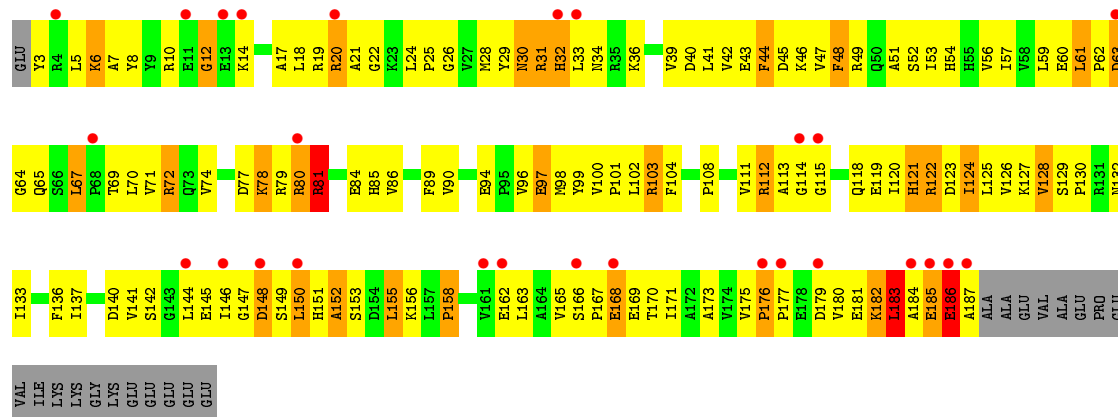
● Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY: 



● Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	202.90 Å 242.63 Å 309.32 Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	49.75 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-2.95) 100.0 (49.75-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.96 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.244 0.225 , 0.255	Depositor DCC
R_{free} test set	30895 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	153829	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, 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	0.41	0/36258	0.70	5/56589 (0.0%)
2	AB	0.26	0/1936	0.46	0/2611
3	AC	0.36	0/1637	0.58	0/2207
4	AD	0.36	0/1733	0.61	0/2318
5	AE	0.46	0/1163	0.67	0/1566
6	AF	0.36	0/856	0.63	0/1154
7	AG	0.36	0/1276	0.62	0/1709
8	AH	0.39	0/1136	0.69	0/1527
9	AI	0.36	0/1029	0.69	0/1379
10	AJ	0.40	0/808	0.69	0/1087
11	AK	0.39	0/900	0.68	0/1213
12	AL	0.42	0/987	0.73	1/1322 (0.1%)
13	AM	0.32	0/948	0.60	0/1272
14	AN	0.41	0/501	0.77	0/664
15	AO	0.37	0/745	0.62	0/992
16	AP	0.40	0/717	0.71	0/965
17	AQ	0.40	0/837	0.69	0/1119
18	AR	0.38	0/579	0.60	0/768
19	AS	0.37	0/706	0.64	0/950
20	AT	0.39	0/765	0.76	0/1007
21	AU	0.43	0/213	0.62	0/279
22	AV	0.84	2/1809 (0.1%)	1.27	7/2819 (0.2%)
23	AX	1.26	2/210 (1.0%)	1.37	2/325 (0.6%)
24	AY	0.33	0/5477	0.61	3/7415 (0.0%)
25	B0	0.29	0/671	0.43	0/892
26	B1	0.37	0/739	0.58	0/983
27	B2	10.54	1/600 (0.2%)	0.42	0/793
28	B3	0.32	0/473	0.50	0/636
29	B4	0.29	0/594	0.45	0/795
30	B5	0.40	0/473	0.70	0/639
31	B6	0.48	0/440	0.80	0/586
32	B7	0.44	0/427	0.71	0/561

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.56	0/516	0.87	1/681 (0.1%)
34	B9	0.45	0/310	0.72	0/407
35	BA	0.46	1/69972 (0.0%)	0.72	25/109230 (0.0%)
36	BB	0.37	0/2853	0.72	1/4451 (0.0%)
37	BC	0.32	0/1766	0.62	0/2380
38	BD	0.47	0/2195	0.82	1/2955 (0.0%)
39	BE	0.42	0/1597	0.71	0/2155
40	BF	0.39	0/1659	0.66	0/2246
41	BG	0.45	0/1483	0.80	1/1994 (0.1%)
42	BH	0.40	0/1371	0.67	0/1853
43	BJ	0.20	0/7	0.87	0/8
46	BN	0.46	0/1132	0.76	0/1527
47	BO	0.44	0/943	0.71	0/1269
48	BP	0.45	0/1131	0.86	4/1504 (0.3%)
49	BQ	0.41	0/1143	0.65	0/1527
50	BR	0.43	0/974	0.75	0/1302
51	BS	0.39	0/779	0.66	0/1038
52	BT	0.42	0/1156	0.66	0/1544
53	BU	0.48	0/975	0.70	0/1297
54	BV	0.40	0/790	0.72	0/1057
55	BW	0.42	0/907	0.71	0/1216
56	BX	0.47	0/740	0.69	1/995 (0.1%)
57	BY	0.52	0/789	0.87	0/1053
58	BZ	0.34	0/1500	0.63	0/2037
All	All	0.77	6/164331 (0.0%)	0.71	52/244868 (0.0%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B2	72	ALA	C-OXT	258.07	6.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1453	U	O3'-P	-17.05	1.40	1.61
22	AV	37	A	N3-C4	7.56	1.39	1.34
22	AV	37	A	C6-N1	7.26	1.40	1.35
23	AX	11	A	N9-C4	5.43	1.41	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	2208	A	P-O3'-C3'	9.92	131.60	119.70
22	AV	37	A	N1-C2-N3	-9.87	124.36	129.30
22	AV	74	C	O4'-C1'-N1	8.40	114.92	108.20
22	AV	37	A	N9-C4-C5	-7.54	102.79	105.80
22	AV	37	A	N1-C6-N6	6.87	122.72	118.60

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(H)	G	Sidechain
24	AY	499	ARG	Sidechain
35	BA	271(H)	G	Sidechain
35	BA	271(Q)	G	Sidechain
35	BA	271(Y)	U	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32391	0	16349	1996	0
2	AB	1901	0	1947	323	1
3	AC	1613	0	1677	223	28
4	AD	1703	0	1765	125	0
5	AE	1147	0	1207	56	0
6	AF	843	0	857	53	0
7	AG	1257	0	1296	138	0
8	AH	1116	0	1177	63	0
9	AI	1010	0	1037	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	114	0
11	AK	885	0	904	56	0
12	AL	971	0	1057	112	0
13	AM	938	0	995	124	0
14	AN	492	0	529	68	0
15	AO	734	0	771	49	0
16	AP	701	0	720	58	0
17	AQ	824	0	891	47	0
18	AR	574	0	644	26	0
19	AS	692	0	714	109	0
20	AT	763	0	861	71	11
21	AU	209	0	221	12	0
22	AV	1619	0	823	58	0
23	AX	188	0	98	7	0
24	AY	5376	0	5433	565	0
25	B0	662	0	688	160	0
26	B1	732	0	808	114	0
27	B2	598	0	651	125	11
28	B3	468	0	523	66	0
29	B4	581	0	577	214	0
30	B5	459	0	478	75	0
31	B6	433	0	461	128	0
32	B7	419	0	467	29	0
33	B8	508	0	576	112	0
34	B9	307	0	335	31	0
35	BA	62476	0	31499	3288	28
36	BB	2551	0	1295	107	0
37	BC	1735	0	1790	277	1
38	BD	2145	0	2234	255	0
39	BE	1564	0	1629	233	0
40	BF	1624	0	1677	220	0
41	BG	1459	0	1516	395	0
42	BH	1345	0	1430	187	0
43	BJ	654	0	156	22	0
44	BK	701	0	168	46	0
45	BL	356	0	86	20	0
46	BN	1105	0	1180	111	0
47	BO	933	0	996	67	0
48	BP	1114	0	1186	302	0
49	BQ	1122	0	1179	111	0
50	BR	960	0	1021	104	0
51	BS	771	0	832	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	BT	1142	0	1200	229	0
53	BU	958	0	1015	122	0
54	BV	779	0	852	147	0
55	BW	896	0	953	56	0
56	BX	726	0	778	47	0
57	BY	776	0	870	164	0
58	BZ	1468	0	1492	216	0
59	AA	198	0	0	0	0
59	AY	1	0	0	0	0
59	B0	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	320	0	0	0	0
59	BC	1	0	0	0	0
59	BU	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
61	AY	32	0	14	11	0
62	AY	2	0	0	2	0
All	All	153829	0	105425	11650	40

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

The worst 5 of 11650 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B5:46:CYS:SG	30:B5:47:PRO:HD2	1.41	1.57
29:B4:12:ALA:H	29:B4:24:THR:CG2	1.16	1.56
9:AI:19:LEU:HA	9:AI:61:ALA:CB	1.39	1.53
52:BT:80:SER:HB3	52:BT:81:PRO:CD	1.40	1.51
9:AI:18:PHE:C	9:AI:61:ALA:HB1	1.27	1.50

The worst 5 of 40 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:100:ILE:CG1	27:B2:43:GLN:CD[2_554]	0.34	1.86
20:AT:100:ILE:CD1	27:B2:43:GLN:NE2[2_554]	0.69	1.51
3:AC:79:ARG:CD	35:BA:2139:C:C4[2_555]	0.83	1.37

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	163 (70%)	44 (19%)	26 (11%)	0	1
3	AC	205/239 (86%)	145 (71%)	32 (16%)	28 (14%)	0	1
4	AD	206/209 (99%)	160 (78%)	35 (17%)	11 (5%)	2	9
5	AE	149/162 (92%)	134 (90%)	12 (8%)	3 (2%)	7	30
6	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	1	7
7	AG	153/156 (98%)	113 (74%)	26 (17%)	14 (9%)	1	2
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	22	56
9	AI	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	3
10	AJ	97/105 (92%)	73 (75%)	15 (16%)	9 (9%)	0	2
11	AK	117/129 (91%)	95 (81%)	19 (16%)	3 (3%)	5	24
12	AL	123/132 (93%)	101 (82%)	11 (9%)	11 (9%)	1	3
13	AM	117/126 (93%)	74 (63%)	32 (27%)	11 (9%)	0	2
14	AN	58/61 (95%)	44 (76%)	7 (12%)	7 (12%)	0	1
15	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	43
16	AP	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	6	26
17	AQ	98/105 (93%)	86 (88%)	10 (10%)	2 (2%)	7	30
18	AR	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	4	21
19	AS	86/93 (92%)	53 (62%)	21 (24%)	12 (14%)	0	1
20	AT	97/106 (92%)	79 (81%)	10 (10%)	8 (8%)	1	3

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	BZ	183/205 (89%)	131 (72%)	30 (16%)	22 (12%)	0	1
All	All	6506/6949 (94%)	4803 (74%)	1007 (16%)	696 (11%)	0	1

5 of 696 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	157 (78%)	45 (22%)	1	3
3	AC	160/188 (85%)	129 (81%)	31 (19%)	1	6
4	AD	180/181 (99%)	155 (86%)	25 (14%)	3	14
5	AE	115/123 (94%)	109 (95%)	6 (5%)	23	56
6	AF	90/90 (100%)	83 (92%)	7 (8%)	12	38
7	AG	126/127 (99%)	108 (86%)	18 (14%)	3	13
8	AH	119/119 (100%)	103 (87%)	16 (13%)	4	15
9	AI	98/99 (99%)	85 (87%)	13 (13%)	4	15
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	16	45
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	45
12	AL	104/109 (95%)	90 (86%)	14 (14%)	4	15
13	AM	94/101 (93%)	84 (89%)	10 (11%)	6	24
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	19
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	26
16	AP	72/74 (97%)	68 (94%)	4 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	53	80
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	27
19	AS	74/80 (92%)	68 (92%)	6 (8%)	11	36
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	24
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	55
24	AY	579/582 (100%)	516 (89%)	63 (11%)	6	23
25	B0	66/66 (100%)	45 (68%)	21 (32%)	0	1
26	B1	78/82 (95%)	60 (77%)	18 (23%)	1	3
27	B2	66/66 (100%)	42 (64%)	24 (36%)	0	0
28	B3	51/52 (98%)	44 (86%)	7 (14%)	3	15
29	B4	63/63 (100%)	48 (76%)	15 (24%)	0	2
30	B5	51/51 (100%)	42 (82%)	9 (18%)	2	8
31	B6	49/51 (96%)	37 (76%)	12 (24%)	0	2
32	B7	41/41 (100%)	39 (95%)	2 (5%)	25	58
33	B8	53/54 (98%)	42 (79%)	11 (21%)	1	4
34	B9	34/34 (100%)	31 (91%)	3 (9%)	10	33
37	BC	179/180 (99%)	160 (89%)	19 (11%)	6	24
38	BD	217/217 (100%)	185 (85%)	32 (15%)	3	12
39	BE	165/166 (99%)	133 (81%)	32 (19%)	1	6
40	BF	165/166 (99%)	146 (88%)	19 (12%)	5	21
41	BG	153/155 (99%)	123 (80%)	30 (20%)	1	6
42	BH	146/148 (99%)	131 (90%)	15 (10%)	7	25
43	BJ	1/1 (100%)	1 (100%)	0	100	100
46	BN	117/119 (98%)	103 (88%)	14 (12%)	5	19
47	BO	100/100 (100%)	93 (93%)	7 (7%)	15	43
48	BP	112/115 (97%)	84 (75%)	28 (25%)	0	2
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	15
50	BR	100/100 (100%)	82 (82%)	18 (18%)	1	7
51	BS	77/87 (88%)	62 (80%)	15 (20%)	1	6
52	BT	120/127 (94%)	94 (78%)	26 (22%)	1	4
53	BU	92/93 (99%)	80 (87%)	12 (13%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BV	82/82 (100%)	65 (79%)	17 (21%)	1	4
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4	16
56	BX	74/77 (96%)	68 (92%)	6 (8%)	11	36
57	BY	84/90 (93%)	65 (77%)	19 (23%)	1	3
58	BZ	162/178 (91%)	138 (85%)	24 (15%)	3	12
All	All	5469/5656 (97%)	4686 (86%)	783 (14%)	3	13

5 of 783 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	B2	44	LEU
37	BC	138	LEU
55	BW	21	VAL
28	B3	8	LEU
31	B6	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
25	B0	17	GLN
37	BC	189	ASN
53	BU	94	ASN
25	B0	70	GLN
28	B3	46	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1519 (99%)	320 (21%)	51 (3%)
22	AV	75/76 (98%)	24 (32%)	2 (2%)
23	AX	8/9 (88%)	3 (37%)	0
35	BA	2897/2915 (99%)	665 (22%)	60 (2%)
36	BB	118/122 (96%)	26 (22%)	2 (1%)
All	All	4603/4641 (99%)	1038 (22%)	115 (2%)

5 of 1038 RNA backbone outliers are listed below:

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

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AV	16	C
35	BA	627	A
35	BA	2439	A
35	BA	49	A
35	BA	331	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 527 ligands modelled in this entry, 526 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	GCP	AY	701	59	26,34,34	3.56	9 (34%)	31,54,54	1.69	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GCP	AY	701	59	-	9/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GCP	C5-C6	-11.22	1.33	1.52
61	AY	701	GCP	C4-N9	-10.76	1.33	1.47
61	AY	701	GCP	C6-N1	4.23	1.40	1.33
61	AY	701	GCP	C8-N9	-3.54	1.33	1.45
61	AY	701	GCP	PB-O2B	-3.45	1.48	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GCP	C4-C5-N7	4.07	107.85	102.46
61	AY	701	GCP	PA-O3A-PB	-3.97	119.98	132.56
61	AY	701	GCP	O1G-PG-C3B	-3.35	104.02	111.24
61	AY	701	GCP	O2B-PB-O1B	2.86	119.61	110.07
61	AY	701	GCP	C4'-O4'-C1'	-2.50	103.96	109.47

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	GCP	PG-C3B-PB-O2B
61	AY	701	GCP	PG-C3B-PB-O3A
61	AY	701	GCP	O4'-C1'-N9-C4
61	AY	701	GCP	C2'-C1'-N9-C4
61	AY	701	GCP	O4'-C4'-C5'-O5'

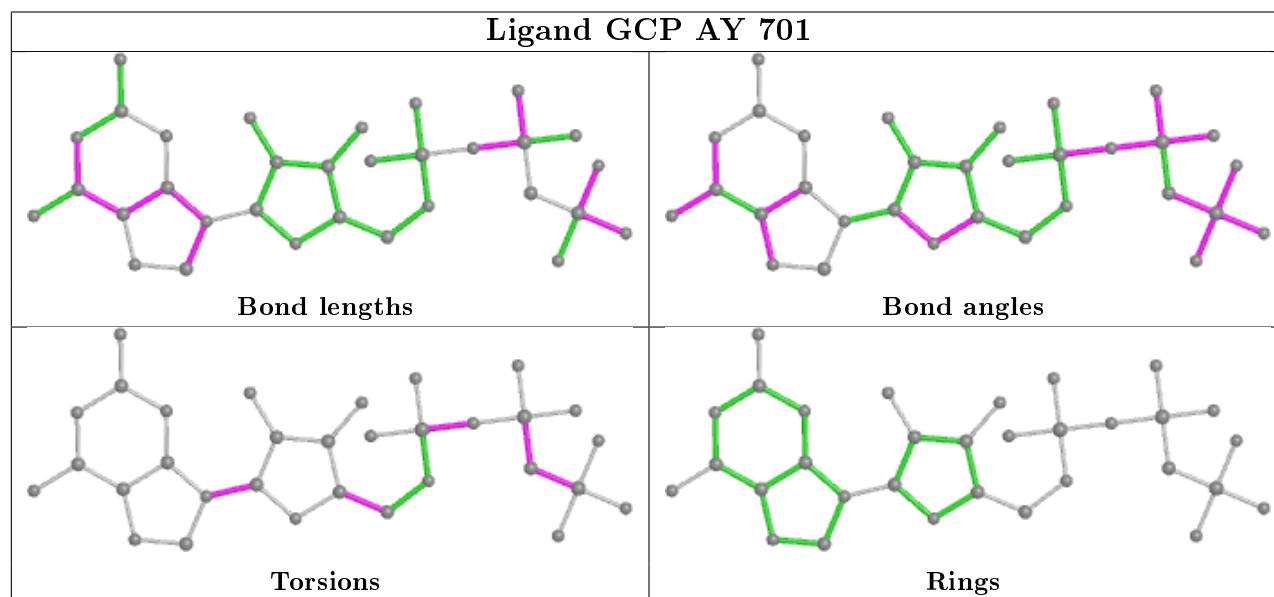
There are no ring outliers.

1 monomer is involved in 11 short contacts:

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

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	BA	3
1	AA	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1507/1519 (99%)	0.18	52 (3%) 44 29	24, 47, 125, 239	0
2	AB	235/256 (91%)	0.47	20 (8%) 10 6	34, 61, 112, 122	0
3	AC	207/239 (86%)	0.33	10 (4%) 30 19	30, 54, 84, 102	0
4	AD	208/209 (99%)	0.14	5 (2%) 59 42	36, 57, 80, 89	0
5	AE	151/162 (93%)	-0.09	2 (1%) 77 61	29, 40, 59, 81	0
6	AF	101/101 (100%)	0.23	3 (2%) 50 34	41, 68, 86, 99	0
7	AG	155/156 (99%)	0.47	10 (6%) 18 11	44, 67, 112, 126	0
8	AH	138/138 (100%)	-0.12	0 100 100	32, 45, 63, 74	0
9	AI	127/128 (99%)	0.40	10 (7%) 12 7	33, 61, 81, 90	0
10	AJ	99/105 (94%)	0.50	9 (9%) 9 5	38, 58, 100, 104	0
11	AK	119/129 (92%)	0.27	4 (3%) 45 29	26, 53, 76, 94	0
12	AL	125/132 (94%)	0.28	7 (5%) 24 15	27, 45, 64, 96	0
13	AM	119/126 (94%)	1.02	19 (15%) 1 1	46, 83, 107, 117	0
14	AN	60/61 (98%)	0.40	7 (11%) 4 2	35, 48, 83, 91	0
15	AO	88/89 (98%)	0.19	2 (2%) 60 43	33, 51, 75, 85	0
16	AP	84/88 (95%)	0.16	1 (1%) 79 63	37, 47, 70, 95	0
17	AQ	100/105 (95%)	-0.08	0 100 100	27, 44, 62, 65	0
18	AR	70/88 (79%)	0.26	2 (2%) 51 35	36, 57, 94, 95	0
19	AS	88/93 (94%)	0.83	8 (9%) 9 5	59, 82, 103, 109	0
20	AT	99/106 (93%)	0.11	3 (3%) 50 34	33, 45, 68, 73	0
21	AU	25/27 (92%)	1.02	2 (8%) 12 7	43, 59, 79, 81	0
22	AV	76/76 (100%)	0.41	5 (6%) 18 10	33, 74, 111, 145	0
23	AX	9/9 (100%)	1.19	3 (33%) 0 0	28, 51, 122, 134	0
24	AY	687/691 (99%)	0.53	62 (9%) 9 5	39, 67, 119, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	84/84 (100%)	1.78	15 (17%) 1 1	43, 56, 121, 140	0
26	B1	94/97 (96%)	0.48	6 (6%) 19 11	26, 47, 76, 88	0
27	B2	71/71 (100%)	0.62	7 (9%) 7 4	41, 57, 88, 112	0
28	B3	60/60 (100%)	0.58	2 (3%) 46 30	35, 56, 75, 100	0
29	B4	71/71 (100%)	3.83	61 (85%) 0 0	129, 151, 159, 159	0
30	B5	59/59 (100%)	0.60	7 (11%) 4 2	20, 42, 109, 122	0
31	B6	50/53 (94%)	1.51	11 (22%) 0 0	41, 72, 91, 98	0
32	B7	48/48 (100%)	0.00	1 (2%) 63 46	18, 30, 60, 86	0
33	B8	64/64 (100%)	0.63	8 (12%) 3 2	32, 49, 70, 87	0
34	B9	37/37 (100%)	0.66	2 (5%) 25 16	40, 52, 62, 76	0
35	BA	2901/2915 (99%)	0.19	107 (3%) 41 27	18, 42, 116, 244	0
36	BB	119/122 (97%)	0.20	1 (0%) 86 73	42, 88, 115, 130	0
37	BC	227/228 (99%)	0.81	35 (15%) 2 1	25, 78, 124, 135	0
38	BD	275/275 (100%)	-0.00	8 (2%) 51 35	18, 32, 58, 93	0
39	BE	205/206 (99%)	0.34	12 (5%) 22 13	23, 42, 78, 86	0
40	BF	208/210 (99%)	0.42	16 (7%) 13 7	17, 52, 104, 121	0
41	BG	179/181 (98%)	1.47	51 (28%) 0 0	94, 122, 138, 144	0
42	BH	176/180 (97%)	0.90	21 (11%) 4 2	52, 75, 97, 108	0
43	BJ	1/130 (0%)	2.80	1 (100%) 0 0	121, 121, 121, 121	0
44	BK	0/140	-	-	-	-
45	BL	0/71	-	-	-	-
46	BN	139/140 (99%)	0.13	5 (3%) 42 28	31, 45, 72, 93	0
47	BO	122/122 (100%)	-0.26	0 100 100	25, 39, 54, 63	0
48	BP	146/149 (97%)	1.24	29 (19%) 1 0	34, 67, 96, 118	0
49	BQ	141/141 (100%)	0.21	3 (2%) 63 46	33, 49, 75, 115	0
50	BR	117/117 (100%)	0.12	4 (3%) 45 29	23, 40, 59, 67	0
51	BS	99/111 (89%)	1.00	15 (15%) 2 1	68, 91, 113, 122	0
52	BT	138/146 (94%)	0.95	24 (17%) 1 1	32, 53, 122, 144	0
53	BU	117/117 (100%)	-0.05	2 (1%) 70 53	28, 42, 69, 85	0
54	BV	101/101 (100%)	0.41	7 (6%) 16 10	25, 62, 83, 87	0
55	BW	113/113 (100%)	0.14	5 (4%) 34 21	26, 38, 69, 104	0
56	BX	93/95 (97%)	-0.15	2 (2%) 62 45	30, 41, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	101/109 (92%)	1.28	23 (22%) 0 0	37, 61, 118, 127	0
58	BZ	185/205 (90%)	0.85	27 (14%) 2 1	25, 81, 96, 109	0
All	All	11218/11801 (95%)	0.38	764 (6%) 17 10	17, 52, 116, 244	0

The worst 5 of 764 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(E)	G	16.7
24	AY	48	GLY	16.3
39	BE	205	ALA	15.5
25	B0	3	HIS	15.2
49	BQ	141	GLN	13.8

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	AA	1781	1/1	0.34	0.27	54,54,54,54	0
59	MG	BA	3247	1/1	0.37	0.36	49,49,49,49	0
59	MG	BA	3179	1/1	0.38	0.43	87,87,87,87	0
59	MG	BA	3194	1/1	0.38	0.35	74,74,74,74	0
59	MG	BA	3215	1/1	0.39	0.60	81,81,81,81	0
59	MG	BA	3252	1/1	0.39	0.60	50,50,50,50	0
59	MG	AA	1780	1/1	0.40	0.18	54,54,54,54	0
59	MG	BA	3281	1/1	0.41	0.46	79,79,79,79	0
59	MG	BA	3204	1/1	0.42	0.39	60,60,60,60	0
59	MG	AA	1712	1/1	0.43	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1740	1/1	0.44	0.75	79,79,79,79	0
59	MG	AA	1777	1/1	0.49	0.31	40,40,40,40	0
59	MG	AA	1628	1/1	0.53	0.42	64,64,64,64	0
59	MG	BA	3174	1/1	0.54	0.64	97,97,97,97	0
59	MG	BA	3019	1/1	0.55	0.71	77,77,77,77	0
59	MG	BA	3282	1/1	0.56	0.30	67,67,67,67	0
59	MG	BA	3030	1/1	0.56	1.26	86,86,86,86	0
59	MG	AA	1754	1/1	0.57	0.40	75,75,75,75	0
59	MG	BA	3279	1/1	0.59	0.44	63,63,63,63	0
59	MG	BA	3268	1/1	0.59	0.35	85,85,85,85	0
59	MG	AA	1762	1/1	0.59	0.41	100,100,100,100	0
59	MG	AA	1773	1/1	0.60	0.56	60,60,60,60	0
59	MG	BA	3263	1/1	0.63	0.33	63,63,63,63	0
59	MG	BA	3012	1/1	0.63	0.44	79,79,79,79	0
59	MG	AA	1779	1/1	0.63	0.53	81,81,81,81	0
59	MG	AA	1677	1/1	0.64	0.38	77,77,77,77	0
59	MG	AA	1632	1/1	0.64	0.25	56,56,56,56	0
59	MG	AA	1716	1/1	0.64	0.37	71,71,71,71	0
59	MG	AA	1760	1/1	0.65	0.67	70,70,70,70	0
59	MG	AA	1753	1/1	0.65	0.53	89,89,89,89	0
59	MG	BA	3136	1/1	0.65	0.30	90,90,90,90	0
59	MG	BA	3275	1/1	0.65	0.38	52,52,52,52	0
59	MG	BC	301	1/1	0.66	0.21	115,115,115,115	0
59	MG	AA	1639	1/1	0.66	0.30	55,55,55,55	0
59	MG	BA	3028	1/1	0.66	0.40	60,60,60,60	0
59	MG	AA	1709	1/1	0.66	0.20	41,41,41,41	0
59	MG	BA	3190	1/1	0.67	0.38	81,81,81,81	0
59	MG	BA	3230	1/1	0.67	0.35	40,40,40,40	0
59	MG	BA	3269	1/1	0.67	0.16	48,48,48,48	0
59	MG	BA	3304	1/1	0.67	0.39	32,32,32,32	0
59	MG	AA	1699	1/1	0.68	0.25	33,33,33,33	0
59	MG	AA	1637	1/1	0.68	0.58	65,65,65,65	0
59	MG	BA	3240	1/1	0.69	0.33	60,60,60,60	0
59	MG	BA	3032	1/1	0.69	0.25	73,73,73,73	0
59	MG	AA	1714	1/1	0.69	0.53	44,44,44,44	0
59	MG	AA	1644	1/1	0.69	0.20	60,60,60,60	0
59	MG	BA	3142	1/1	0.70	0.20	48,48,48,48	0
59	MG	BA	3265	1/1	0.71	0.55	65,65,65,65	0
59	MG	AA	1743	1/1	0.71	0.39	38,38,38,38	0
59	MG	BA	3147	1/1	0.72	0.55	119,119,119,119	0
59	MG	BA	3284	1/1	0.72	0.42	61,61,61,61	0
59	MG	BA	3016	1/1	0.72	0.62	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3155	1/1	0.72	0.29	60,60,60,60	0
59	MG	AA	1703	1/1	0.72	0.42	81,81,81,81	0
59	MG	BA	3242	1/1	0.73	0.44	78,78,78,78	0
59	MG	AA	1741	1/1	0.73	0.46	58,58,58,58	0
59	MG	AA	1635	1/1	0.73	0.21	65,65,65,65	0
59	MG	AA	1607	1/1	0.74	0.34	97,97,97,97	0
59	MG	AA	1724	1/1	0.74	0.41	48,48,48,48	0
59	MG	BA	3085	1/1	0.74	0.22	25,25,25,25	0
59	MG	AA	1755	1/1	0.74	0.35	60,60,60,60	0
59	MG	BA	3025	1/1	0.74	0.32	42,42,42,42	0
59	MG	BA	3125	1/1	0.74	0.38	122,122,122,122	0
59	MG	BA	3128	1/1	0.74	0.26	38,38,38,38	0
59	MG	AA	1771	1/1	0.74	0.23	40,40,40,40	0
59	MG	AA	1647	1/1	0.75	0.45	79,79,79,79	0
59	MG	AA	1674	1/1	0.75	0.44	74,74,74,74	0
59	MG	AA	1715	1/1	0.75	0.24	42,42,42,42	0
59	MG	AA	1666	1/1	0.76	0.53	83,83,83,83	0
59	MG	BA	3026	1/1	0.76	0.36	67,67,67,67	0
59	MG	AA	1606	1/1	0.76	0.53	60,60,60,60	0
59	MG	BA	3225	1/1	0.76	0.15	44,44,44,44	0
59	MG	AA	1766	1/1	0.76	0.29	58,58,58,58	0
59	MG	BA	3239	1/1	0.76	0.27	87,87,87,87	0
59	MG	AA	1790	1/1	0.76	0.25	57,57,57,57	0
59	MG	BA	3264	1/1	0.76	0.56	77,77,77,77	0
59	MG	AA	1636	1/1	0.77	0.51	60,60,60,60	0
59	MG	AA	1650	1/1	0.77	0.27	36,36,36,36	0
59	MG	AA	1638	1/1	0.77	0.17	38,38,38,38	0
59	MG	BA	3218	1/1	0.77	0.23	58,58,58,58	0
59	MG	BA	3276	1/1	0.77	0.51	46,46,46,46	0
59	MG	BA	3258	1/1	0.77	0.32	51,51,51,51	0
59	MG	AA	1695	1/1	0.77	0.34	50,50,50,50	0
59	MG	AA	1728	1/1	0.77	0.32	47,47,47,47	0
59	MG	BA	3064	1/1	0.77	0.12	62,62,62,62	0
59	MG	BA	3267	1/1	0.77	0.34	62,62,62,62	0
59	MG	AA	1711	1/1	0.77	0.19	34,34,34,34	0
59	MG	BA	3009	1/1	0.77	0.72	77,77,77,77	0
59	MG	BA	3209	1/1	0.77	0.63	81,81,81,81	0
59	MG	AA	1758	1/1	0.77	0.39	75,75,75,75	0
59	MG	AA	1796	1/1	0.78	0.28	44,44,44,44	0
59	MG	BA	3201	1/1	0.78	0.41	64,64,64,64	0
59	MG	BA	3067	1/1	0.79	0.28	71,71,71,71	0
59	MG	AA	1640	1/1	0.79	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3175	1/1	0.79	0.18	62,62,62,62	0
59	MG	BA	3315	1/1	0.79	0.35	52,52,52,52	0
59	MG	BA	3197	1/1	0.79	0.56	58,58,58,58	0
59	MG	BA	3040	1/1	0.79	0.42	71,71,71,71	0
59	MG	BA	3160	1/1	0.79	0.17	55,55,55,55	0
59	MG	BA	3280	1/1	0.79	0.24	87,87,87,87	0
59	MG	BA	3292	1/1	0.79	0.36	64,64,64,64	0
59	MG	AA	1745	1/1	0.80	0.45	66,66,66,66	0
59	MG	AA	1621	1/1	0.80	0.40	68,68,68,68	0
59	MG	AA	1744	1/1	0.80	0.21	90,90,90,90	0
59	MG	BA	3042	1/1	0.80	0.37	45,45,45,45	0
59	MG	AA	1611	1/1	0.80	0.34	75,75,75,75	0
59	MG	AA	1643	1/1	0.80	0.23	38,38,38,38	0
59	MG	AA	1764	1/1	0.80	0.27	61,61,61,61	0
59	MG	BA	3305	1/1	0.80	0.10	52,52,52,52	0
59	MG	BA	3295	1/1	0.80	0.30	32,32,32,32	0
59	MG	AA	1601	1/1	0.80	0.23	97,97,97,97	0
59	MG	AA	1797	1/1	0.80	0.19	58,58,58,58	0
59	MG	BA	3260	1/1	0.80	0.46	72,72,72,72	0
59	MG	BA	3168	1/1	0.80	0.11	58,58,58,58	0
59	MG	BA	3214	1/1	0.80	0.31	39,39,39,39	0
59	MG	BA	3095	1/1	0.80	0.38	47,47,47,47	0
59	MG	BA	3166	1/1	0.80	0.28	68,68,68,68	0
59	MG	AA	1789	1/1	0.81	0.28	61,61,61,61	0
59	MG	AA	1707	1/1	0.81	0.23	60,60,60,60	0
59	MG	BA	3187	1/1	0.81	0.89	68,68,68,68	0
59	MG	BA	3283	1/1	0.81	0.21	73,73,73,73	0
59	MG	AA	1634	1/1	0.81	0.22	43,43,43,43	0
59	MG	AA	1697	1/1	0.81	0.12	61,61,61,61	0
59	MG	BA	3219	1/1	0.81	0.16	44,44,44,44	0
59	MG	BA	3045	1/1	0.81	0.69	54,54,54,54	0
59	MG	BA	3148	1/1	0.81	0.28	53,53,53,53	0
59	MG	BA	3236	1/1	0.81	0.24	52,52,52,52	0
59	MG	AA	1792	1/1	0.81	0.12	37,37,37,37	0
59	MG	AA	1701	1/1	0.81	0.16	30,30,30,30	0
59	MG	BA	3193	1/1	0.81	0.53	64,64,64,64	0
59	MG	AA	1676	1/1	0.82	0.24	62,62,62,62	0
59	MG	BA	3270	1/1	0.82	0.34	70,70,70,70	0
59	MG	BA	3116	1/1	0.82	0.28	78,78,78,78	0
59	MG	BA	3132	1/1	0.82	0.33	59,59,59,59	0
59	MG	BA	3041	1/1	0.82	0.21	75,75,75,75	0
59	MG	AA	1684	1/1	0.82	0.85	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3154	1/1	0.82	0.60	59,59,59,59	0
59	MG	BA	3226	1/1	0.82	0.34	56,56,56,56	0
59	MG	AA	1722	1/1	0.82	0.23	32,32,32,32	0
59	MG	AA	1763	1/1	0.82	0.30	51,51,51,51	0
59	MG	AA	1726	1/1	0.82	0.21	45,45,45,45	0
59	MG	BA	3248	1/1	0.83	0.45	58,58,58,58	0
59	MG	BA	3251	1/1	0.83	0.28	44,44,44,44	0
59	MG	BA	3140	1/1	0.83	0.13	45,45,45,45	0
59	MG	BA	3107	1/1	0.83	0.30	44,44,44,44	0
59	MG	BA	3055	1/1	0.83	0.16	33,33,33,33	0
59	MG	BA	3036	1/1	0.83	0.28	47,47,47,47	0
59	MG	BA	3261	1/1	0.83	0.14	67,67,67,67	0
59	MG	AA	1794	1/1	0.83	0.27	53,53,53,53	0
59	MG	AA	1689	1/1	0.83	0.41	79,79,79,79	0
59	MG	BA	3106	1/1	0.84	0.22	47,47,47,47	0
59	MG	AA	1691	1/1	0.84	0.11	65,65,65,65	0
59	MG	BA	3126	1/1	0.84	0.42	55,55,55,55	0
59	MG	BA	3163	1/1	0.84	0.30	55,55,55,55	0
59	MG	BA	3087	1/1	0.84	0.34	41,41,41,41	0
59	MG	BA	3250	1/1	0.84	0.24	53,53,53,53	0
59	MG	BA	3253	1/1	0.84	0.41	98,98,98,98	0
59	MG	BA	3206	1/1	0.84	0.23	65,65,65,65	0
59	MG	BA	3072	1/1	0.84	0.63	70,70,70,70	0
59	MG	BA	3237	1/1	0.84	0.20	94,94,94,94	0
59	MG	BA	3020	1/1	0.84	0.22	63,63,63,63	0
59	MG	AA	1788	1/1	0.84	0.32	73,73,73,73	0
59	MG	AA	1756	1/1	0.84	0.39	54,54,54,54	0
59	MG	BA	3271	1/1	0.84	0.34	28,28,28,28	0
59	MG	AA	1668	1/1	0.85	0.17	34,34,34,34	0
59	MG	BA	3153	1/1	0.85	0.24	54,54,54,54	0
59	MG	AA	1748	1/1	0.85	0.36	56,56,56,56	0
59	MG	AA	1604	1/1	0.85	0.41	59,59,59,59	0
59	MG	BA	3186	1/1	0.85	0.15	50,50,50,50	0
59	MG	BA	3238	1/1	0.85	0.29	42,42,42,42	0
59	MG	BA	3112	1/1	0.85	0.70	51,51,51,51	0
59	MG	AA	1698	1/1	0.85	0.31	58,58,58,58	0
59	MG	AA	1620	1/1	0.85	0.43	75,75,75,75	0
59	MG	AA	1624	1/1	0.85	0.84	61,61,61,61	0
59	MG	BA	3169	1/1	0.85	0.37	43,43,43,43	0
59	MG	AA	1669	1/1	0.86	0.20	40,40,40,40	0
59	MG	AA	1793	1/1	0.86	0.22	50,50,50,50	0
59	MG	AA	1663	1/1	0.86	0.47	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3207	1/1	0.86	0.29	30,30,30,30	0
59	MG	BA	3143	1/1	0.86	0.21	57,57,57,57	0
59	MG	BA	3233	1/1	0.86	0.20	42,42,42,42	0
59	MG	AA	1729	1/1	0.86	0.47	45,45,45,45	0
59	MG	AA	1661	1/1	0.86	0.29	40,40,40,40	0
59	MG	BA	3299	1/1	0.86	0.41	53,53,53,53	0
59	MG	BA	3234	1/1	0.86	0.20	63,63,63,63	0
59	MG	BA	3108	1/1	0.86	0.27	34,34,34,34	0
59	MG	BA	3167	1/1	0.86	0.17	61,61,61,61	0
59	MG	AA	1747	1/1	0.86	0.08	23,23,23,23	0
59	MG	AA	1761	1/1	0.86	0.21	30,30,30,30	0
59	MG	BA	3255	1/1	0.86	0.24	35,35,35,35	0
59	MG	BA	3243	1/1	0.86	0.22	32,32,32,32	0
59	MG	AA	1627	1/1	0.86	0.24	74,74,74,74	0
59	MG	AA	1642	1/1	0.86	0.26	61,61,61,61	0
59	MG	B0	101	1/1	0.86	0.77	72,72,72,72	0
59	MG	BA	3137	1/1	0.86	0.16	49,49,49,49	0
59	MG	BA	3145	1/1	0.86	0.23	32,32,32,32	0
59	MG	AA	1787	1/1	0.86	0.27	55,55,55,55	0
59	MG	AA	1798	1/1	0.87	0.07	39,39,39,39	0
59	MG	AA	1731	1/1	0.87	0.09	48,48,48,48	0
59	MG	BA	3134	1/1	0.87	0.30	65,65,65,65	0
59	MG	BA	3133	1/1	0.87	0.31	39,39,39,39	0
59	MG	BA	3079	1/1	0.87	0.34	34,34,34,34	0
59	MG	BA	3029	1/1	0.87	0.33	73,73,73,73	0
59	MG	BA	3054	1/1	0.87	0.28	31,31,31,31	0
59	MG	AA	1656	1/1	0.87	0.15	46,46,46,46	0
59	MG	AA	1608	1/1	0.87	0.37	48,48,48,48	0
59	MG	AA	1768	1/1	0.87	0.46	34,34,34,34	0
59	MG	BA	3129	1/1	0.87	0.29	51,51,51,51	0
59	MG	AA	1732	1/1	0.87	0.25	20,20,20,20	0
59	MG	AA	1737	1/1	0.87	0.18	61,61,61,61	0
59	MG	BA	3181	1/1	0.87	0.17	32,32,32,32	0
59	MG	AA	1757	1/1	0.87	0.30	57,57,57,57	0
59	MG	AA	1734	1/1	0.87	0.12	41,41,41,41	0
61	GCP	AY	701	32/32	0.87	0.20	41,53,61,63	0
59	MG	BA	3027	1/1	0.88	0.30	71,71,71,71	0
59	MG	BA	3196	1/1	0.88	0.38	53,53,53,53	0
59	MG	BA	3075	1/1	0.88	0.23	31,31,31,31	0
59	MG	BA	3144	1/1	0.88	0.23	28,28,28,28	0
59	MG	AA	1615	1/1	0.88	0.75	51,51,51,51	0
59	MG	BA	3198	1/1	0.88	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1767	1/1	0.88	0.29	60,60,60,60	0
59	MG	BA	3273	1/1	0.88	0.65	72,72,72,72	0
59	MG	AA	1749	1/1	0.88	0.13	38,38,38,38	0
59	MG	AA	1651	1/1	0.88	0.20	68,68,68,68	0
59	MG	AA	1783	1/1	0.88	0.13	43,43,43,43	0
59	MG	BA	3212	1/1	0.88	0.28	46,46,46,46	0
59	MG	AA	1784	1/1	0.88	0.17	37,37,37,37	0
59	MG	BA	3274	1/1	0.88	0.18	79,79,79,79	0
59	MG	BA	3105	1/1	0.88	0.20	69,69,69,69	0
59	MG	AA	1786	1/1	0.88	0.15	35,35,35,35	0
59	MG	AA	1772	1/1	0.88	0.58	79,79,79,79	0
59	MG	AA	1696	1/1	0.88	0.35	35,35,35,35	0
59	MG	B5	101	1/1	0.88	0.27	47,47,47,47	0
59	MG	BA	3024	1/1	0.88	0.28	44,44,44,44	0
59	MG	BA	3138	1/1	0.88	0.47	57,57,57,57	0
59	MG	BA	3073	1/1	0.88	0.33	83,83,83,83	0
59	MG	BA	3097	1/1	0.89	0.41	37,37,37,37	0
59	MG	BA	3141	1/1	0.89	0.20	29,29,29,29	0
59	MG	AA	1630	1/1	0.89	0.53	56,56,56,56	0
59	MG	AA	1658	1/1	0.89	0.20	25,25,25,25	0
59	MG	BA	3289	1/1	0.89	0.21	51,51,51,51	0
59	MG	BA	3088	1/1	0.89	0.24	27,27,27,27	0
59	MG	BA	3164	1/1	0.89	0.24	49,49,49,49	0
59	MG	BA	3015	1/1	0.89	0.53	63,63,63,63	0
59	MG	BA	3046	1/1	0.89	0.27	27,27,27,27	0
59	MG	BA	3162	1/1	0.89	0.27	45,45,45,45	0
59	MG	AA	1602	1/1	0.89	0.48	42,42,42,42	0
59	MG	BA	3232	1/1	0.89	0.24	33,33,33,33	0
59	MG	AA	1735	1/1	0.89	0.41	62,62,62,62	0
59	MG	BA	3191	1/1	0.89	0.39	72,72,72,72	0
59	MG	BA	3302	1/1	0.89	0.39	52,52,52,52	0
59	MG	BA	3293	1/1	0.89	0.49	76,76,76,76	0
59	MG	BA	3122	1/1	0.89	0.17	26,26,26,26	0
59	MG	BA	3146	1/1	0.89	0.23	29,29,29,29	0
59	MG	BA	3018	1/1	0.89	0.56	43,43,43,43	0
59	MG	AA	1738	1/1	0.90	0.17	53,53,53,53	0
59	MG	BA	3090	1/1	0.90	0.31	56,56,56,56	0
59	MG	BA	3184	1/1	0.90	0.24	40,40,40,40	0
59	MG	BA	3228	1/1	0.90	0.32	23,23,23,23	0
59	MG	AA	1752	1/1	0.90	0.22	59,59,59,59	0
59	MG	AA	1751	1/1	0.90	0.14	46,46,46,46	0
59	MG	BA	3023	1/1	0.90	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3213	1/1	0.90	0.36	31,31,31,31	0
59	MG	BA	3262	1/1	0.90	0.15	68,68,68,68	0
59	MG	BA	3296	1/1	0.90	0.38	38,38,38,38	0
59	MG	AA	1708	1/1	0.90	0.26	57,57,57,57	0
59	MG	BA	3182	1/1	0.90	0.27	73,73,73,73	0
59	MG	AA	1746	1/1	0.90	0.39	47,47,47,47	0
59	MG	AA	1686	1/1	0.90	0.25	34,34,34,34	0
59	MG	BA	3037	1/1	0.90	0.40	49,49,49,49	0
59	MG	BA	3202	1/1	0.90	0.39	43,43,43,43	0
59	MG	AA	1662	1/1	0.90	0.33	34,34,34,34	0
59	MG	BA	3221	1/1	0.90	0.09	43,43,43,43	0
59	MG	BA	3056	1/1	0.90	0.37	38,38,38,38	0
59	MG	BA	3098	1/1	0.90	0.23	25,25,25,25	0
59	MG	AA	1727	1/1	0.90	0.14	55,55,55,55	0
59	MG	BA	3241	1/1	0.90	0.19	65,65,65,65	0
59	MG	BA	3117	1/1	0.90	0.18	26,26,26,26	0
59	MG	BA	3060	1/1	0.90	0.39	31,31,31,31	0
59	MG	BA	3285	1/1	0.91	0.28	40,40,40,40	0
59	MG	AA	1613	1/1	0.91	0.18	65,65,65,65	0
59	MG	AA	1739	1/1	0.91	0.42	28,28,28,28	0
59	MG	BA	3093	1/1	0.91	0.42	69,69,69,69	0
59	MG	AA	1774	1/1	0.91	0.62	51,51,51,51	0
59	MG	AA	1648	1/1	0.91	0.35	29,29,29,29	0
59	MG	AA	1769	1/1	0.91	0.36	33,33,33,33	0
59	MG	BA	3185	1/1	0.91	0.43	36,36,36,36	0
59	MG	BA	3310	1/1	0.91	0.29	20,20,20,20	0
59	MG	AA	1775	1/1	0.91	0.13	45,45,45,45	0
59	MG	BA	3022	1/1	0.91	0.55	65,65,65,65	0
59	MG	AA	1742	1/1	0.91	0.22	45,45,45,45	0
59	MG	BA	3254	1/1	0.91	0.27	18,18,18,18	0
59	MG	BA	3053	1/1	0.91	0.33	24,24,24,24	0
59	MG	BA	3048	1/1	0.91	0.39	28,28,28,28	0
59	MG	AA	1765	1/1	0.91	0.56	63,63,63,63	0
59	MG	BA	3211	1/1	0.91	0.65	58,58,58,58	0
59	MG	AA	1622	1/1	0.91	0.47	49,49,49,49	0
59	MG	AA	1700	1/1	0.91	0.32	27,27,27,27	0
59	MG	BA	3068	1/1	0.91	0.19	33,33,33,33	0
59	MG	BA	3208	1/1	0.91	0.24	34,34,34,34	0
59	MG	AA	1626	1/1	0.92	0.42	59,59,59,59	0
59	MG	AA	1646	1/1	0.92	0.38	34,34,34,34	0
59	MG	BA	3287	1/1	0.92	0.17	41,41,41,41	0
59	MG	BA	3266	1/1	0.92	0.31	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3244	1/1	0.92	0.21	41,41,41,41	0
59	MG	BA	3227	1/1	0.92	0.28	27,27,27,27	0
59	MG	BU	201	1/1	0.92	0.14	28,28,28,28	0
59	MG	AA	1657	1/1	0.92	0.10	32,32,32,32	0
59	MG	BA	3192	1/1	0.92	0.36	51,51,51,51	0
59	MG	BA	3301	1/1	0.92	0.41	45,45,45,45	0
59	MG	AA	1670	1/1	0.92	0.21	57,57,57,57	0
59	MG	BA	3291	1/1	0.92	0.32	27,27,27,27	0
59	MG	AA	1704	1/1	0.92	0.37	25,25,25,25	0
59	MG	AA	1685	1/1	0.92	0.42	40,40,40,40	0
59	MG	BA	3121	1/1	0.92	0.34	33,33,33,33	0
59	MG	AA	1683	1/1	0.92	0.23	25,25,25,25	0
59	MG	BA	3297	1/1	0.92	0.18	39,39,39,39	0
59	MG	BA	3130	1/1	0.92	0.55	56,56,56,56	0
59	MG	BA	3216	1/1	0.92	0.20	54,54,54,54	0
59	MG	BA	3115	1/1	0.92	0.30	52,52,52,52	0
59	MG	AA	1693	1/1	0.92	0.17	30,30,30,30	0
59	MG	BA	3049	1/1	0.92	0.46	47,47,47,47	0
59	MG	BA	3089	1/1	0.92	0.24	18,18,18,18	0
59	MG	BA	3078	1/1	0.92	0.20	26,26,26,26	0
59	MG	BA	3031	1/1	0.92	0.35	35,35,35,35	0
59	MG	AA	1713	1/1	0.92	0.16	40,40,40,40	0
59	MG	BA	3259	1/1	0.92	0.12	39,39,39,39	0
59	MG	AA	1645	1/1	0.92	0.26	22,22,22,22	0
59	MG	BA	3314	1/1	0.92	0.10	49,49,49,49	0
59	MG	BA	3286	1/1	0.93	0.33	42,42,42,42	0
59	MG	BA	3061	1/1	0.93	0.05	37,37,37,37	0
59	MG	BA	3157	1/1	0.93	0.17	17,17,17,17	0
59	MG	AA	1725	1/1	0.93	0.25	35,35,35,35	0
59	MG	BA	3127	1/1	0.93	0.24	38,38,38,38	0
59	MG	AA	1672	1/1	0.93	0.17	42,42,42,42	0
59	MG	BA	3298	1/1	0.93	0.17	20,20,20,20	0
59	MG	AA	1750	1/1	0.93	0.30	42,42,42,42	0
59	MG	BA	3189	1/1	0.93	0.19	26,26,26,26	0
59	MG	AA	1652	1/1	0.93	0.44	41,41,41,41	0
59	MG	BA	3300	1/1	0.93	0.17	65,65,65,65	0
59	MG	BA	3188	1/1	0.93	0.41	34,34,34,34	0
59	MG	AA	1654	1/1	0.93	0.26	24,24,24,24	0
59	MG	AA	1721	1/1	0.93	0.12	17,17,17,17	0
59	MG	BA	3084	1/1	0.93	0.54	38,38,38,38	0
59	MG	AA	1694	1/1	0.93	0.13	19,19,19,19	0
59	MG	AA	1719	1/1	0.93	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3303	1/1	0.93	0.09	42,42,42,42	0
59	MG	BA	3038	1/1	0.93	0.31	40,40,40,40	0
59	MG	AA	1733	1/1	0.93	0.31	67,67,67,67	0
59	MG	BA	3170	1/1	0.93	0.52	41,41,41,41	0
59	MG	BA	3013	1/1	0.93	0.49	37,37,37,37	0
59	MG	BA	3294	1/1	0.93	0.20	42,42,42,42	0
59	MG	BA	3220	1/1	0.93	0.19	56,56,56,56	0
59	MG	BA	3139	1/1	0.93	0.29	35,35,35,35	0
59	MG	AA	1664	1/1	0.93	0.39	29,29,29,29	0
59	MG	AY	702	1/1	0.93	0.08	23,23,23,23	0
59	MG	BA	3007	1/1	0.93	0.45	26,26,26,26	0
59	MG	AA	1649	1/1	0.93	0.40	23,23,23,23	0
59	MG	BA	3200	1/1	0.93	0.31	71,71,71,71	0
59	MG	AA	1692	1/1	0.93	0.23	48,48,48,48	0
59	MG	BA	3111	1/1	0.93	0.32	30,30,30,30	0
59	MG	BA	3114	1/1	0.93	0.21	29,29,29,29	0
59	MG	BA	3011	1/1	0.94	0.28	46,46,46,46	0
59	MG	AA	1660	1/1	0.94	0.10	19,19,19,19	0
59	MG	BA	3312	1/1	0.94	0.52	44,44,44,44	0
59	MG	BA	3277	1/1	0.94	0.45	57,57,57,57	0
59	MG	AA	1616	1/1	0.94	0.41	30,30,30,30	0
59	MG	AA	1603	1/1	0.94	0.41	38,38,38,38	0
59	MG	AA	1631	1/1	0.94	0.20	40,40,40,40	0
59	MG	BA	3152	1/1	0.94	0.41	64,64,64,64	0
59	MG	BA	3272	1/1	0.94	0.43	52,52,52,52	0
59	MG	AA	1605	1/1	0.94	0.43	40,40,40,40	0
59	MG	BA	3050	1/1	0.94	0.15	23,23,23,23	0
59	MG	BA	3306	1/1	0.94	0.23	39,39,39,39	0
59	MG	AA	1717	1/1	0.94	0.43	41,41,41,41	0
59	MG	BA	3246	1/1	0.94	0.31	34,34,34,34	0
59	MG	AA	1665	1/1	0.94	0.42	28,28,28,28	0
59	MG	AA	1655	1/1	0.94	0.40	30,30,30,30	0
59	MG	BA	3071	1/1	0.94	0.37	22,22,22,22	0
59	MG	BA	3051	1/1	0.94	0.37	31,31,31,31	0
59	MG	BA	3199	1/1	0.94	0.27	26,26,26,26	0
59	MG	AA	1736	1/1	0.94	0.19	29,29,29,29	0
59	MG	BA	3307	1/1	0.94	0.16	40,40,40,40	0
59	MG	BA	3290	1/1	0.94	0.42	43,43,43,43	0
59	MG	BA	3195	1/1	0.94	0.25	32,32,32,32	0
59	MG	BA	3077	1/1	0.94	0.35	31,31,31,31	0
59	MG	BA	3257	1/1	0.94	0.22	43,43,43,43	0
59	MG	BA	3177	1/1	0.94	0.40	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3203	1/1	0.94	0.27	30,30,30,30	0
59	MG	AA	1653	1/1	0.94	0.31	19,19,19,19	0
59	MG	AA	1673	1/1	0.94	0.21	35,35,35,35	0
59	MG	BA	3059	1/1	0.94	0.45	45,45,45,45	0
59	MG	BA	3100	1/1	0.94	0.10	24,24,24,24	0
59	MG	AA	1688	1/1	0.94	0.25	30,30,30,30	0
59	MG	BA	3210	1/1	0.95	0.29	23,23,23,23	0
59	MG	BA	3151	1/1	0.95	0.13	33,33,33,33	0
59	MG	AA	1610	1/1	0.95	0.66	46,46,46,46	0
59	MG	AA	1690	1/1	0.95	0.47	35,35,35,35	0
59	MG	AA	1675	1/1	0.95	0.26	45,45,45,45	0
59	MG	BA	3245	1/1	0.95	0.23	25,25,25,25	0
59	MG	BA	3223	1/1	0.95	0.34	32,32,32,32	0
59	MG	BA	3217	1/1	0.95	0.18	35,35,35,35	0
59	MG	BA	3308	1/1	0.95	0.12	58,58,58,58	0
59	MG	BA	3057	1/1	0.95	0.29	29,29,29,29	0
59	MG	BA	3249	1/1	0.95	0.31	22,22,22,22	0
59	MG	BA	3173	1/1	0.95	0.27	20,20,20,20	0
59	MG	AA	1687	1/1	0.95	0.20	30,30,30,30	0
59	MG	AA	1718	1/1	0.95	0.50	35,35,35,35	0
59	MG	AA	1720	1/1	0.95	0.47	37,37,37,37	0
59	MG	BA	3183	1/1	0.95	0.14	58,58,58,58	0
59	MG	AA	1706	1/1	0.95	0.16	43,43,43,43	0
59	MG	BA	3180	1/1	0.95	0.34	47,47,47,47	0
59	MG	AA	1710	1/1	0.95	0.06	35,35,35,35	0
59	MG	BA	3086	1/1	0.95	0.26	46,46,46,46	0
59	MG	BA	3205	1/1	0.95	0.12	35,35,35,35	0
59	MG	BA	3316	1/1	0.95	0.38	34,34,34,34	0
59	MG	BA	3256	1/1	0.95	0.44	52,52,52,52	0
59	MG	AA	1609	1/1	0.95	0.42	40,40,40,40	0
59	MG	AA	1791	1/1	0.95	0.09	57,57,57,57	0
59	MG	BA	3082	1/1	0.95	0.49	23,23,23,23	0
59	MG	BA	3120	1/1	0.95	0.38	43,43,43,43	0
59	MG	BA	3135	1/1	0.95	0.25	58,58,58,58	0
59	MG	BA	3176	1/1	0.95	0.46	23,23,23,23	0
59	MG	BA	3158	1/1	0.95	0.30	27,27,27,27	0
59	MG	AA	1633	1/1	0.95	0.54	52,52,52,52	0
59	MG	BA	3161	1/1	0.95	0.42	30,30,30,30	0
59	MG	BA	3118	1/1	0.95	0.30	29,29,29,29	0
59	MG	BA	3311	1/1	0.96	0.34	22,22,22,22	0
59	MG	BA	3047	1/1	0.96	0.37	42,42,42,42	0
59	MG	AA	1680	1/1	0.96	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1617	1/1	0.96	0.49	49,49,49,49	0
59	MG	BA	3001	1/1	0.96	0.11	35,35,35,35	0
59	MG	BA	3224	1/1	0.96	0.46	32,32,32,32	0
59	MG	BA	3017	1/1	0.96	0.33	37,37,37,37	0
59	MG	BA	3309	1/1	0.96	0.17	50,50,50,50	0
59	MG	AA	1776	1/1	0.96	0.29	25,25,25,25	0
59	MG	AA	1723	1/1	0.96	0.14	10,10,10,10	0
59	MG	BA	3229	1/1	0.96	0.13	5,5,5,5	0
59	MG	AA	1671	1/1	0.96	0.65	43,43,43,43	0
59	MG	BA	3102	1/1	0.96	0.23	30,30,30,30	0
59	MG	BA	3313	1/1	0.96	0.26	36,36,36,36	0
59	MG	BA	3235	1/1	0.96	0.21	29,29,29,29	0
59	MG	AA	1795	1/1	0.96	0.15	46,46,46,46	0
59	MG	AA	1681	1/1	0.96	0.45	34,34,34,34	0
59	MG	AA	1614	1/1	0.96	0.40	26,26,26,26	0
59	MG	BA	3156	1/1	0.96	0.19	25,25,25,25	0
59	MG	BA	3014	1/1	0.96	0.34	53,53,53,53	0
59	MG	BA	3008	1/1	0.96	0.46	45,45,45,45	0
59	MG	BA	3034	1/1	0.96	0.25	36,36,36,36	0
59	MG	AA	1730	1/1	0.96	0.12	62,62,62,62	0
59	MG	AA	1770	1/1	0.96	0.29	41,41,41,41	0
59	MG	BA	3319	1/1	0.96	0.11	35,35,35,35	0
59	MG	AA	1678	1/1	0.96	0.35	29,29,29,29	0
59	MG	AA	1785	1/1	0.96	0.08	47,47,47,47	0
59	MG	AA	1782	1/1	0.96	0.09	39,39,39,39	0
59	MG	AA	1682	1/1	0.96	0.27	53,53,53,53	0
59	MG	BA	3003	1/1	0.96	0.34	20,20,20,20	0
59	MG	AA	1619	1/1	0.96	0.36	37,37,37,37	0
60	ZN	AD	301	1/1	0.96	0.35	54,54,54,54	0
59	MG	BA	3222	1/1	0.96	0.30	44,44,44,44	0
59	MG	BA	3021	1/1	0.96	0.32	37,37,37,37	0
59	MG	AA	1625	1/1	0.96	0.36	17,17,17,17	0
59	MG	AA	1612	1/1	0.96	0.46	47,47,47,47	0
59	MG	BA	3278	1/1	0.96	0.24	91,91,91,91	0
59	MG	BA	3149	1/1	0.96	0.48	29,29,29,29	0
59	MG	BA	3172	1/1	0.96	0.45	31,31,31,31	0
59	MG	BA	3092	1/1	0.96	0.59	37,37,37,37	0
59	MG	BA	3101	1/1	0.97	0.35	29,29,29,29	0
59	MG	BA	3231	1/1	0.97	0.34	13,13,13,13	0
59	MG	BA	3113	1/1	0.97	0.52	32,32,32,32	0
59	MG	BA	3074	1/1	0.97	0.36	3,3,3,3	0
59	MG	BA	3052	1/1	0.97	0.31	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3062	1/1	0.97	0.15	13,13,13,13	0
59	MG	BA	3110	1/1	0.97	0.49	31,31,31,31	0
59	MG	BA	3103	1/1	0.97	0.20	35,35,35,35	0
59	MG	BA	3044	1/1	0.97	0.40	21,21,21,21	0
59	MG	BA	3063	1/1	0.97	0.15	22,22,22,22	0
59	MG	AA	1641	1/1	0.97	0.17	17,17,17,17	0
59	MG	AA	1778	1/1	0.97	0.12	6,6,6,6	0
59	MG	AA	1702	1/1	0.97	0.53	44,44,44,44	0
59	MG	AA	1659	1/1	0.97	0.39	34,34,34,34	0
59	MG	AA	1618	1/1	0.97	0.38	47,47,47,47	0
59	MG	BA	3006	1/1	0.97	0.41	30,30,30,30	0
59	MG	BA	3083	1/1	0.97	0.42	23,23,23,23	0
59	MG	BA	3005	1/1	0.97	0.49	16,16,16,16	0
59	MG	BA	3159	1/1	0.97	0.20	36,36,36,36	0
59	MG	BA	3035	1/1	0.97	0.51	31,31,31,31	0
59	MG	BA	3069	1/1	0.97	0.33	18,18,18,18	0
59	MG	AA	1705	1/1	0.97	0.07	23,23,23,23	0
59	MG	BA	3131	1/1	0.97	0.43	33,33,33,33	0
59	MG	BA	3039	1/1	0.97	0.39	38,38,38,38	0
59	MG	BA	3091	1/1	0.97	0.22	21,21,21,21	0
59	MG	BA	3004	1/1	0.97	0.38	24,24,24,24	0
59	MG	BA	3058	1/1	0.97	0.31	31,31,31,31	0
59	MG	BA	3099	1/1	0.97	0.21	19,19,19,19	0
59	MG	BA	3043	1/1	0.97	0.23	28,28,28,28	0
59	MG	AA	1667	1/1	0.97	0.35	33,33,33,33	0
59	MG	BA	3066	1/1	0.97	0.16	27,27,27,27	0
59	MG	AA	1759	1/1	0.97	0.33	37,37,37,37	0
59	MG	AA	1629	1/1	0.97	0.28	44,44,44,44	0
59	MG	BA	3171	1/1	0.97	0.23	19,19,19,19	0
59	MG	BA	3080	1/1	0.98	0.41	38,38,38,38	0
59	MG	BA	3320	1/1	0.98	0.13	39,39,39,39	0
59	MG	BA	3123	1/1	0.98	0.49	32,32,32,32	0
59	MG	BA	3096	1/1	0.98	0.20	23,23,23,23	0
59	MG	BA	3094	1/1	0.98	0.32	25,25,25,25	0
59	MG	BA	3081	1/1	0.98	0.28	23,23,23,23	0
59	MG	BA	3109	1/1	0.98	0.44	20,20,20,20	0
59	MG	BA	3033	1/1	0.98	0.21	41,41,41,41	0
59	MG	BA	3317	1/1	0.98	0.28	29,29,29,29	0
59	MG	BA	3104	1/1	0.98	0.32	30,30,30,30	0
59	MG	BA	3010	1/1	0.98	0.41	33,33,33,33	0
59	MG	BA	3076	1/1	0.98	0.29	18,18,18,18	0
59	MG	BA	3119	1/1	0.98	0.26	24,24,24,24	0

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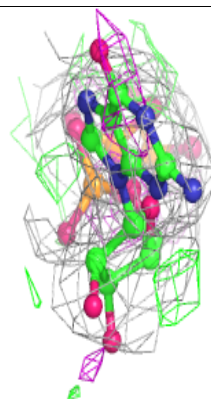
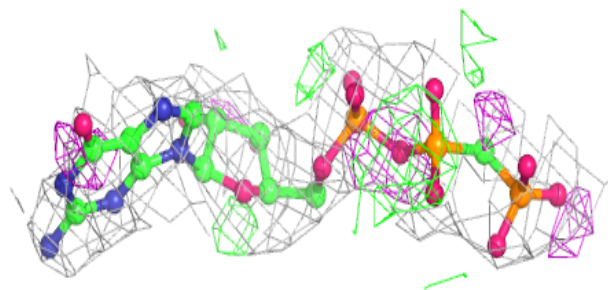
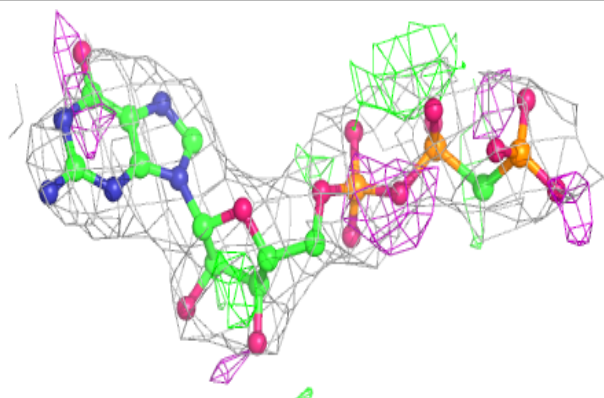
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3002	1/1	0.98	0.13	39,39,39,39	0
59	MG	BA	3178	1/1	0.98	0.27	43,43,43,43	0
59	MG	BA	3065	1/1	0.98	0.29	21,21,21,21	0
59	MG	AA	1623	1/1	0.98	0.52	33,33,33,33	0
59	MG	BA	3288	1/1	0.98	0.18	24,24,24,24	0
59	MG	BA	3150	1/1	0.98	0.16	15,15,15,15	0
59	MG	AA	1679	1/1	0.98	0.55	32,32,32,32	0
59	MG	BA	3070	1/1	0.98	0.45	25,25,25,25	0
59	MG	BA	3124	1/1	0.99	0.27	15,15,15,15	0
59	MG	BA	3165	1/1	0.99	0.45	29,29,29,29	0
59	MG	BA	3318	1/1	0.99	0.08	46,46,46,46	0
60	ZN	B9	101	1/1	1.00	0.06	49,49,49,49	0
60	ZN	AN	101	1/1	1.00	0.13	45,45,45,45	0

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

Electron density around GCP AY 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.