



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:47 am GMT

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

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

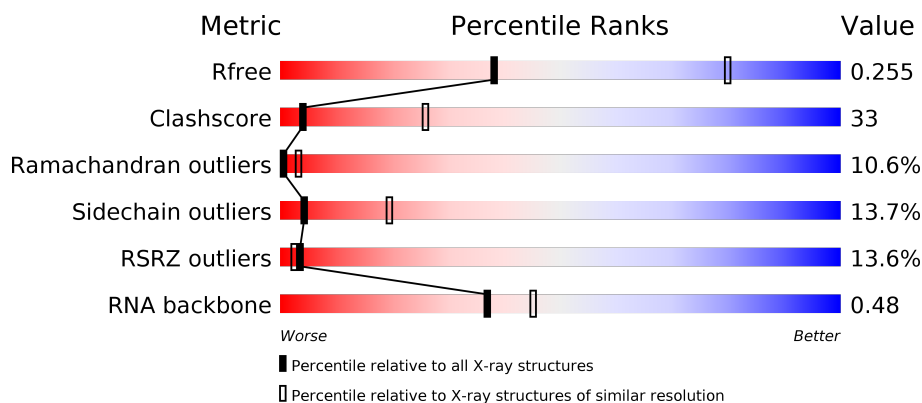
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1533	<div> <div>8%</div> <div>28%</div> <div>57%</div> <div>15%</div> <div>.</div> </div>
2	AB	241	<div> <div>27%</div> <div>25%</div> <div>45%</div> <div>17%</div> <div>.</div> <div>10%</div> </div>
3	AC	233	<div> <div>9%</div> <div>30%</div> <div>44%</div> <div>13%</div> <div>.</div> <div>12%</div> </div>
4	AD	206	<div> <div>29%</div> <div>27%</div> <div>57%</div> <div>15%</div> <div>.</div> </div>

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	KBE	AY	1	-	-	X	-
24	UAL	AY	5	-	-	X	-
24	5OH	AY	6	-	-	X	-
57	MG	AA	1601	-	-	-	X
57	MG	AA	1603	-	-	-	X
57	MG	AA	1604	-	-	-	X
57	MG	AA	1606	-	-	-	X
57	MG	AA	1607	-	-	-	X
57	MG	AA	1611	-	-	-	X
57	MG	AA	1616	-	-	-	X
57	MG	AA	1618	-	-	-	X
57	MG	AA	1622	-	-	-	X
57	MG	AA	1631	-	-	-	X
57	MG	AA	1633	-	-	-	X
57	MG	AA	1647	-	-	-	X
57	MG	AA	1650	-	-	-	X
57	MG	AA	1655	-	-	-	X
57	MG	AA	1665	-	-	-	X
57	MG	AA	1668	-	-	-	X
57	MG	AA	1673	-	-	-	X
57	MG	AA	1677	-	-	-	X
57	MG	AA	1689	-	-	-	X
57	MG	BA	3001	-	-	-	X
57	MG	BA	3003	-	-	-	X
57	MG	BA	3005	-	-	-	X
57	MG	BA	3007	-	-	-	X
57	MG	BA	3009	-	-	-	X
57	MG	BA	3011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3013	-	-	-	X
57	MG	BA	3014	-	-	-	X
57	MG	BA	3016	-	-	-	X
57	MG	BA	3018	-	-	-	X
57	MG	BA	3020	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3024	-	-	-	X
57	MG	BA	3026	-	-	-	X
57	MG	BA	3032	-	-	-	X
57	MG	BA	3034	-	-	-	X
57	MG	BA	3039	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3042	-	-	-	X
57	MG	BA	3045	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3061	-	-	-	X
57	MG	BA	3066	-	-	-	X
57	MG	BA	3068	-	-	-	X
57	MG	BA	3070	-	-	-	X
57	MG	BA	3072	-	-	-	X
57	MG	BA	3073	-	-	-	X
57	MG	BA	3074	-	-	-	X
57	MG	BA	3078	-	-	-	X
57	MG	BA	3083	-	-	-	X
57	MG	BA	3084	-	-	-	X
57	MG	BA	3090	-	-	-	X
57	MG	BA	3091	-	-	-	X
57	MG	BA	3092	-	-	-	X
57	MG	BA	3096	-	-	-	X
57	MG	BA	3097	-	-	-	X
57	MG	BA	3099	-	-	-	X
57	MG	BA	3102	-	-	-	X
57	MG	BA	3103	-	-	-	X
57	MG	BA	3104	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3130	-	-	-	X
57	MG	BA	3138	-	-	-	X
57	MG	BA	3148	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3150	-	-	-	X
57	MG	BA	3151	-	-	-	X
57	MG	BA	3153	-	-	-	X
57	MG	BA	3174	-	-	-	X
57	MG	BA	3177	-	-	-	X
57	MG	BA	3181	-	-	-	X
57	MG	BA	3182	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3201	-	-	-	X
57	MG	BA	3206	-	-	-	X
57	MG	BA	3223	-	-	-	X
57	MG	BA	3244	-	-	-	X
57	MG	BA	3262	-	-	-	X
57	MG	BA	3269	-	-	-	X
57	MG	BA	3276	-	-	-	X
57	MG	BA	3280	-	-	-	X
57	MG	BA	3283	-	-	-	X
57	MG	BA	3294	-	-	-	X
57	MG	BA	3298	-	-	-	X
57	MG	BA	3316	-	-	-	X
57	MG	BA	3341	-	-	-	X
57	MG	BD	302	-	-	-	X
57	MG	BD	304	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 147221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called messenger RNA.

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

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

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

- Molecule 24 is a protein called Viomycin.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

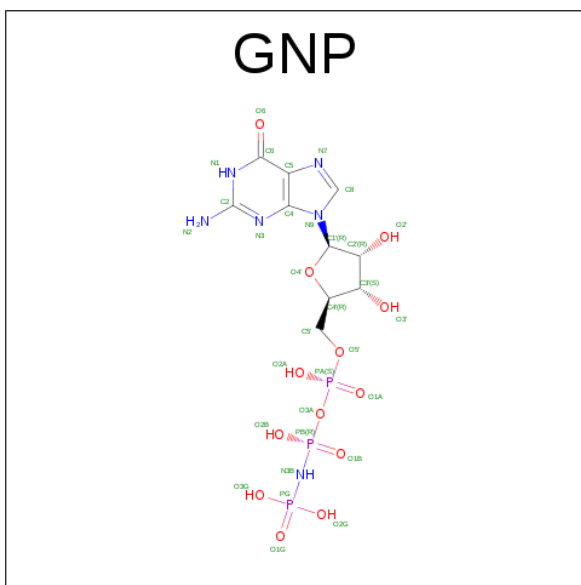
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BT	1	Total	Mg	0	0
			1	1		
57	BB	9	Total	Mg	0	0
			9	9		
57	BO	1	Total	Mg	0	0
			1	1		
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	357	Total	Mg	0	0
			357	357		
57	BN	1	Total	Mg	0	0
			1	1		
57	B2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AH	1	Total 1	Mg 1	0	0
57	BD	5	Total 5	Mg 5	0	0
57	BE	1	Total 1	Mg 1	0	0
57	AW	1	Total 1	Mg 1	0	0
57	AA	102	Total 102	Mg 102	0	0
57	BQ	1	Total 1	Mg 1	0	0
57	BC	1	Total 1	Mg 1	0	0
57	B0	3	Total 3	Mg 3	0	0
57	BX	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	BR	2	Total 2	Mg 2	0	0
57	AF	1	Total 1	Mg 1	0	0
57	AM	1	Total 1	Mg 1	0	0

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



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

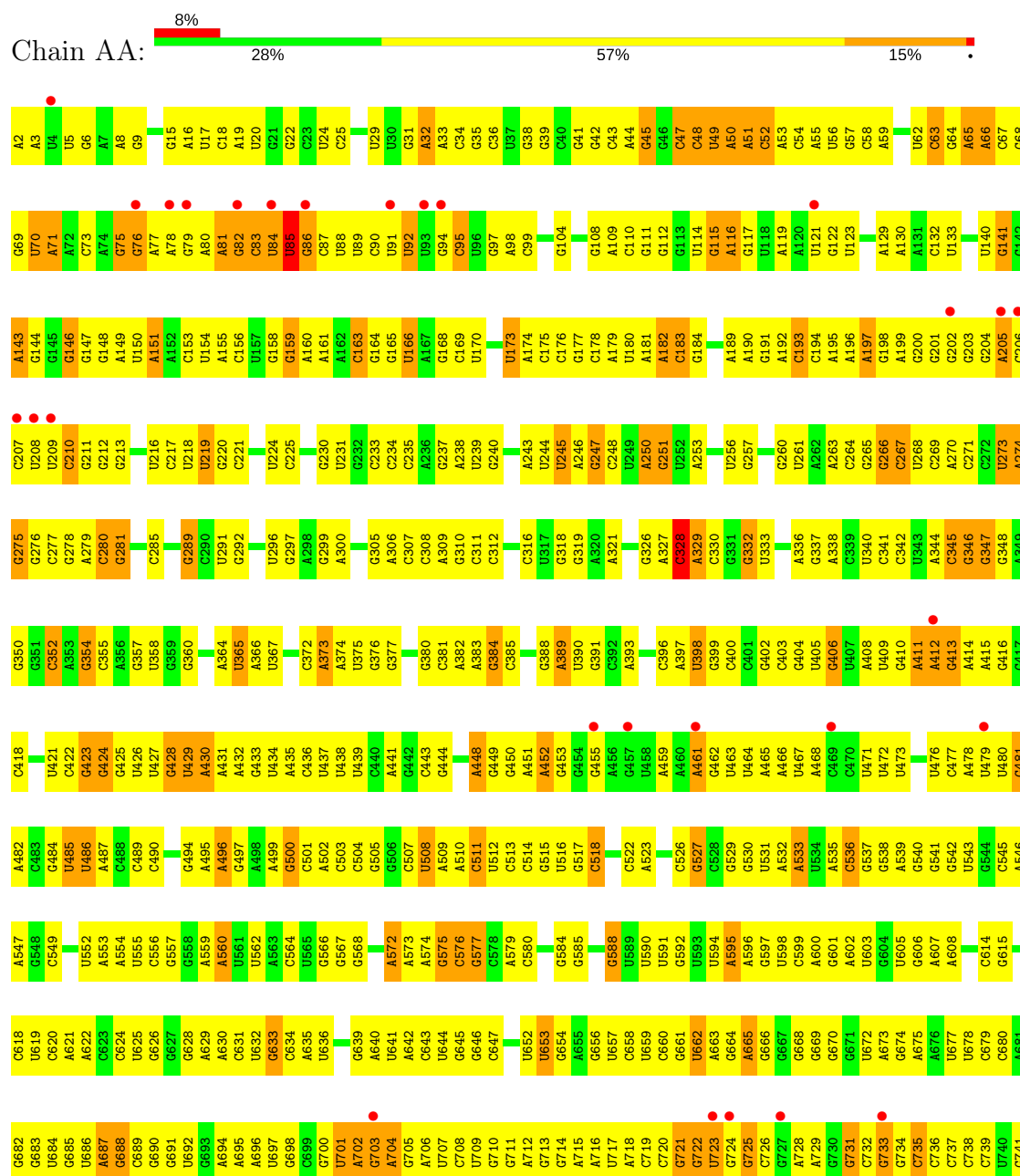
- Molecule 59 is water.

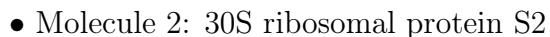
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AW	2	Total O 2 2	0	0
59	B8	1	Total O 1 1	0	0
59	BA	8	Total O 8 8	0	0
59	BC	2	Total O 2 2	0	0
59	BD	1	Total O 1 1	0	0
59	BF	1	Total O 1 1	0	0
59	BG	1	Total O 1 1	0	0
59	BW	1	Total O 1 1	0	0

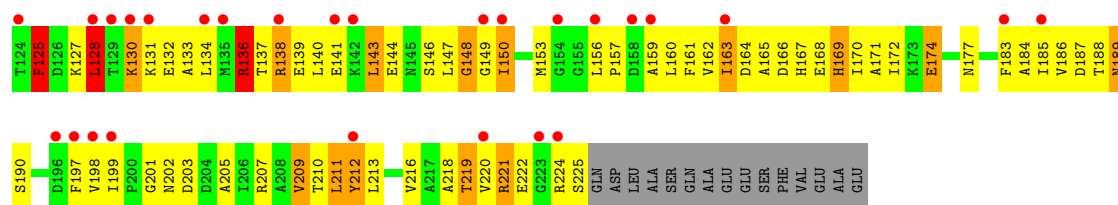
3 Residue-property plots

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

• Molecule 1: 16S rRNA

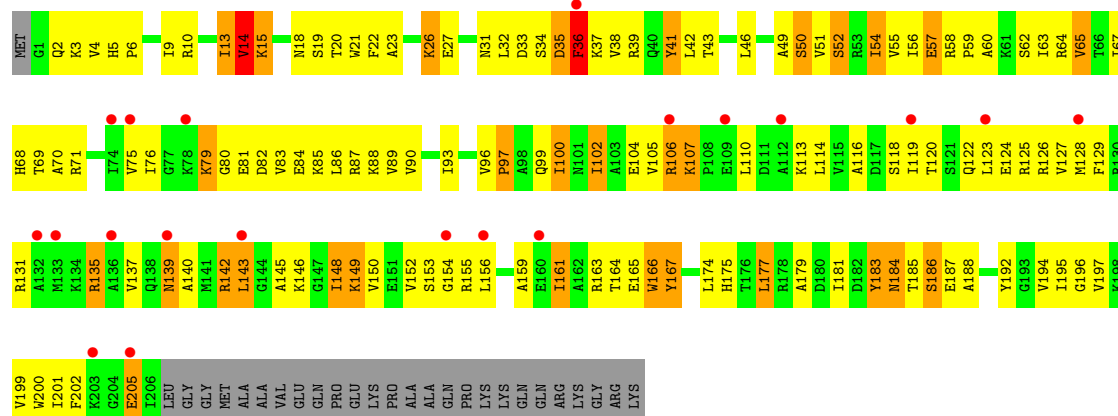






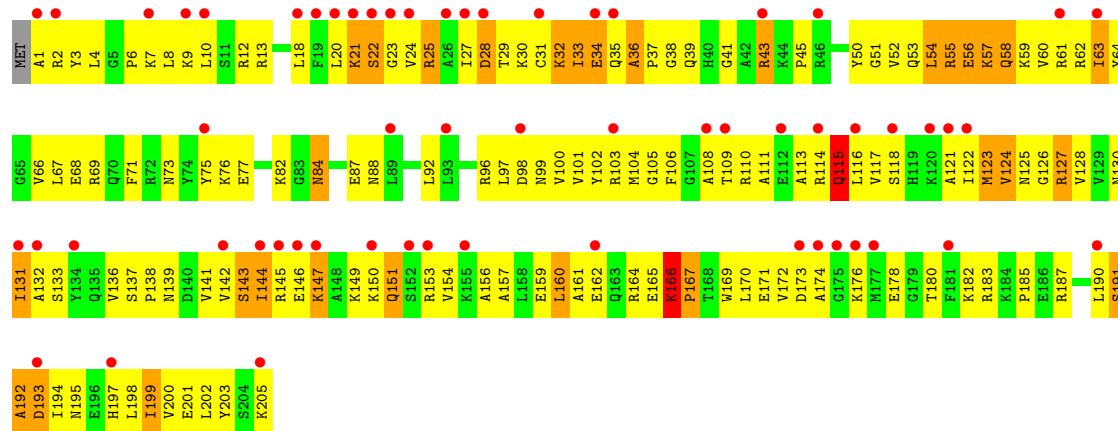
• Molecule 3: 30S ribosomal protein S3

Chain AC: 9% 30% 44% 13% 12%



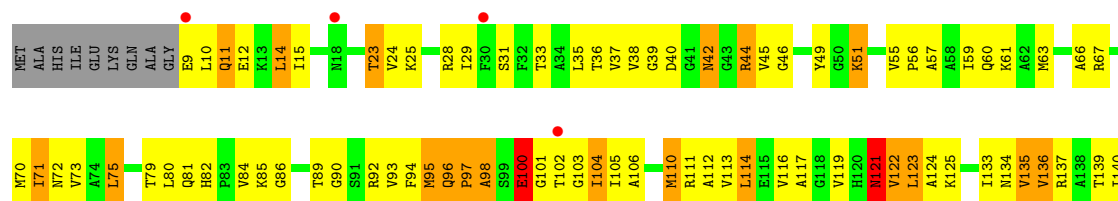
• Molecule 4: 30S ribosomal protein S4

Chain AD: 29% 27% 57% 15%



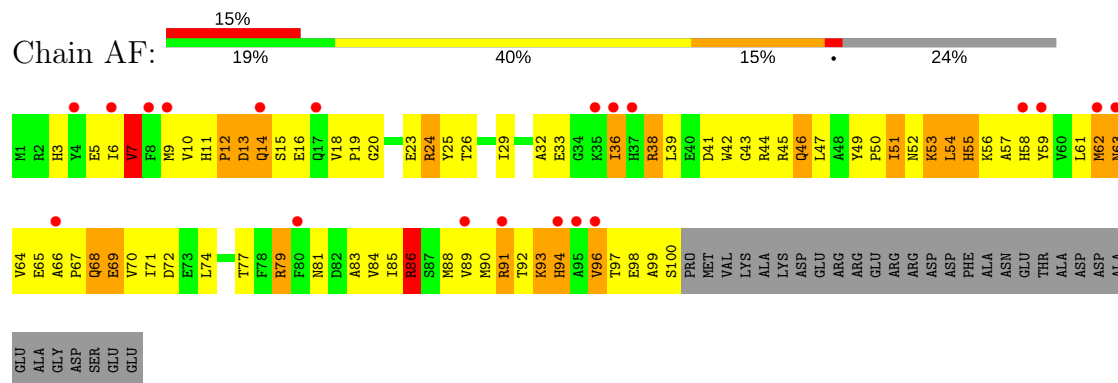
• Molecule 5: 30S ribosomal protein S5

Chain AE: 2% 31% 44% 14% 10%

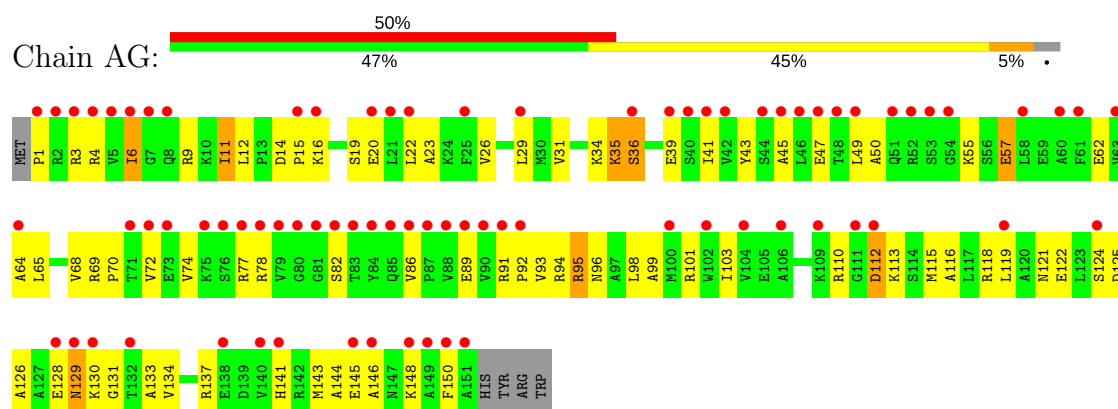




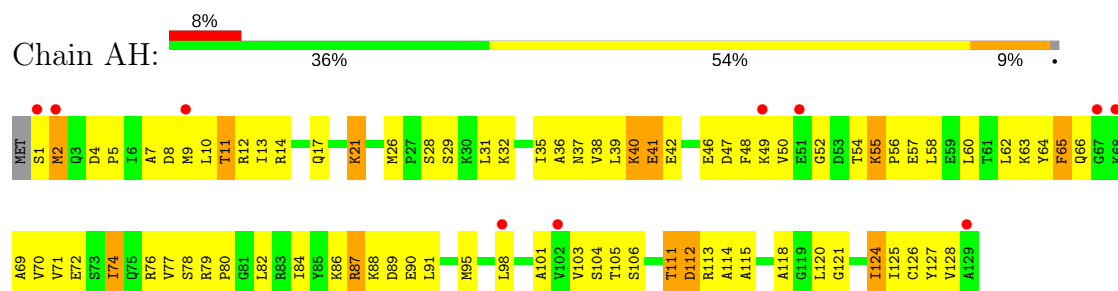
• Molecule 6: 30S ribosomal protein S6 1



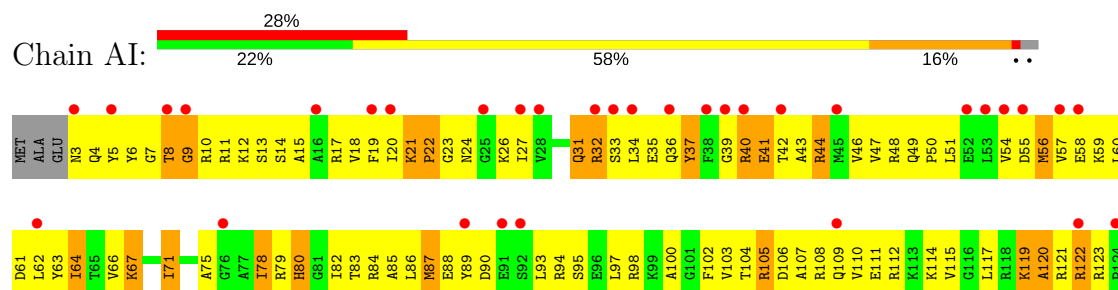
• Molecule 7: 30S ribosomal protein S7

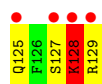


• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

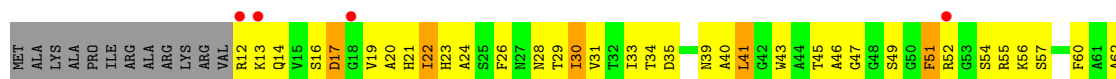




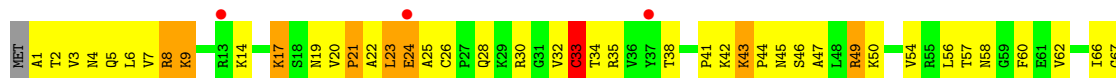
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



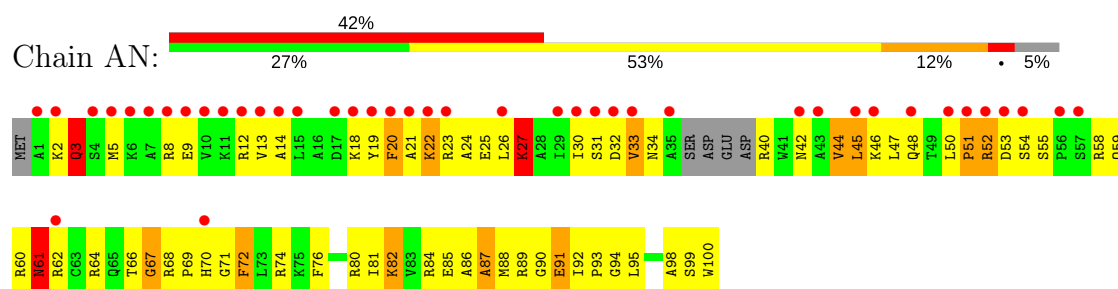
- Molecule 12: 30S ribosomal protein S12 1



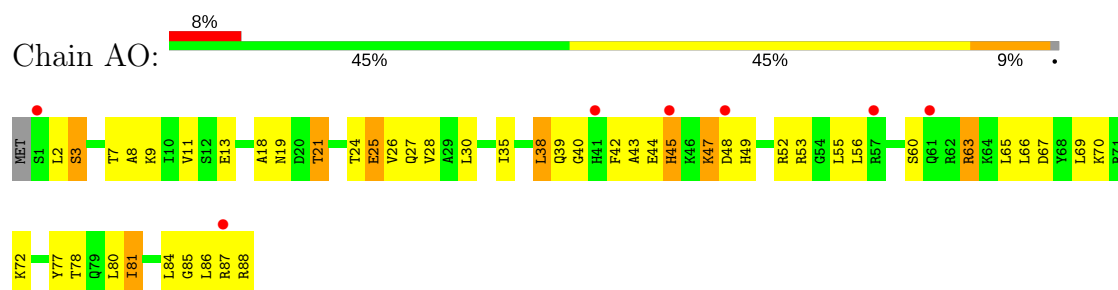
- Molecule 13: 30S ribosomal protein S13



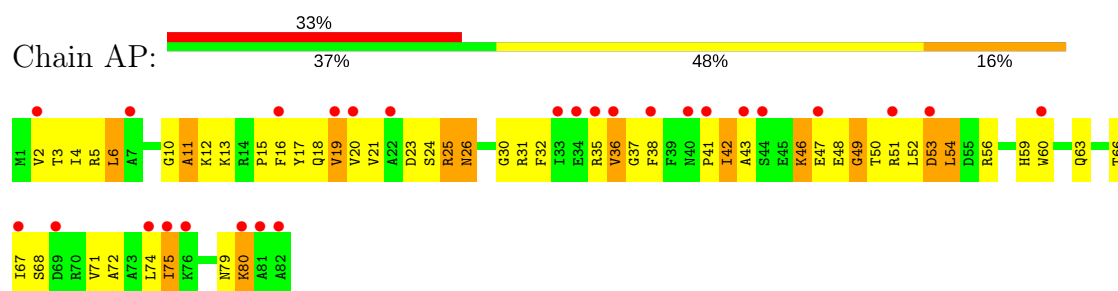
- Molecule 14: 30S ribosomal protein S14



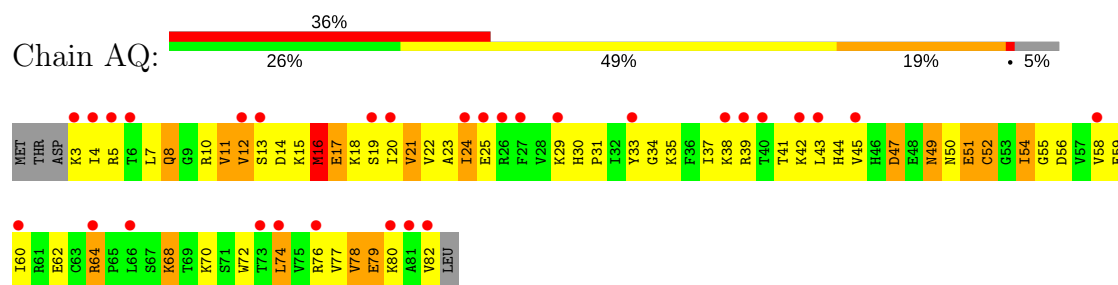
- Molecule 15: 30S ribosomal protein S15 1



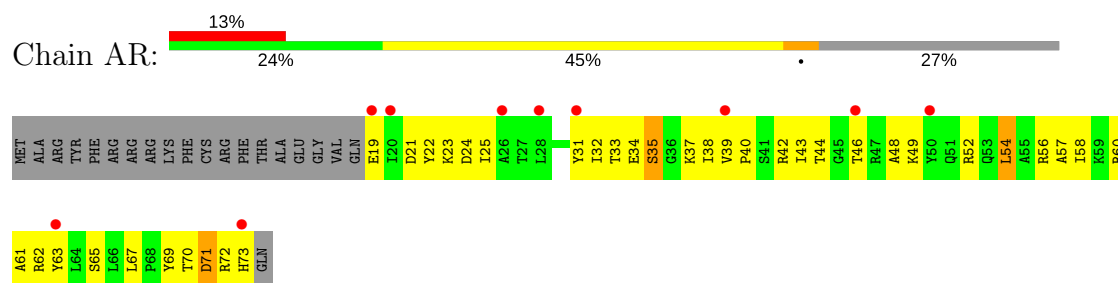
- Molecule 16: 30S ribosomal protein S16



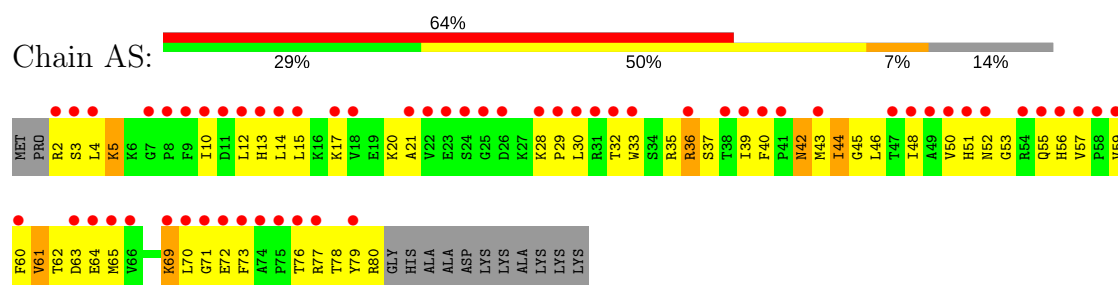
- Molecule 17: 30S ribosomal protein S17



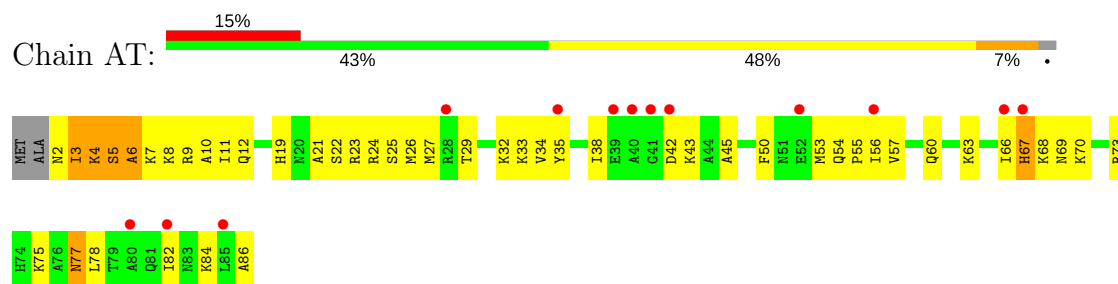
- Molecule 18: 30S ribosomal protein S18



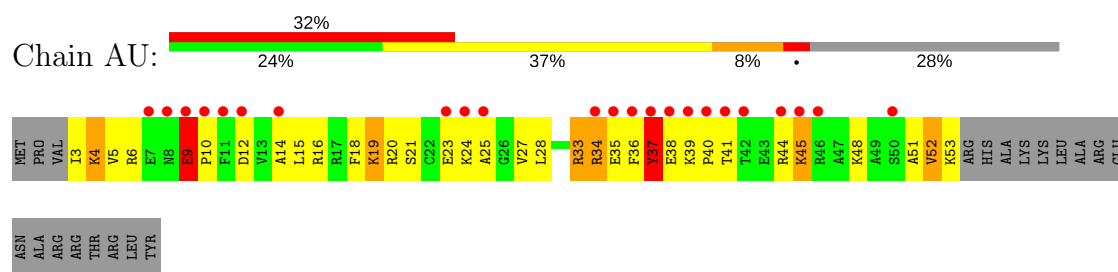
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



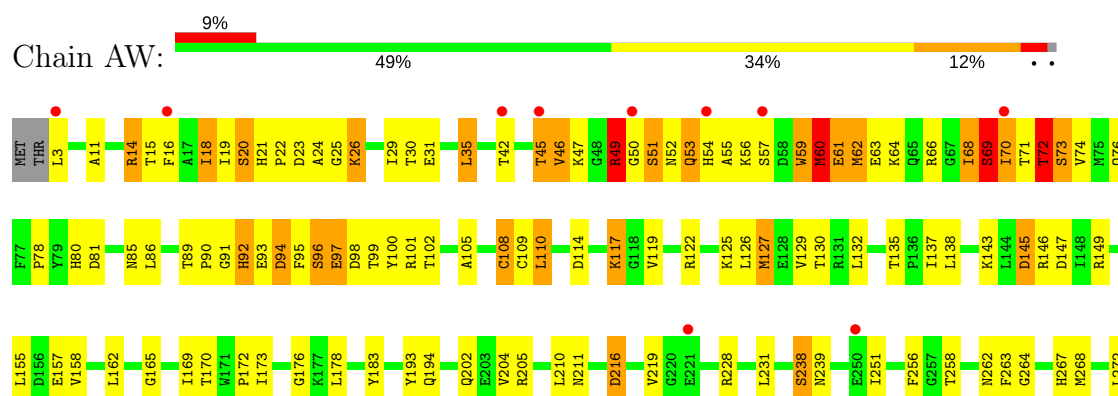
- Molecule 21: 30S ribosomal protein S21

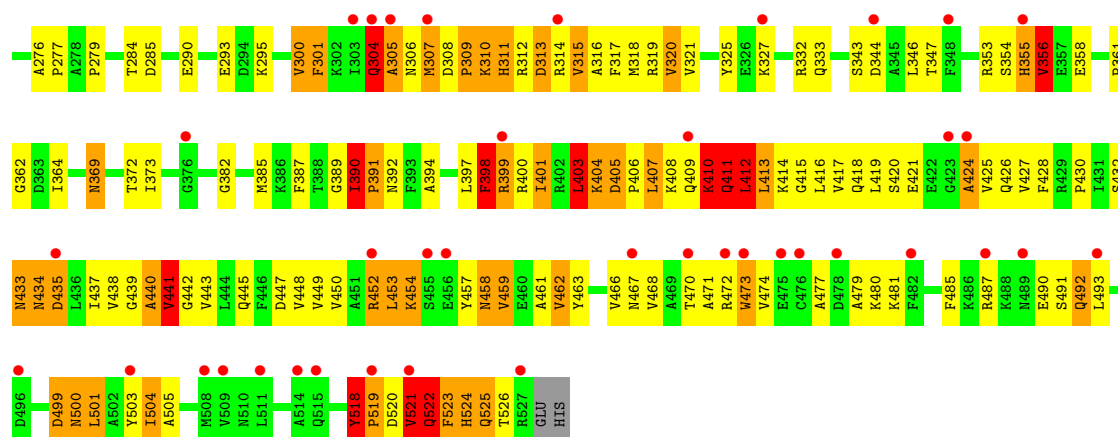


- Molecule 22: messenger RNA

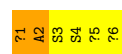


- Molecule 23: Peptide chain release factor 3

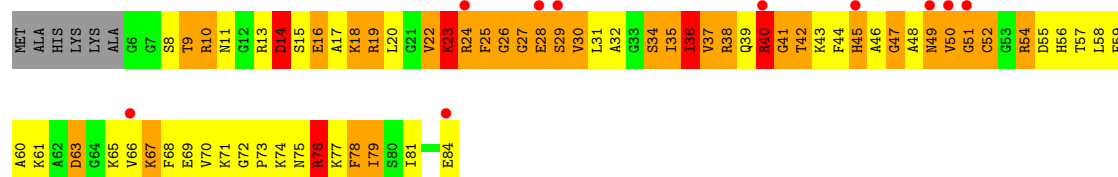




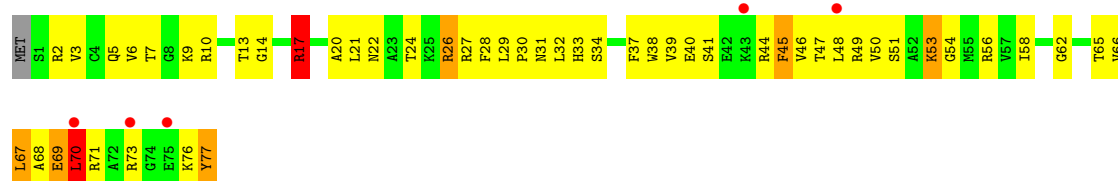
• Molecule 24: Viomycin



• Molecule 25: 50S ribosomal protein L27



• Molecule 26: 50S ribosomal protein L28

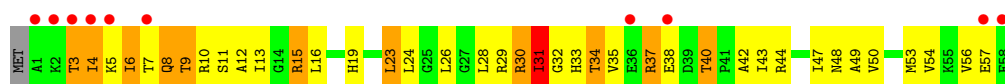


• Molecule 27: 50S ribosomal protein L29



• Molecule 28: 50S ribosomal protein L30

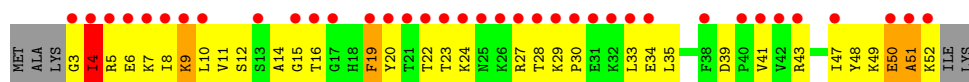




- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36 1

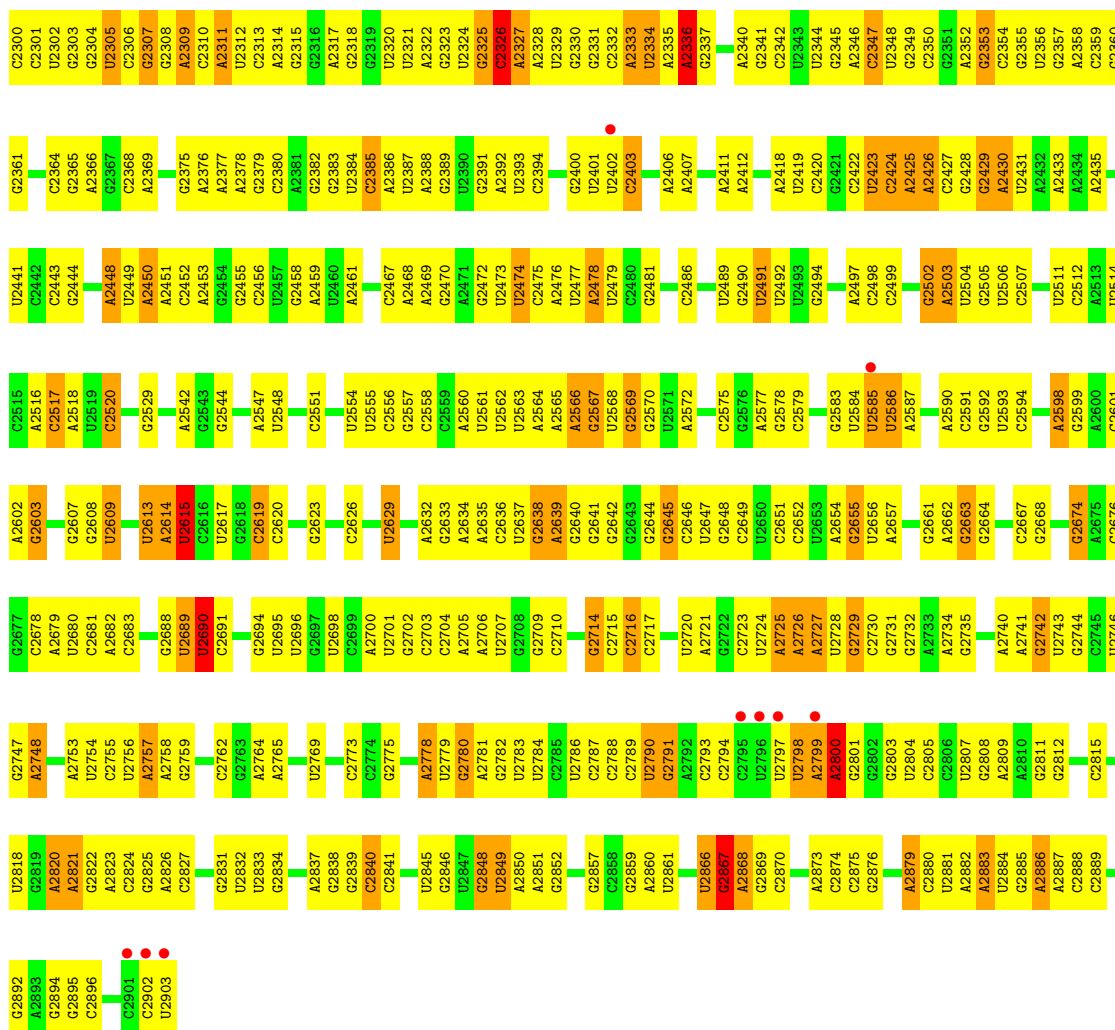


- Molecule 34: 23S rRNA



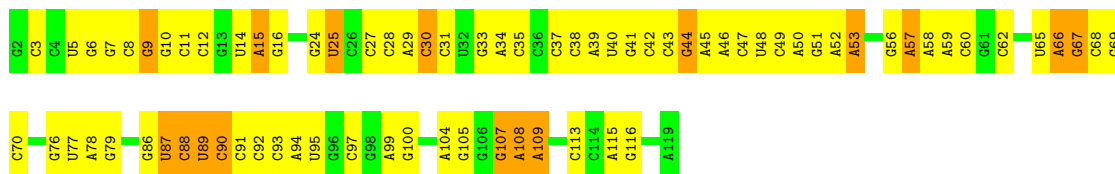
A1134	G1063	C992	G862	C796	U724	G651	A582	C509	C444	G372	C305	U234	U162
C1136	C1064	G993	A863	G797	G725	U652	G883	C510	C445	U373	U306	U235	C163
G1137	U1065	C994	G864	G798	G726	U653	G884	U511	G446	A374	G308	C236	C164
U1066	U929	C995	C865	G799	A727	A654	G885	G512	A447	C378	A309	G242	A167
G1138	A1067	A996	A866	A800	G728	A655	A586	A513	U448	G379	A310	U243	G168
U1069	G997	G997	C867	G801	G729	G656	U588	G518	A449	U380	A311	A244	G169
C1140	A1069	C998	U868	A802	A730	U657	U589	U519	C450	G381	G312	G245	U170
U1070	A1070	U999	C869	U803	C731	U658	A590	G520	U451	G382	A312	G246	U171
A1142	C1071	A1000	U870	A804	C732	G659	A591	U521	A452	C383	C314	G247	A172
A1143	A1001	G935	U871	G805	G733	C660	U591	A522	A454	C383	G315	G248	A173
A1144	U1072	G1002	U872	C809	C736	G662	U593	C523	C455	G386	G319	C249	
	G1074	C1005	G873	C812		G663	U594	G524		U387	A320	G250	A176
A1147	C1075	C1006	G874	C813	A739			U525	G458	G388	A321	A251	G177
U1148	G1076		G875	U813		A666	A599	U526	U459	U389	U321	G252	G178
G1149	U1077	A1010	C876	C814	A742	U667	G600	A527	U460	U390	A322	G253	C179
C1150	U1078	G1011	A877	C815	A743	A668	A601	A528	C461	U391	C323	G254	G180
A1151	C1079	U1012	A878	C816	U744	G669	G602	C531	C462	U392	A324	A255	A181
C1152	A1080	C1013	G879	C817	G745	A670	A603	A532	G463	C393	G325		A182
C1153	U1081	A1014	G880	C818	U746	C671	G604	A533	A466	G396	U328	G259	C183
G1154	U1082	U1015	G881	G819	U747	C672		G533	A467	U397	G329	G260	C184
A1155	U1083	G1016	G882	A819	A748	G673	A609	U534	C468	U398	A330	A265	G188
A1156	G948	U1017	U883	A820	A749	C674	C610	A538	C469	U399	G331	G266	G189
G1157	G949	G1018	U884	A821	A750	A675	G611	C540	A470	G400	A401	C267	A190
	G950	U1019	C885	C822	A752		G612		A471	G401	A402	C268	A191
C1161	A1086	A1020	A	C823	A753	C679	A613		A472	G402	A403	C269	C192
G1162	U1088	A1021	U	U824	A754	C680	A614		A473	U403	A404	A270	
A1165	A1089	G1022	C	A825	U755		U615		G474	U404	A405	G271	A195
G1166	A1090	U1023	C	U826	U756	U683	A616		G475	U405	A406	A272	A196
C1167	G956	G1024	C	U827	A756	U684	G617		G476	U406	A407	G273	A197
G1168	C957	G1025	G	U828		A685			A477	G408	C341	G274	C198
U1169	U958	G1026	A	A829	G760	U686	G620		A478	G409	A342	C275	A199
		A1027		C830	A761		A621		A479	G410	C343	U276	U200
C1170	C961	U1028	U894	U832	A764	A689	G622		A480	G411	A344	C277	C201
U1171	G962	A1029	U895	A833		G690	C623		C481	A412	A345	A278	U202
G1172	U963	C1030	A896	C834	G768	C691	A627		A482	C413	A346	A279	A203
C1173	C964	G1031	C897	C835	U769	C692	G628		A483	C414	A347	U280	A204
U1174	C964	A1032	C898	C836	G770	A693	G629		C486	U415	A348	C281	G205
A1175	U967	U1033	A899	G837	G771	U694	G630			C417	U349	A282	U206
	C968	U1034	A900	U839	C772		A631		C490	C418	A352	G283	A213
C1176	G971	A1035	C901	C838	G775	U702	A632		C491	C419	C353	U284	G214
G1177	A972	G1040	G902	C839	G776	G704	A633		A492	U419	C354	U285	G215
C1178	G974	U1041	G903	U840	G777	A705	C634		C493	C420	U355	U286	A216
U1180	A975	G1042	G904	C843	G778	A706	C635		C494	G424	U358	G287	A217
G1182	C976	C1043	G907	A844	G779	G707	A636		C495	C425	U359	U288	A218
U1183	A979	U1044	A910	A845	U779	G708	A637		C496	C426	U360	U289	G219
C1184	A980	G1045	A911	U846	U780	G709	G638		A497	U427	G361	U290	A220
G1185	A981	A1046	C912	U847	A781	U710	G639		C498	U428	A362	U293	A221
U1186	U982	A1047	U913	U848	A782	G711	C640		U499	A432	A363	A294	A222
C1187	C982	G1048	C914	U849	G783	G712	U641		G500	C433	G364	U295	C225
U1188	A983	U1049	C915	U850	G784	G713	A643		A501	U434	U365	U296	
G1189	A984	A1050	G916	U851	G785	U714	A644		A502	C435	G297	G298	C228
A1126	C985	G1055	A917	C855	C786	A715	C645		A503	C436	G366		C229
U1129	C986	G1056	A918	C856	A788	U716	C646		A504	U437	G367		G230
U1198	C987	U1057	U919	C857	A789	C717	G647		A505	U441	A368	G301	A231
U1199	A988	G1058	A920	C858			G648		G506	G442	U369	C302	G232
C1200	G989	U1060	C921	C859	A794	A721	G649		A507	G443	G370	G303	
A1205	A990	G1062	G922	U860	A795	A722			A508	A443	A371	U304	A233
	C991		G923	A861	C795	C723							

U2229	G	C2096	G1945	C1870	G1799	C1726	U1629	G1560	G1489	G1416	C1349	G1278	G1206
G2230	C	A2097	U1946	A1871	C1800	C1727	C1638	C1561	A1490	C1417	C1352	G1279	C1211
U2231	C	G2102	C1947	A1872	A1801	C1728	C1639	U1562	G1491	G1418	U1352	G1280	G1212
U2233	C	C2103	A1952	G1873	G	U1729	C1638	U1563	G1492	A1419	A1353	A1286	A1213
U2234	A	C2104	A1962	C1874	A1805	G1730	C1644	C1564	C1493	A1420	A1354	A1287	G1216
G2237	C	U2105	G1954	C1875	A1808	G1731	G	A1566	A1494	G1421	G1355	G1288	G1217
G2238	U	U2106	U1955	A1876	A1809	C1732	U1647	A1567	A1495	G1422	G1358	C1289	U1218
G2239	U	G2107	U1956	G1884	A1810	G1733	U1648	G1568	A1497	A1427	A1359	C1290	U1219
U2243	A	A2108	C1957	A1885	G1811	G1734	U1649	A1569	C1498	G1428	A1360	G1291	G1223
U2244	A	U2109	U1986	A1886	G1812	A1735	A1650	A1570	C1499	G1429	G1361	G1292	U1224
U2245	A	U	C1962	C1887	G1813	G1737	G1651	A1571	G1500	G1430	C1362	C1293	G1225
G2248	U	G	U1963	G1888	G1814	G1738	A1652	U1572	G1501	A1431	C1363	G1297	
U2249	A	U	G1964	A1889	A1815	A1739	G1653	G	A1502	G1432	G1364	G1297	
U2250	A	U	C1965	C1893	G1816	G1740	A1654	U1576	A1503	A1434	A1365	G1300	C1229
G2255	C	A	A1966	C1894	U1818	C1741	A1655	C1577	A1504	A1434	G1368	A1301	U1230
G2256	C	G	G1967	C1895	U1819	U1742	C1656	U1578	A1505	G1435	G1368	A1302	U1231
G2257	C	A	G1968	C1900	A1820	G1743	U1657	G	U1506	G1436	G1371	G1303	G1232
G2258	C	U	A1969	A1900	A1821	A1744	A1665	G1581	C1507	C1437	G1371	G1304	C1233
G2259	C	U	A1970	A1901	G1822	A1745	A1666	U1582	A1508	U1443	G1374	C1305	U1234
G2260	C	U	U1971	A1902	G1823	G	G1667	U1584	A1509	G1444	U1375	C1306	G1235
G2261	C	U	G1972	G1903	G1824	U1746	A1668	U1585	G1510	G1444	C1376	C1307	G1236
G2262	C	U	G1973	G1904	G1825	A1747	A1669	A1586	G1511	G1450	C1377	A1308	A1237
G2263	C	U	C1974	C1905	G1826	G1756	G	G1587	A1515	G1451	A1378	G1309	G1238
G2264	C	U	U1984	G1906	U1827	A1757	G1674	G1588	G1516	G1452	U1379	G1313	G1239
A2268	U	U2194	C1985	C1908	G1828	U1758	C1675	U1589	C1517	A1453	G1380	C1314	U1240
G2269	U	U2195	U1986	C1909	U1829	A1759	A1676	A1590	C1518	G1454	G1381	C1314	A1244
G2270	U	U2196	C1986	G1910	G1830	C1760	A1677	C1591	G1519	G1455	C1382	C1315	G1245
A2273	U	U2187	C1986	G1910	G1831	C1761	A1677	C1592	G1520	G1456	A1383	U1316	
A2274	U	U2188	C1990	G1911	G1832	G1762	U1682	A1593	G1521	G1457	A1384	G1317	G1248
G2275	U	U2189	U1991	A1912	C1833	C1764	U1683	U1594	A1522	U1458	A1385	U1318	G1249
G2276	U	U2190	G1992	A1913	G1838	U1765	G1687	U1595	U1523	G1459	C1386	C1319	U1249
G2277	U	U2191	U1993	C1914	G1839	A1773	U1688	A1596	G1524	C1461	A1387	C1320	G1250
A2278	U	U2192	C1996	U1915	G1840	C1774	U1688	U1597	A1525	C1462	A1388	C1321	C1251
G2279	U	U2193	C1997	G1917	U1841	U1775	U1692	U1599	G1530	G1463	C1389	C1322	G1252
G2280	U	U2194	A1998	A1918	G1842	G1776	U1693	C1600	C1531	G1464	U1390	C1323	A1253
G2281	U	U2195	C1999	A1919	G1843	U1777	U1694	G1601	A1532	G1465	A1392	U1255	U1254
G2282	U	U2196	C2000	C1920	G1844	U1778	G1695	U1602	C1533	U1466	A1393	G1324	G1256
G2283	U	U2197	G2004	G1921	G1846	U1779	A1701	A1603	U1534	U1467	U1394	A1328	C1257
G2284	U	U2198	A2005	G1922	A1847	A1780	A1701	G1604	A1535	U1468	A1395	U1329	U1258
G2285	U	U2199	C2006	G1923	G1848	U1781	A1705	C1605	G1536	A1469	U1396	G1259	G1260
G2286	U	U2200	A2013	C1924	G1850	U1782	A1705	G1537	G1538	A1470	C1397	G1332	A1261
G2287	U	U2201	A2014	U1925	U1851	A1783	C1706	A1608	G1539	U1474	C1398	G1333	A1262
G2288	U	U2202	A2015	A1926	U1852	A1784	C1707	A1609	U1539	G1475	C1399	G1334	A1263
G2289	U	U2203	A2016	A1927	A1853	A1785	C1708	A1610	G1540	U1476	U1400	C1335	A1264
G2290	U	U2204	U2016	A1928	A1854	U1786	U1709	G1613	C1541	A1477	G1401	A1336	G1265
G2291	U	U2205	U2017	G1929	U1855	A1787	G1710	U1614	U1542	U1478	U1402	G1337	G1266
G2292	U	U2206	U2018	U1930	U1856	C1788	G1718	C1615	G1543	G1479	C1403	G1338	U1267
G2293	U	U2207	A2019	U1931	G1857	A1789	U1714	A1616	A1544	C1480	C1404	G1339	A1268
G2294	U	U2208	A2020	C1934	U1858	A1791	G1715	A1617	A1545	U1481	U1405	C1340	A1269
G2295	U	U2209	A2021	U1935	A1859	A1792	A1716	C1617	G1546	U1482	U1406	G1341	C1270
G2296	U	U2210	A2022	A1936	G1860	C1793	A1717	A1618	C1550	G1483	U1409	C1342	G1271
G2297	U	U2211	C2023	A1937	G1861	U1794	G1718	G1619	C1551	U1484	U1410	G1343	A1272
G2298	U	U2212	G2024	A1938	G1862	C1795	A1722	U1621	A1552	U1485	U1411	C1345	A1273
G2299	U	U2213	G2025	U1943	U1864	U1796	G1723	G1622	C1558	U1486	C1414	G1346	A1274
G2300	U	U2214	U2026	U1944	G1869	U1797	G1724	G1623	C1559	U1487	A1415	A1347	A1275
G2301	U	U2215	G2027			U1798	U1725	G1628		U1488		C1348	G1277



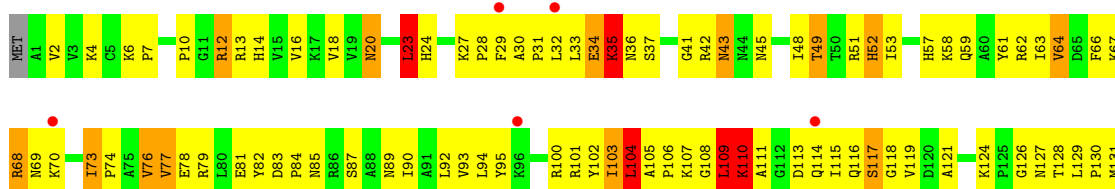
• Molecule 35: 5S ribosomal RNA

Chain BB: 36% 51% 14%



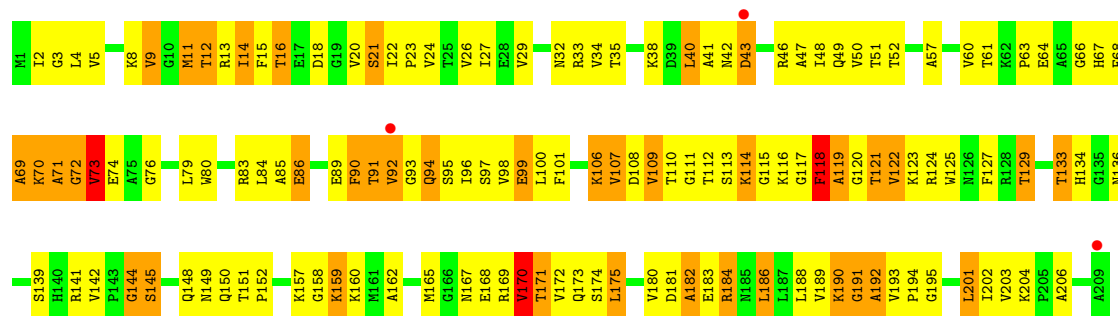
• Molecule 36: 50S ribosomal protein L2

Chain BC: 4% 32% 51% 15%

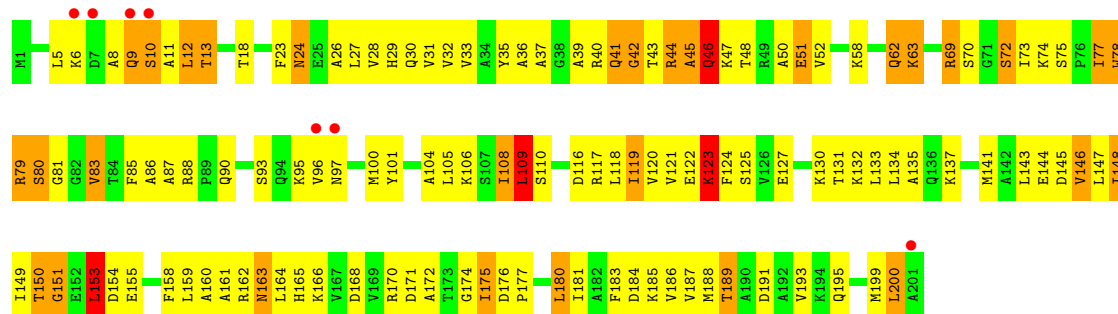




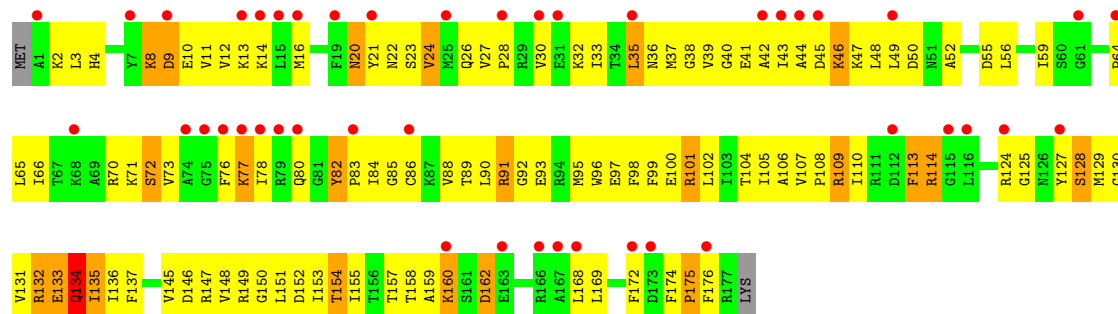
• Molecule 37: 50S ribosomal protein L3



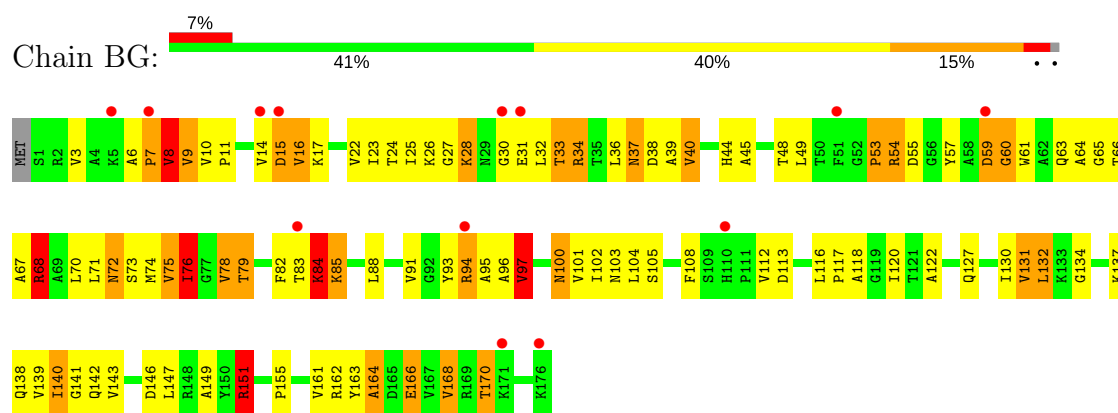
• Molecule 38: 50S ribosomal protein L4



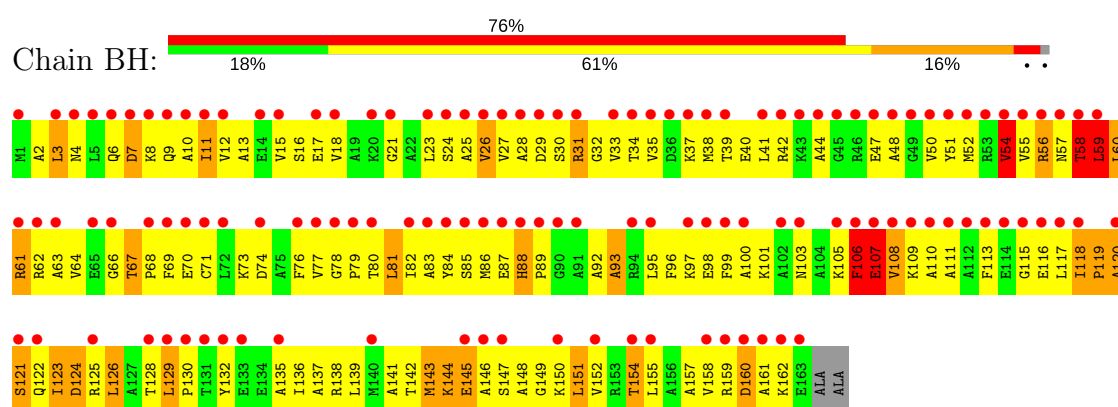
• Molecule 39: 50S ribosomal protein L5



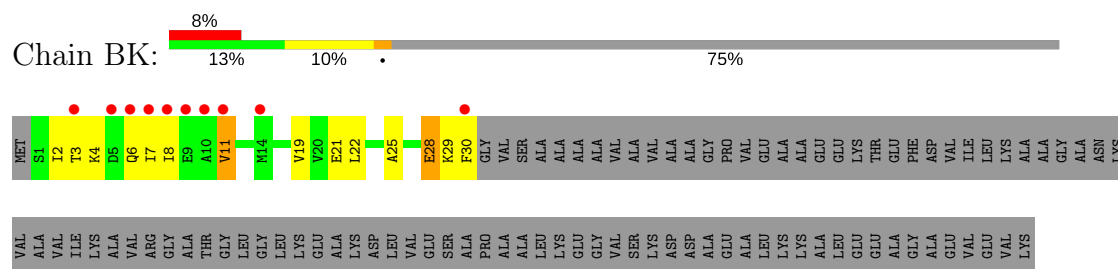
- Molecule 40: 50S ribosomal protein L6



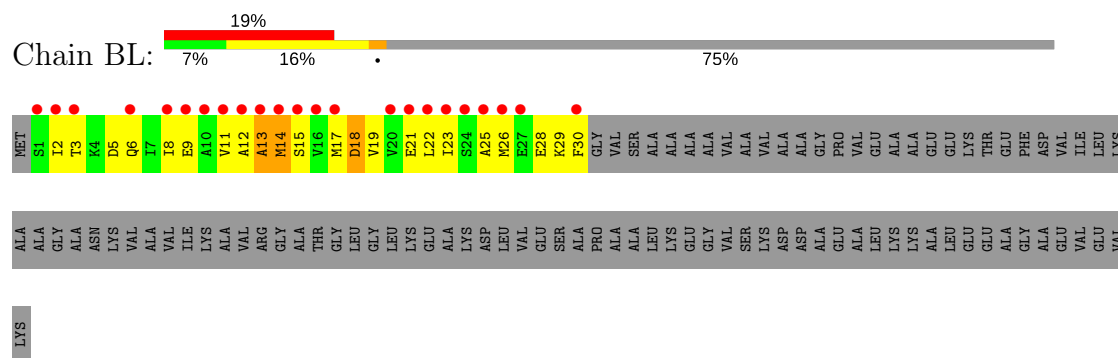
- Molecule 41: 50S ribosomal protein L10



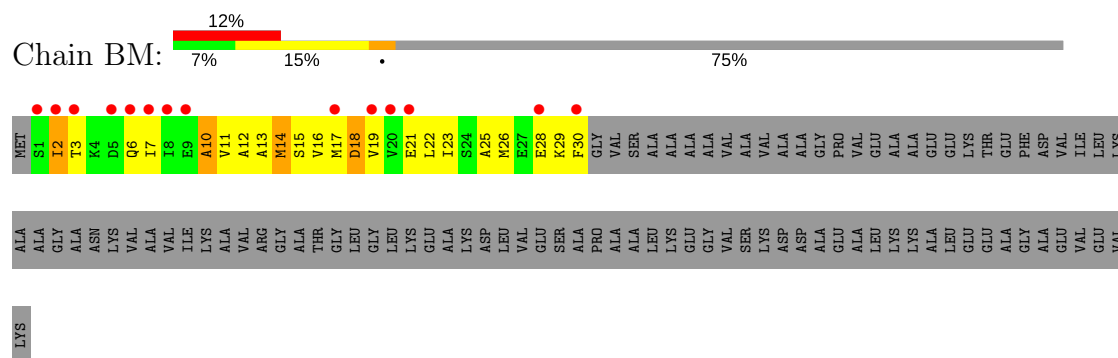
- Molecule 43: 50S ribosomal protein L7/L12



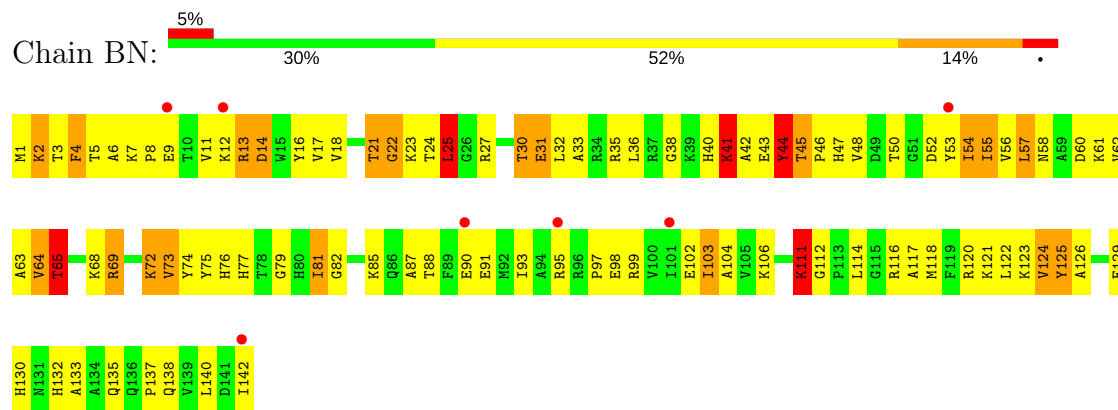
- Molecule 43: 50S ribosomal protein L7/L12



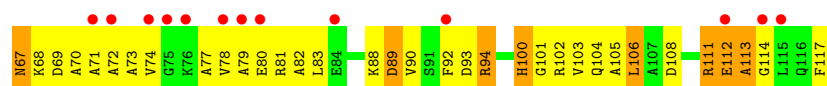
- Molecule 43: 50S ribosomal protein L7/L12



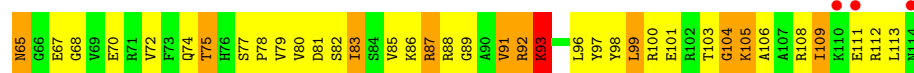
- Molecule 44: 50S ribosomal protein L13



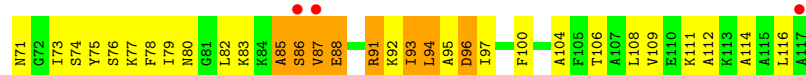
- Molecule 45: 50S ribosomal protein L14



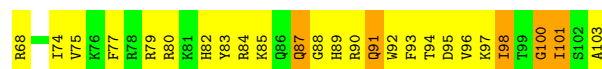
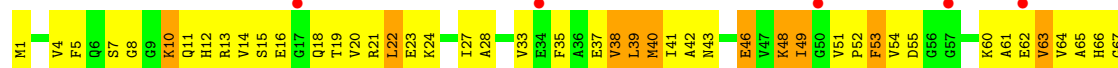
- Molecule 50: 50S ribosomal protein L19



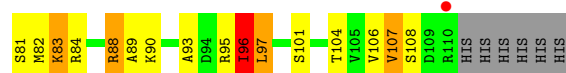
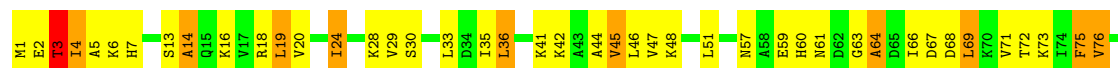
- Molecule 51: 50S ribosomal protein L20



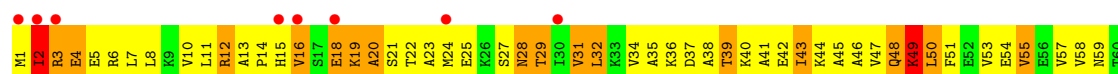
- Molecule 52: 50S ribosomal protein L21

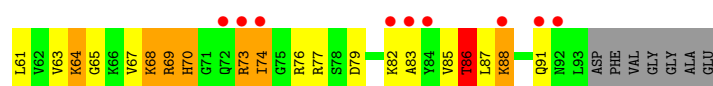


- Molecule 53: 50S ribosomal protein L22

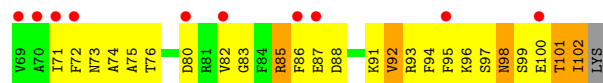
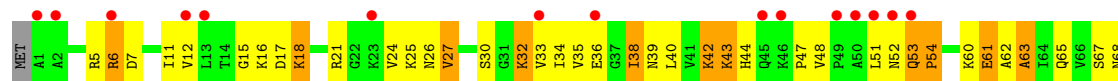


- Molecule 54: 50S ribosomal protein L23

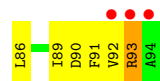




- Molecule 55: 50S ribosomal protein L24 1



- Molecule 56: 50S ribosomal protein L25 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 59.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 99.9 (59.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2, phenix	Depositor
R, R_{free}	0.210 , 0.250 0.228 , 0.255	Depositor DCC
R_{free} test set	21747 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	147221	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	AL	0	1
23	AW	0	2
24	AY	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	2106	U	O3'-P	20.78	1.86	1.61
34	BA	2183	A	O3'-P	15.69	1.79	1.61
34	BA	974	G	O3'-P	-15.38	1.42	1.61
34	BA	973	A	O3'-P	-13.70	1.44	1.61
34	BA	974	G	N7-C5	-6.57	1.35	1.39

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

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

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32873	0	16542	1452	0
2	AB	1704	0	1732	189	0
3	AC	1624	0	1699	162	7
4	AD	1643	0	1710	196	0
5	AE	1105	0	1148	135	0
6	AF	817	0	808	102	0
7	AG	1181	0	1240	70	0
8	AH	979	0	1034	91	0
9	AI	1022	0	1070	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	786	0	828	97	0
11	AK	877	0	887	104	0
12	AL	955	0	1019	123	0
13	AM	883	0	944	96	0
14	AN	774	0	827	90	0
15	AO	714	0	737	45	0
16	AP	649	0	666	63	0
17	AQ	648	0	691	62	0
18	AR	455	0	478	41	0
19	AS	637	0	665	70	0
20	AT	665	0	714	60	0
21	AU	425	0	449	67	0
22	AV	129	0	65	9	0
23	AW	4144	0	4127	284	0
24	AY	48	0	40	31	0
25	B0	596	0	610	166	0
26	B1	625	0	655	54	0
27	B2	509	0	543	40	0
28	B3	449	0	491	53	0
29	B4	444	0	461	33	0
30	B5	409	0	440	39	0
31	B6	377	0	418	20	0
32	B7	504	0	574	49	0
33	B8	302	0	340	40	0
34	BA	61252	0	30808	2055	7
35	BB	2529	0	1281	94	0
36	BC	2082	0	2157	226	0
37	BD	1565	0	1616	201	0
38	BE	1552	0	1619	151	0
39	BF	1410	0	1447	142	0
40	BG	1323	0	1374	134	0
41	BH	1230	0	1282	253	0
42	BI	1032	0	1088	85	0
43	BJ	227	0	237	48	0
43	BK	227	0	237	23	0
43	BL	227	0	237	38	0
43	BM	227	0	237	47	0
44	BN	1129	0	1162	147	0
45	BO	938	0	1012	117	0
46	BP	1045	0	1117	108	0
47	BQ	1074	0	1157	79	0
48	BR	960	0	1000	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	BS	892	0	923	77	0
50	BT	917	0	965	123	0
51	BU	947	0	1022	108	0
52	BV	816	0	839	96	0
53	BW	856	0	922	55	0
54	BX	738	0	807	110	0
55	BY	779	0	834	74	0
56	BZ	753	0	780	54	0
57	AA	102	0	0	0	0
57	AF	1	0	0	0	0
57	AH	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	1	0	0	0	0
57	AW	1	0	0	0	0
57	B0	3	0	0	0	0
57	B2	1	0	0	0	0
57	B4	1	0	0	0	0
57	BA	357	0	0	0	0
57	BB	9	0	0	0	0
57	BC	1	0	0	0	0
57	BD	5	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	BR	2	0	0	0	0
57	BT	1	0	0	0	0
57	BX	1	0	0	0	0
58	AW	32	0	13	6	0
59	AW	2	0	0	2	0
59	B8	1	0	0	0	0
59	BA	8	0	0	0	0
59	BC	2	0	0	0	0
59	BD	1	0	0	0	0
59	BF	1	0	0	0	0
59	BG	1	0	0	0	0
59	BW	1	0	0	1	0
All	All	147221	0	100825	8116	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 8116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1495:U:O4	24:AY:1:KBE:CE	1.84	1.26
1:AA:1494:G:N7	24:AY:1:KBE:HGA	1.52	1.24
1:AA:1494:G:O6	24:AY:1:KBE:HG	1.35	1.22
1:AA:1495:U:C4	24:AY:1:KBE:HE	1.75	1.20
51:BU:63:ARG:NH1	51:BU:96:ASP:HA	1.58	1.18

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BM	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	9
44	BN	140/142 (99%)	101 (72%)	24 (17%)	15 (11%)	0	3
45	BO	120/123 (98%)	88 (73%)	19 (16%)	13 (11%)	0	3
46	BP	141/144 (98%)	88 (62%)	34 (24%)	19 (14%)	0	1
47	BQ	134/136 (98%)	104 (78%)	18 (13%)	12 (9%)	1	5
48	BR	118/127 (93%)	86 (73%)	20 (17%)	12 (10%)	1	4
49	BS	114/117 (97%)	90 (79%)	14 (12%)	10 (9%)	1	5
50	BT	112/115 (97%)	74 (66%)	21 (19%)	17 (15%)	0	1
51	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	13
52	BV	101/103 (98%)	75 (74%)	18 (18%)	8 (8%)	1	7
53	BW	108/116 (93%)	89 (82%)	15 (14%)	4 (4%)	4	26
54	BX	91/100 (91%)	49 (54%)	23 (25%)	19 (21%)	0	0
55	BY	100/104 (96%)	65 (65%)	22 (22%)	13 (13%)	0	2
56	BZ	92/94 (98%)	72 (78%)	14 (15%)	6 (6%)	1	11
All	All	6272/6999 (90%)	4427 (71%)	1181 (19%)	664 (11%)	0	3

5 of 664 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	145 (81%)	35 (19%)	1	8
3	AC	170/190 (90%)	146 (86%)	24 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	152 (88%)	20 (12%)	6	27
5	AE	113/126 (90%)	95 (84%)	18 (16%)	3	13
6	AF	87/112 (78%)	73 (84%)	14 (16%)	3	13
7	AG	124/129 (96%)	121 (98%)	3 (2%)	54	84
8	AH	104/105 (99%)	94 (90%)	10 (10%)	10	37
9	AI	105/107 (98%)	92 (88%)	13 (12%)	5	24
10	AJ	86/90 (96%)	70 (81%)	16 (19%)	2	9
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	10
12	AL	103/104 (99%)	89 (86%)	14 (14%)	4	20
13	AM	92/96 (96%)	87 (95%)	5 (5%)	26	65
14	AN	79/84 (94%)	71 (90%)	8 (10%)	9	34
15	AO	76/77 (99%)	66 (87%)	10 (13%)	5	21
16	AP	65/65 (100%)	57 (88%)	8 (12%)	5	25
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	10
18	AR	48/65 (74%)	44 (92%)	4 (8%)	13	46
19	AS	70/79 (89%)	64 (91%)	6 (9%)	12	43
20	AT	65/66 (98%)	60 (92%)	5 (8%)	15	50
21	AU	44/61 (72%)	37 (84%)	7 (16%)	3	13
23	AW	447/453 (99%)	381 (85%)	66 (15%)	3	16
24	AY	2/2 (100%)	2 (100%)	0	100	100
25	B0	59/63 (94%)	42 (71%)	17 (29%)	0	1
26	B1	67/68 (98%)	56 (84%)	11 (16%)	2	12
27	B2	55/55 (100%)	46 (84%)	9 (16%)	2	12
28	B3	48/49 (98%)	39 (81%)	9 (19%)	2	9
29	B4	47/48 (98%)	40 (85%)	7 (15%)	3	16
30	B5	45/49 (92%)	42 (93%)	3 (7%)	19	56
31	B6	38/38 (100%)	34 (90%)	4 (10%)	8	32
32	B7	51/52 (98%)	48 (94%)	3 (6%)	23	62
33	B8	34/34 (100%)	32 (94%)	2 (6%)	23	62
36	BC	216/218 (99%)	177 (82%)	39 (18%)	2	10
37	BD	164/164 (100%)	143 (87%)	21 (13%)	5	23

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

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

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

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

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

5.3.3 RNA ⓘ

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

5 of 893 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	KBE	AY	1	24	8,8,9	0.56	0	7,8,10	1.28	1 (14%)
24	DPP	AY	2	24	4,5,6	1.97	1 (25%)	1,5,7	3.37	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	UAL	AY	5	24	8,8,9	2.32	3 (37%)	4,9,11	1.31	1 (25%)
24	5OH	AY	6	24	8,12,13	1.07	1 (12%)	5,16,18	0.81	0

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	5	UAL	C1-N1	-2.87	1.35	1.40
24	AY	5	UAL	CB-CA	2.19	1.41	1.35
24	AY	6	5OH	CA-C	2.73	1.53	1.50
24	AY	2	DPP	CA-C	3.40	1.54	1.50
24	AY	5	UAL	C-CA	4.97	1.53	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	2	DPP	O-C-CA	-3.37	115.72	125.02
24	AY	5	UAL	O-C-CA	-2.38	122.42	125.47
24	AY	1	KBE	CB-CA-C	2.73	116.38	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	GNP	AW	602	-	27,34,34	2.89	6 (22%)	26,54,54	1.90	8 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GNP	AW	602	-	-	0/16/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AW	602	GNP	C4-N9	-8.15	1.36	1.47
58	AW	602	GNP	C5-C6	-7.89	1.38	1.53
58	AW	602	GNP	C8-N9	-3.06	1.37	1.46
58	AW	602	GNP	PB-O3A	-2.52	1.56	1.59
58	AW	602	GNP	C6-N1	3.56	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AW	602	GNP	PA-O3A-PB	-4.62	116.08	132.38
58	AW	602	GNP	O3G-PG-O1G	-2.92	105.98	113.41
58	AW	602	GNP	C5'-C4'-C3'	-2.20	106.90	115.29
58	AW	602	GNP	O1G-PG-N3B	-2.18	108.53	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	AW	602	GNP	O1B-PB-N3B	2.77	115.94	111.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1532/1533 (99%)	0.45	120 (7%) 14 8	51, 102, 197, 245	0
2	AB	218/241 (90%)	1.47	65 (29%) 1 1	91, 120, 142, 158	0
3	AC	206/233 (88%)	0.54	20 (9%) 8 5	75, 114, 132, 139	0
4	AD	205/206 (99%)	1.36	59 (28%) 1 1	86, 110, 132, 147	0
5	AE	150/167 (89%)	0.22	4 (2%) 55 40	73, 94, 129, 143	0
6	AF	100/131 (76%)	0.94	20 (20%) 1 1	98, 122, 135, 145	0
7	AG	151/156 (96%)	2.24	78 (51%) 0 0	107, 144, 159, 163	0
8	AH	129/130 (99%)	0.66	10 (7%) 14 8	77, 97, 121, 139	0
9	AI	127/130 (97%)	1.63	37 (29%) 1 1	77, 122, 148, 159	0
10	AJ	98/103 (95%)	1.22	19 (19%) 1 1	89, 106, 143, 156	0
11	AK	117/129 (90%)	0.61	9 (7%) 14 8	73, 105, 133, 150	0
12	AL	123/124 (99%)	0.58	5 (4%) 38 25	55, 74, 111, 143	0
13	AM	114/118 (96%)	3.29	71 (62%) 0 0	137, 149, 163, 165	0
14	AN	96/101 (95%)	2.49	42 (43%) 0 0	79, 128, 152, 160	0
15	AO	88/89 (98%)	0.51	7 (7%) 13 7	79, 101, 131, 142	0
16	AP	82/82 (100%)	1.59	27 (32%) 0 0	72, 95, 131, 147	0
17	AQ	80/84 (95%)	1.93	30 (37%) 0 0	78, 111, 136, 147	0
18	AR	55/75 (73%)	1.20	10 (18%) 1 1	77, 101, 126, 165	0
19	AS	79/92 (85%)	4.26	59 (74%) 0 0	131, 153, 159, 164	0
20	AT	85/87 (97%)	0.95	13 (15%) 2 1	80, 105, 126, 142	0
21	AU	51/71 (71%)	2.07	23 (45%) 0 0	106, 132, 153, 157	0
22	AV	6/27 (22%)	5.59	6 (100%) 0 0	181, 198, 202, 206	0
23	AW	525/529 (99%)	0.59	49 (9%) 9 6	47, 99, 188, 267	0
24	AY	2/6 (33%)	-0.15	0 100 100	85, 85, 85, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	79/85 (92%)	1.02	10 (12%) 4 3	62, 87, 115, 129	0
26	B1	77/78 (98%)	0.59	5 (6%) 20 11	55, 71, 124, 126	0
27	B2	63/63 (100%)	0.18	4 (6%) 21 12	69, 101, 126, 140	0
28	B3	58/59 (98%)	0.85	10 (17%) 2 1	63, 75, 121, 129	0
29	B4	56/57 (98%)	0.22	4 (7%) 17 10	42, 63, 97, 125	0
30	B5	50/55 (90%)	3.28	37 (74%) 0 0	114, 128, 137, 151	0
31	B6	46/46 (100%)	0.42	2 (4%) 36 23	43, 56, 77, 114	0
32	B7	64/65 (98%)	0.37	0 100 100	57, 68, 83, 90	0
33	B8	38/38 (100%)	0.51	0 100 100	61, 78, 90, 105	0
34	BA	2853/2903 (98%)	0.28	132 (4%) 33 20	35, 67, 195, 445	0
35	BB	118/118 (100%)	0.02	0 100 100	61, 106, 152, 188	0
36	BC	271/273 (99%)	0.27	10 (3%) 42 27	36, 66, 83, 108	0
37	BD	209/209 (100%)	0.01	3 (1%) 75 63	37, 57, 89, 99	0
38	BE	201/201 (100%)	0.18	7 (3%) 44 29	37, 76, 109, 131	0
39	BF	177/179 (98%)	1.32	44 (24%) 1 1	106, 128, 152, 165	0
40	BG	176/177 (99%)	0.41	13 (7%) 15 9	54, 80, 117, 131	0
41	BH	163/165 (98%)	4.73	125 (76%) 0 0	80, 145, 163, 185	1 (0%)
42	BI	141/142 (99%)	3.87	111 (78%) 0 0	135, 157, 169, 176	0
43	BJ	30/121 (24%)	1.38	7 (23%) 1 1	126, 137, 143, 145	0
43	BK	30/121 (24%)	1.64	10 (33%) 0 0	133, 146, 152, 156	0
43	BL	30/121 (24%)	4.10	23 (76%) 0 0	132, 148, 158, 163	0
43	BM	30/121 (24%)	2.72	14 (46%) 0 0	128, 142, 149, 151	0
44	BN	142/142 (100%)	0.47	7 (4%) 30 18	45, 65, 91, 117	0
45	BO	122/123 (99%)	0.24	3 (2%) 58 43	41, 61, 84, 104	0
46	BP	143/144 (99%)	0.60	14 (9%) 8 5	41, 84, 112, 132	0
47	BQ	136/136 (100%)	0.42	6 (4%) 35 22	47, 70, 100, 126	0
48	BR	120/127 (94%)	0.30	3 (2%) 58 43	40, 56, 72, 138	0
49	BS	116/117 (99%)	1.43	33 (28%) 1 1	81, 100, 121, 128	0
50	BT	114/115 (99%)	0.25	5 (4%) 35 22	48, 71, 112, 121	0
51	BU	117/118 (99%)	0.10	3 (2%) 56 41	37, 59, 94, 108	0
52	BV	103/103 (100%)	0.35	5 (4%) 30 18	43, 86, 111, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
53	BW	110/116 (94%)	-0.04	1 (0%) 84 75	41, 54, 82, 127	0
54	BX	93/100 (93%)	1.03	17 (18%) 1 1	50, 81, 134, 144	0
55	BY	102/104 (98%)	1.29	25 (24%) 1 1	63, 84, 126, 141	0
56	BZ	94/94 (100%)	0.63	9 (9%) 9 5	68, 94, 113, 126	0
All	All	10891/11580 (94%)	0.77	1485 (13%) 3 2	35, 89, 165, 445	1 (0%)

The worst 5 of 1485 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	BH	88	HIS	21.3
34	BA	2903	U	20.8
19	AS	55	GLN	17.4
41	BH	84	TYR	17.3
41	BH	112	ALA	16.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
24	DPP	AY	2	6/7	0.81	0.31	-	79,82,82,84	0
24	UAL	AY	5	9/10	0.72	0.30	-	81,82,83,84	0
24	KBE	AY	1	9/10	0.51	0.60	-	78,79,82,82	0
24	5OH	AY	6	12/13	0.81	0.30	-	84,89,92,94	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
57	MG	BA	3223	1/1	0.83	1.05	44.83	75,75,75,75	0
57	MG	BA	3244	1/1	0.93	0.46	41.06	76,76,76,76	0
57	MG	AA	1603	1/1	0.96	0.44	37.43	42,42,42,42	0
57	MG	BA	3011	1/1	0.99	0.50	28.30	23,23,23,23	0
57	MG	BA	3341	1/1	0.93	0.52	19.53	57,57,57,57	0
57	MG	BA	3182	1/1	0.97	0.57	18.44	48,48,48,48	0
57	MG	BA	3099	1/1	0.94	0.45	17.87	44,44,44,44	0
57	MG	BA	3073	1/1	0.98	0.49	17.08	42,42,42,42	0
57	MG	BA	3096	1/1	0.94	0.36	16.35	44,44,44,44	0
57	MG	BA	3054	1/1	0.97	0.43	16.19	36,36,36,36	0
57	MG	BA	3013	1/1	0.99	0.38	15.99	20,20,20,20	0
57	MG	BA	3074	1/1	0.95	0.40	15.89	44,44,44,44	0
57	MG	BA	3052	1/1	0.99	0.38	15.79	39,39,39,39	0
57	MG	BA	3177	1/1	0.85	0.48	15.64	59,59,59,59	0
57	MG	BA	3001	1/1	0.97	0.42	15.01	42,42,42,42	0
57	MG	BD	304	1/1	0.98	0.41	14.72	28,28,28,28	0
57	MG	BA	3047	1/1	0.90	0.42	14.27	51,51,51,51	0
57	MG	BA	3024	1/1	0.98	0.43	13.94	32,32,32,32	0
57	MG	BA	3130	1/1	0.91	0.43	13.93	41,41,41,41	0
57	MG	BA	3039	1/1	0.98	0.40	13.88	31,31,31,31	0
57	MG	BA	3003	1/1	0.97	0.42	13.81	18,18,18,18	0
57	MG	BA	3066	1/1	0.98	0.49	13.41	41,41,41,41	0
57	MG	AA	1677	1/1	0.88	0.48	13.06	57,57,57,57	0
57	MG	BA	3092	1/1	0.98	0.54	12.96	43,43,43,43	0
57	MG	BA	3138	1/1	0.90	0.33	11.63	58,58,58,58	0
57	MG	BA	3280	1/1	0.73	0.35	11.30	73,73,73,73	0
57	MG	BA	3045	1/1	0.97	0.46	10.85	35,35,35,35	0
57	MG	BA	3032	1/1	0.96	0.54	10.40	38,38,38,38	0
57	MG	BA	3042	1/1	0.98	0.33	9.85	27,27,27,27	0
57	MG	AA	1631	1/1	0.81	0.32	9.80	60,60,60,60	0
57	MG	BA	3070	1/1	0.92	0.34	9.80	44,44,44,44	0
57	MG	AA	1611	1/1	0.96	0.40	9.42	44,44,44,44	0
57	MG	AA	1606	1/1	0.89	0.36	9.21	45,45,45,45	0
57	MG	AA	1604	1/1	0.90	0.50	9.14	42,42,42,42	0
57	MG	BA	3016	1/1	0.94	0.38	8.95	39,39,39,39	0
57	MG	BA	3316	1/1	0.80	0.32	8.67	61,61,61,61	0
57	MG	BA	3151	1/1	0.86	0.33	8.52	47,47,47,47	0
57	MG	AA	1616	1/1	0.95	0.35	8.40	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3294	1/1	0.82	0.27	8.11	43,43,43,43	0
57	MG	BA	3090	1/1	0.98	0.46	7.91	40,40,40,40	0
57	MG	BA	3125	1/1	0.85	0.53	7.79	53,53,53,53	0
57	MG	BA	3262	1/1	0.89	0.29	7.60	85,85,85,85	0
57	MG	BA	3083	1/1	0.93	0.35	7.50	47,47,47,47	0
57	MG	BA	3103	1/1	0.97	0.33	7.30	28,28,28,28	0
57	MG	BA	3150	1/1	0.80	0.40	7.18	53,53,53,53	0
57	MG	BA	3174	1/1	0.91	0.26	6.94	49,49,49,49	0
57	MG	BD	302	1/1	0.87	0.48	6.61	53,53,53,53	0
57	MG	BA	3084	1/1	0.99	0.32	6.25	21,21,21,21	0
57	MG	BA	3181	1/1	0.85	0.27	6.23	44,44,44,44	0
57	MG	BA	3188	1/1	0.92	0.27	6.16	51,51,51,51	0
57	MG	BA	3022	1/1	0.95	0.29	5.95	28,28,28,28	0
57	MG	BA	3102	1/1	0.96	0.31	5.86	36,36,36,36	0
57	MG	BA	3026	1/1	0.95	0.30	5.86	24,24,24,24	0
57	MG	BA	3009	1/1	0.97	0.33	5.63	14,14,14,14	0
57	MG	AA	1607	1/1	0.94	0.33	5.55	33,33,33,33	0
57	MG	BA	3034	1/1	0.97	0.30	5.39	36,36,36,36	0
57	MG	AA	1668	1/1	0.83	0.28	5.32	51,51,51,51	0
57	MG	AA	1601	1/1	0.98	0.27	5.29	22,22,22,22	0
57	MG	BA	3283	1/1	0.96	0.33	5.26	25,25,25,25	0
57	MG	BA	3007	1/1	0.95	0.37	4.95	17,17,17,17	0
57	MG	BA	3041	1/1	0.96	0.29	4.81	27,27,27,27	0
57	MG	BA	3078	1/1	0.94	0.42	4.74	32,32,32,32	0
57	MG	BA	3298	1/1	0.81	0.26	4.62	76,76,76,76	0
57	MG	AA	1665	1/1	0.94	0.53	4.57	56,56,56,56	0
57	MG	BA	3091	1/1	0.90	0.40	4.50	42,42,42,42	0
57	MG	BA	3118	1/1	0.95	0.26	4.37	40,40,40,40	0
57	MG	BA	3061	1/1	0.94	0.27	4.16	48,48,48,48	0
57	MG	BA	3104	1/1	0.87	0.25	4.11	45,45,45,45	0
57	MG	AA	1673	1/1	0.95	0.50	4.06	84,84,84,84	0
57	MG	BA	3269	1/1	0.95	0.26	3.98	51,51,51,51	0
57	MG	AA	1618	1/1	0.97	0.27	3.94	49,49,49,49	0
57	MG	AA	1622	1/1	0.94	0.29	3.93	42,42,42,42	0
57	MG	BA	3018	1/1	0.97	0.25	3.92	16,16,16,16	0
57	MG	BA	3020	1/1	0.97	0.40	3.82	29,29,29,29	0
57	MG	BA	3058	1/1	0.98	0.32	3.61	35,35,35,35	0
57	MG	BA	3005	1/1	0.98	0.25	3.55	20,20,20,20	0
57	MG	AA	1647	1/1	0.84	0.26	3.46	60,60,60,60	0
57	MG	BA	3153	1/1	0.97	0.26	3.24	59,59,59,59	0
57	MG	BA	3068	1/1	0.97	0.30	3.16	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3276	1/1	0.95	0.30	3.02	58,58,58,58	0
57	MG	BA	3148	1/1	0.87	0.22	2.74	50,50,50,50	0
57	MG	BA	3206	1/1	0.87	0.24	2.74	52,52,52,52	0
57	MG	AA	1655	1/1	0.87	0.26	2.61	60,60,60,60	0
57	MG	AA	1650	1/1	0.93	0.23	2.60	67,67,67,67	0
57	MG	BA	3014	1/1	0.94	0.22	2.50	27,27,27,27	0
57	MG	AA	1689	1/1	0.88	0.28	2.47	69,69,69,69	0
57	MG	AA	1633	1/1	0.88	0.29	2.37	53,53,53,53	0
57	MG	BA	3072	1/1	0.94	0.22	2.21	36,36,36,36	0
57	MG	BA	3201	1/1	0.89	0.20	2.05	47,47,47,47	0
57	MG	BA	3051	1/1	0.96	0.26	1.78	33,33,33,33	0
57	MG	BA	3097	1/1	0.87	0.40	1.48	48,48,48,48	0
57	MG	BA	3115	1/1	0.95	0.24	1.48	37,37,37,37	0
57	MG	BA	3111	1/1	0.98	0.23	1.24	29,29,29,29	0
57	MG	BA	3145	1/1	0.93	0.23	1.17	55,55,55,55	0
57	MG	BA	3122	1/1	0.97	0.22	1.12	38,38,38,38	0
57	MG	BA	3236	1/1	0.98	0.21	0.89	46,46,46,46	0
57	MG	BA	3106	1/1	0.97	0.23	0.87	37,37,37,37	0
57	MG	BA	3085	1/1	0.98	0.23	0.80	40,40,40,40	0
57	MG	BA	3264	1/1	0.90	0.20	0.62	67,67,67,67	0
57	MG	BA	3161	1/1	0.93	0.20	0.60	42,42,42,42	0
57	MG	BA	3056	1/1	0.97	0.22	0.60	26,26,26,26	0
57	MG	BA	3330	1/1	0.94	0.15	0.60	83,83,83,83	0
57	MG	AL	201	1/1	0.83	0.30	0.43	54,54,54,54	0
57	MG	BA	3327	1/1	0.80	0.23	0.24	64,64,64,64	0
57	MG	AA	1641	1/1	0.87	0.24	0.12	67,67,67,67	0
57	MG	BA	3142	1/1	0.93	0.23	0.09	50,50,50,50	0
57	MG	AA	1613	1/1	0.93	0.18	-0.04	58,58,58,58	0
57	MG	B0	102	1/1	0.98	0.30	-0.12	33,33,33,33	0
57	MG	BA	3143	1/1	0.98	0.19	-0.12	32,32,32,32	0
57	MG	BD	301	1/1	0.72	0.21	-0.13	49,49,49,49	0
57	MG	AA	1612	1/1	0.95	0.22	-0.14	29,29,29,29	0
57	MG	BA	3355	1/1	0.75	0.24	-0.14	69,69,69,69	0
57	MG	BA	3108	1/1	0.93	0.18	-0.31	42,42,42,42	0
57	MG	AA	1669	1/1	0.75	0.17	-0.35	71,71,71,71	0
57	MG	BB	203	1/1	0.69	0.19	-0.35	51,51,51,51	0
57	MG	BA	3038	1/1	0.95	0.19	-0.45	21,21,21,21	0
57	MG	AA	1644	1/1	0.88	0.18	-0.50	49,49,49,49	0
57	MG	BN	201	1/1	0.95	0.30	-0.62	51,51,51,51	0
57	MG	AA	1701	1/1	0.74	0.16	-0.64	79,79,79,79	0
57	MG	BA	3059	1/1	0.97	0.20	-0.65	43,43,43,43	0
57	MG	AH	201	1/1	0.92	0.21	-0.68	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BR	202	1/1	0.97	0.18	-0.81	51,51,51,51	0
57	MG	BA	3109	1/1	0.94	0.13	-0.88	38,38,38,38	0
57	MG	AA	1608	1/1	0.96	0.19	-0.88	59,59,59,59	0
57	MG	AA	1698	1/1	0.95	0.16	-0.96	51,51,51,51	0
57	MG	BA	3332	1/1	0.55	0.23	-0.99	96,96,96,96	0
57	MG	BA	3002	1/1	0.98	0.19	-1.02	13,13,13,13	0
57	MG	BA	3175	1/1	0.91	0.15	-1.09	44,44,44,44	0
57	MG	BA	3338	1/1	0.65	0.13	-1.11	61,61,61,61	0
57	MG	AA	1626	1/1	0.81	0.19	-1.14	45,45,45,45	0
58	GNP	AW	602	32/32	0.95	0.16	-1.14	58,71,81,83	0
57	MG	AA	1646	1/1	0.85	0.18	-1.24	50,50,50,50	0
57	MG	AA	1697	1/1	0.96	0.11	-1.42	64,64,64,64	0
57	MG	BA	3299	1/1	0.89	0.17	-1.44	64,64,64,64	0
57	MG	BA	3140	1/1	0.93	0.16	-1.47	46,46,46,46	0
57	MG	BA	3288	1/1	0.65	0.18	-1.51	95,95,95,95	0
57	MG	AM	201	1/1	0.83	0.12	-1.54	80,80,80,80	0
57	MG	BA	3180	1/1	0.94	0.12	-1.57	45,45,45,45	0
57	MG	BR	201	1/1	0.96	0.15	-1.59	69,69,69,69	0
57	MG	BA	3274	1/1	0.90	0.12	-1.71	52,52,52,52	0
57	MG	BB	205	1/1	0.90	0.12	-1.78	79,79,79,79	0
57	MG	BA	3309	1/1	0.98	0.15	-1.82	62,62,62,62	0
57	MG	BT	201	1/1	0.92	0.12	-1.99	40,40,40,40	0
57	MG	BA	3195	1/1	0.82	0.15	-2.10	47,47,47,47	0
57	MG	BA	3248	1/1	0.93	0.16	-2.33	52,52,52,52	0
57	MG	AA	1639	1/1	0.86	0.17	-2.68	49,49,49,49	0
57	MG	AA	1695	1/1	0.96	0.10	-3.02	62,62,62,62	0
57	MG	BA	3191	1/1	0.97	0.10	-3.74	57,57,57,57	0
57	MG	BA	3168	1/1	0.93	0.15	-4.03	32,32,32,32	0
57	MG	AA	1637	1/1	0.82	0.09	-4.27	54,54,54,54	0
57	MG	BA	3243	1/1	0.95	0.07	-5.07	62,62,62,62	0
57	MG	BA	3189	1/1	0.87	0.12	-5.49	51,51,51,51	0
57	MG	BA	3184	1/1	0.94	0.14	-5.59	37,37,37,37	0
57	MG	BB	206	1/1	0.91	0.08	-5.97	65,65,65,65	0
57	MG	BA	3173	1/1	0.94	0.11	-7.68	36,36,36,36	0
57	MG	BA	3271	1/1	0.84	0.48	-	53,53,53,53	0
57	MG	BA	3113	1/1	0.99	0.27	-	34,34,34,34	0
57	MG	BA	3305	1/1	0.85	0.19	-	71,71,71,71	0
57	MG	BA	3179	1/1	0.93	0.16	-	46,46,46,46	0
57	MG	BA	3198	1/1	0.92	0.15	-	60,60,60,60	0
57	MG	BA	3093	1/1	0.90	0.24	-	42,42,42,42	0
57	MG	BA	3321	1/1	0.80	0.14	-	73,73,73,73	0
57	MG	BA	3226	1/1	0.92	0.24	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3076	1/1	0.95	0.20	-	36,36,36,36	0
57	MG	BA	3159	1/1	0.88	0.49	-	49,49,49,49	0
57	MG	BA	3301	1/1	0.95	0.23	-	64,64,64,64	0
57	MG	BA	3241	1/1	0.92	0.25	-	57,57,57,57	0
57	MG	BA	3209	1/1	0.95	0.10	-	42,42,42,42	0
57	MG	BA	3139	1/1	0.92	0.42	-	43,43,43,43	0
57	MG	BX	201	1/1	0.92	0.29	-	47,47,47,47	0
57	MG	AA	1692	1/1	0.90	0.15	-	67,67,67,67	0
57	MG	AA	1619	1/1	0.95	0.18	-	40,40,40,40	0
57	MG	BA	3240	1/1	0.81	0.51	-	56,56,56,56	0
57	MG	BA	3310	1/1	0.95	0.17	-	75,75,75,75	0
57	MG	BA	3303	1/1	0.80	0.38	-	56,56,56,56	0
57	MG	BA	3053	1/1	0.99	0.51	-	31,31,31,31	0
57	MG	BA	3069	1/1	0.99	0.24	-	39,39,39,39	0
57	MG	BA	3187	1/1	0.92	0.10	-	56,56,56,56	0
57	MG	BA	3190	1/1	0.94	0.58	-	43,43,43,43	0
57	MG	BA	3116	1/1	0.90	0.23	-	41,41,41,41	0
57	MG	AA	1621	1/1	0.94	0.38	-	57,57,57,57	0
57	MG	AA	1659	1/1	0.93	0.12	-	55,55,55,55	0
57	MG	BA	3124	1/1	0.95	0.56	-	42,42,42,42	0
57	MG	BA	3137	1/1	0.88	0.57	-	42,42,42,42	0
57	MG	BA	3165	1/1	0.88	0.50	-	52,52,52,52	0
57	MG	BA	3307	1/1	0.95	0.22	-	52,52,52,52	0
57	MG	BA	3154	1/1	0.93	0.56	-	43,43,43,43	0
57	MG	BA	3010	1/1	0.99	0.28	-	33,33,33,33	0
57	MG	BA	3235	1/1	0.90	0.22	-	64,64,64,64	0
57	MG	BA	3343	1/1	0.84	0.07	-	71,71,71,71	0
57	MG	BA	3031	1/1	0.93	0.38	-	25,25,25,25	0
57	MG	BA	3293	1/1	0.90	0.37	-	53,53,53,53	0
57	MG	BA	3004	1/1	0.98	0.24	-	21,21,21,21	0
57	MG	BA	3337	1/1	0.84	0.27	-	55,55,55,55	0
57	MG	AA	1629	1/1	0.95	0.26	-	41,41,41,41	0
57	MG	BA	3322	1/1	0.82	0.20	-	62,62,62,62	0
57	MG	BA	3315	1/1	0.94	0.19	-	63,63,63,63	0
57	MG	BA	3094	1/1	0.97	0.19	-	47,47,47,47	0
57	MG	BA	3044	1/1	0.96	0.42	-	37,37,37,37	0
57	MG	BA	3006	1/1	0.99	0.37	-	22,22,22,22	0
57	MG	BA	3158	1/1	0.94	0.26	-	35,35,35,35	0
57	MG	AF	201	1/1	0.86	0.33	-	65,65,65,65	0
57	MG	BA	3193	1/1	0.94	0.48	-	61,61,61,61	0
57	MG	BA	3286	1/1	0.89	0.20	-	48,48,48,48	0
57	MG	BA	3270	1/1	0.91	0.29	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3258	1/1	0.97	0.13	-	50,50,50,50	0
57	MG	BA	3043	1/1	0.99	0.46	-	26,26,26,26	0
57	MG	BA	3055	1/1	0.98	0.43	-	24,24,24,24	0
57	MG	AA	1680	1/1	0.92	0.07	-	55,55,55,55	0
57	MG	BB	202	1/1	0.91	0.25	-	43,43,43,43	0
57	MG	BB	208	1/1	0.81	0.29	-	59,59,59,59	0
57	MG	BA	3229	1/1	0.90	0.09	-	46,46,46,46	0
57	MG	BA	3313	1/1	0.73	0.35	-	67,67,67,67	0
57	MG	BA	3356	1/1	0.79	0.23	-	61,61,61,61	0
57	MG	BA	3205	1/1	0.92	0.21	-	50,50,50,50	0
57	MG	BA	3333	1/1	0.51	0.82	-	77,77,77,77	0
57	MG	BA	3156	1/1	0.95	0.17	-	41,41,41,41	0
57	MG	BA	3312	1/1	0.73	0.26	-	56,56,56,56	0
57	MG	BA	3335	1/1	0.91	0.17	-	58,58,58,58	0
57	MG	BA	3008	1/1	0.97	0.29	-	22,22,22,22	0
57	MG	AA	1630	1/1	0.95	0.44	-	48,48,48,48	0
57	MG	BA	3211	1/1	0.86	0.54	-	48,48,48,48	0
57	MG	BA	3123	1/1	0.96	0.30	-	36,36,36,36	0
57	MG	BA	3086	1/1	0.97	0.43	-	43,43,43,43	0
57	MG	AA	1656	1/1	0.91	0.15	-	73,73,73,73	0
57	MG	AA	1688	1/1	0.84	0.07	-	77,77,77,77	0
57	MG	BA	3245	1/1	0.96	0.49	-	46,46,46,46	0
57	MG	BA	3306	1/1	0.66	0.35	-	67,67,67,67	0
57	MG	BD	305	1/1	0.98	0.17	-	16,16,16,16	0
57	MG	BA	3292	1/1	0.91	0.28	-	54,54,54,54	0
57	MG	BA	3334	1/1	0.82	0.26	-	56,56,56,56	0
57	MG	BA	3284	1/1	0.77	0.33	-	73,73,73,73	0
57	MG	BA	3220	1/1	0.89	0.32	-	56,56,56,56	0
57	MG	AA	1632	1/1	0.96	0.44	-	40,40,40,40	0
57	MG	BA	3204	1/1	0.54	0.52	-	72,72,72,72	0
57	MG	BA	3035	1/1	0.96	0.33	-	26,26,26,26	0
57	MG	BB	207	1/1	0.86	0.12	-	47,47,47,47	0
57	MG	BA	3304	1/1	0.94	0.45	-	50,50,50,50	0
57	MG	BA	3317	1/1	0.44	0.36	-	88,88,88,88	0
57	MG	BA	3255	1/1	0.89	0.34	-	66,66,66,66	0
57	MG	AA	1683	1/1	0.90	0.22	-	63,63,63,63	0
57	MG	BA	3178	1/1	0.95	0.26	-	49,49,49,49	0
57	MG	BA	3171	1/1	0.93	0.27	-	57,57,57,57	0
57	MG	AA	1694	1/1	0.85	0.11	-	75,75,75,75	0
57	MG	BA	3136	1/1	0.93	0.66	-	53,53,53,53	0
57	MG	AA	1634	1/1	0.94	0.34	-	55,55,55,55	0
57	MG	AA	1623	1/1	0.90	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3152	1/1	0.93	0.07	-	41,41,41,41	0
57	MG	BA	3300	1/1	0.89	0.54	-	69,69,69,69	0
57	MG	BA	3237	1/1	0.95	0.14	-	51,51,51,51	0
57	MG	BA	3324	1/1	0.86	0.25	-	59,59,59,59	0
57	MG	BA	3046	1/1	0.98	0.42	-	27,27,27,27	0
57	MG	BA	3227	1/1	0.88	0.25	-	63,63,63,63	0
57	MG	BA	3048	1/1	0.93	0.39	-	40,40,40,40	0
57	MG	AA	1666	1/1	0.95	0.35	-	62,62,62,62	0
57	MG	BA	3079	1/1	0.97	0.67	-	44,44,44,44	0
57	MG	BA	3166	1/1	0.99	0.07	-	50,50,50,50	0
57	MG	BA	3279	1/1	0.92	0.11	-	50,50,50,50	0
57	MG	BA	3080	1/1	0.95	0.22	-	43,43,43,43	0
57	MG	BA	3323	1/1	0.85	0.29	-	64,64,64,64	0
57	MG	BA	3277	1/1	0.93	0.26	-	42,42,42,42	0
57	MG	BA	3225	1/1	0.82	0.41	-	60,60,60,60	0
57	MG	BA	3266	1/1	0.91	0.30	-	56,56,56,56	0
57	MG	BA	3021	1/1	0.97	0.34	-	18,18,18,18	0
57	MG	BA	3063	1/1	0.96	0.44	-	32,32,32,32	0
57	MG	BA	3141	1/1	0.94	0.18	-	54,54,54,54	0
57	MG	BA	3121	1/1	0.94	0.48	-	39,39,39,39	0
57	MG	BA	3219	1/1	0.63	0.75	-	69,69,69,69	0
57	MG	BA	3215	1/1	0.82	0.12	-	53,53,53,53	0
57	MG	BA	3199	1/1	0.95	0.43	-	42,42,42,42	0
57	MG	BA	3027	1/1	0.97	0.42	-	40,40,40,40	0
57	MG	BA	3087	1/1	0.92	0.46	-	42,42,42,42	0
57	MG	BB	209	1/1	0.96	0.34	-	36,36,36,36	0
57	MG	BA	3186	1/1	0.96	0.23	-	47,47,47,47	0
57	MG	BA	3128	1/1	0.94	0.28	-	33,33,33,33	0
57	MG	AA	1662	1/1	0.95	0.34	-	57,57,57,57	0
57	MG	AA	1642	1/1	0.98	0.28	-	53,53,53,53	0
57	MG	BA	3350	1/1	0.81	0.25	-	80,80,80,80	0
57	MG	AA	1664	1/1	0.98	0.19	-	41,41,41,41	0
57	MG	AA	1649	1/1	0.96	0.39	-	49,49,49,49	0
57	MG	BA	3160	1/1	0.86	0.35	-	49,49,49,49	0
57	MG	BA	3253	1/1	0.90	0.14	-	65,65,65,65	0
57	MG	BA	3112	1/1	0.97	0.27	-	41,41,41,41	0
57	MG	BA	3275	1/1	0.89	0.12	-	59,59,59,59	0
57	MG	BA	3351	1/1	0.89	0.19	-	58,58,58,58	0
57	MG	BA	3110	1/1	0.93	0.29	-	38,38,38,38	0
57	MG	BA	3098	1/1	0.96	0.13	-	47,47,47,47	0
57	MG	BA	3203	1/1	0.98	0.31	-	50,50,50,50	0
57	MG	BA	3028	1/1	0.91	0.37	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3295	1/1	0.69	0.20	-	57,57,57,57	0
57	MG	AA	1636	1/1	0.95	0.16	-	36,36,36,36	0
57	MG	BA	3212	1/1	0.97	0.21	-	45,45,45,45	0
57	MG	AA	1617	1/1	0.93	0.20	-	47,47,47,47	0
57	MG	BA	3228	1/1	0.88	0.23	-	42,42,42,42	0
57	MG	BA	3347	1/1	0.94	0.14	-	76,76,76,76	0
57	MG	B2	101	1/1	0.95	0.12	-	49,49,49,49	0
57	MG	BA	3062	1/1	0.94	0.33	-	42,42,42,42	0
57	MG	BA	3320	1/1	0.88	0.21	-	52,52,52,52	0
57	MG	BA	3278	1/1	0.93	0.32	-	48,48,48,48	0
57	MG	BA	3162	1/1	0.96	0.11	-	56,56,56,56	0
57	MG	AL	202	1/1	0.95	0.15	-	73,73,73,73	0
57	MG	AA	1693	1/1	0.84	0.28	-	56,56,56,56	0
57	MG	BA	3222	1/1	0.91	0.14	-	50,50,50,50	0
57	MG	BA	3065	1/1	0.90	0.36	-	46,46,46,46	0
57	MG	AA	1627	1/1	0.86	0.26	-	40,40,40,40	0
57	MG	BA	3247	1/1	0.92	0.17	-	61,61,61,61	0
57	MG	BA	3217	1/1	0.95	0.06	-	56,56,56,56	0
57	MG	BA	3149	1/1	0.94	0.32	-	42,42,42,42	0
57	MG	BA	3037	1/1	0.93	0.45	-	36,36,36,36	0
57	MG	BA	3100	1/1	0.98	0.42	-	36,36,36,36	0
57	MG	AA	1635	1/1	0.91	0.29	-	58,58,58,58	0
57	MG	BA	3183	1/1	0.95	0.25	-	48,48,48,48	0
57	MG	BA	3105	1/1	0.87	0.42	-	49,49,49,49	0
57	MG	BA	3200	1/1	0.93	0.40	-	44,44,44,44	0
57	MG	AA	1670	1/1	0.64	0.36	-	62,62,62,62	0
57	MG	BA	3131	1/1	0.86	0.23	-	40,40,40,40	0
57	MG	BA	3057	1/1	0.98	0.30	-	33,33,33,33	0
57	MG	BA	3268	1/1	0.91	0.28	-	52,52,52,52	0
57	MG	BA	3107	1/1	0.98	0.31	-	36,36,36,36	0
57	MG	AA	1672	1/1	0.85	0.17	-	52,52,52,52	0
57	MG	BA	3012	1/1	0.97	0.43	-	18,18,18,18	0
57	MG	BA	3261	1/1	0.91	0.21	-	63,63,63,63	0
57	MG	BA	3218	1/1	0.94	0.22	-	50,50,50,50	0
57	MG	BB	201	1/1	0.80	0.33	-	54,54,54,54	0
57	MG	AA	1628	1/1	0.99	0.28	-	44,44,44,44	0
57	MG	BA	3082	1/1	0.98	0.39	-	36,36,36,36	0
57	MG	BA	3019	1/1	0.94	0.23	-	15,15,15,15	0
57	MG	BA	3308	1/1	0.92	0.44	-	82,82,82,82	0
57	MG	AA	1691	1/1	0.84	0.37	-	63,63,63,63	0
57	MG	BA	3242	1/1	0.69	0.27	-	72,72,72,72	0
57	MG	AA	1682	1/1	0.90	0.12	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3127	1/1	0.87	0.27	-	38,38,38,38	0
57	MG	BA	3238	1/1	0.89	0.17	-	50,50,50,50	0
57	MG	BA	3260	1/1	0.91	0.24	-	50,50,50,50	0
57	MG	AA	1684	1/1	0.89	0.50	-	60,60,60,60	0
57	MG	BA	3263	1/1	0.92	0.23	-	53,53,53,53	0
57	MG	AA	1648	1/1	0.88	0.13	-	54,54,54,54	0
57	MG	BA	3135	1/1	0.95	0.14	-	45,45,45,45	0
57	MG	BA	3196	1/1	0.87	0.53	-	46,46,46,46	0
57	MG	BA	3231	1/1	0.93	0.10	-	56,56,56,56	0
57	MG	BA	3167	1/1	0.93	0.41	-	48,48,48,48	0
57	MG	BA	3133	1/1	0.93	0.26	-	45,45,45,45	0
57	MG	B4	101	1/1	0.93	0.42	-	40,40,40,40	0
57	MG	BA	3194	1/1	0.97	0.24	-	49,49,49,49	0
57	MG	BE	301	1/1	0.88	0.09	-	67,67,67,67	0
57	MG	BA	3017	1/1	0.92	0.33	-	30,30,30,30	0
57	MG	BA	3089	1/1	0.92	0.07	-	52,52,52,52	0
57	MG	AA	1699	1/1	0.85	0.38	-	49,49,49,49	0
57	MG	BA	3015	1/1	0.98	0.57	-	38,38,38,38	0
57	MG	BA	3060	1/1	0.94	0.39	-	27,27,27,27	0
57	MG	BA	3132	1/1	0.89	0.27	-	52,52,52,52	0
57	MG	AA	1602	1/1	0.93	0.31	-	37,37,37,37	0
57	MG	BA	3163	1/1	0.97	0.21	-	49,49,49,49	0
57	MG	AA	1671	1/1	0.79	0.16	-	53,53,53,53	0
57	MG	BA	3185	1/1	0.82	0.28	-	52,52,52,52	0
57	MG	AA	1652	1/1	0.83	0.26	-	60,60,60,60	0
57	MG	BA	3239	1/1	0.86	0.17	-	71,71,71,71	0
57	MG	AA	1681	1/1	0.91	0.15	-	38,38,38,38	0
57	MG	BA	3252	1/1	0.89	0.33	-	49,49,49,49	0
57	MG	BQ	201	1/1	0.90	0.18	-	44,44,44,44	0
57	MG	BA	3176	1/1	0.93	0.28	-	50,50,50,50	0
57	MG	BA	3120	1/1	0.97	0.09	-	31,31,31,31	0
57	MG	AA	1663	1/1	0.85	0.26	-	74,74,74,74	0
57	MG	BA	3144	1/1	0.93	0.12	-	68,68,68,68	0
57	MG	BA	3272	1/1	0.84	0.26	-	55,55,55,55	0
57	MG	AA	1614	1/1	0.97	0.18	-	42,42,42,42	0
57	MG	AA	1660	1/1	0.97	0.17	-	46,46,46,46	0
57	MG	BA	3129	1/1	0.95	0.21	-	43,43,43,43	0
57	MG	BA	3075	1/1	0.88	0.13	-	43,43,43,43	0
57	MG	BA	3155	1/1	0.97	0.69	-	51,51,51,51	0
57	MG	BA	3192	1/1	0.82	0.44	-	59,59,59,59	0
57	MG	AA	1679	1/1	0.84	0.30	-	62,62,62,62	0
57	MG	BA	3345	1/1	0.71	0.43	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3233	1/1	0.78	0.49	-	46,46,46,46	0
57	MG	B0	103	1/1	0.91	0.52	-	54,54,54,54	0
57	MG	BA	3208	1/1	0.91	0.25	-	62,62,62,62	0
57	MG	BA	3049	1/1	0.97	0.24	-	31,31,31,31	0
57	MG	BA	3249	1/1	0.92	0.09	-	49,49,49,49	0
57	MG	BA	3169	1/1	0.85	0.26	-	39,39,39,39	0
57	MG	BA	3254	1/1	0.95	0.22	-	59,59,59,59	0
57	MG	BA	3265	1/1	0.92	0.32	-	45,45,45,45	0
57	MG	AA	1657	1/1	0.69	0.36	-	83,83,83,83	0
57	MG	BA	3282	1/1	0.88	0.25	-	55,55,55,55	0
57	MG	BA	3214	1/1	0.88	0.23	-	43,43,43,43	0
57	MG	BA	3296	1/1	0.86	0.28	-	60,60,60,60	0
57	MG	BA	3348	1/1	0.69	0.29	-	67,67,67,67	0
57	MG	BA	3319	1/1	0.81	0.20	-	68,68,68,68	0
57	MG	BA	3213	1/1	0.92	0.31	-	46,46,46,46	0
57	MG	BA	3354	1/1	0.90	0.12	-	62,62,62,62	0
57	MG	BA	3357	1/1	0.83	0.22	-	81,81,81,81	0
57	MG	BA	3257	1/1	0.85	0.31	-	48,48,48,48	0
57	MG	BA	3267	1/1	0.88	0.21	-	52,52,52,52	0
57	MG	BA	3342	1/1	0.91	0.26	-	54,54,54,54	0
57	MG	BA	3147	1/1	0.93	0.22	-	46,46,46,46	0
57	MG	BA	3221	1/1	0.95	0.37	-	43,43,43,43	0
57	MG	AA	1609	1/1	0.97	0.49	-	40,40,40,40	0
57	MG	BA	3040	1/1	0.97	0.41	-	43,43,43,43	0
57	MG	BA	3114	1/1	0.95	0.34	-	32,32,32,32	0
57	MG	BA	3289	1/1	0.92	0.17	-	62,62,62,62	0
57	MG	AA	1686	1/1	0.44	0.62	-	93,93,93,93	0
57	MG	AA	1702	1/1	0.89	0.32	-	58,58,58,58	0
57	MG	AA	1640	1/1	0.97	0.09	-	41,41,41,41	0
57	MG	BA	3036	1/1	0.95	0.28	-	43,43,43,43	0
57	MG	AA	1685	1/1	0.46	0.24	-	64,64,64,64	0
57	MG	BA	3326	1/1	0.97	0.14	-	42,42,42,42	0
57	MG	BA	3234	1/1	0.93	0.47	-	49,49,49,49	0
57	MG	BA	3077	1/1	0.95	0.57	-	41,41,41,41	0
57	MG	AA	1667	1/1	0.78	0.15	-	87,87,87,87	0
57	MG	BA	3023	1/1	0.95	0.41	-	39,39,39,39	0
57	MG	BA	3230	1/1	0.96	0.21	-	46,46,46,46	0
57	MG	BA	3273	1/1	0.97	0.56	-	72,72,72,72	0
57	MG	BA	3353	1/1	0.76	0.53	-	73,73,73,73	0
57	MG	BA	3232	1/1	0.83	0.34	-	54,54,54,54	0
57	MG	BA	3050	1/1	0.93	0.39	-	33,33,33,33	0
57	MG	B0	101	1/1	0.94	0.11	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3224	1/1	0.96	0.13	-	41,41,41,41	0
57	MG	BA	3101	1/1	0.96	0.23	-	43,43,43,43	0
57	MG	BA	3134	1/1	0.95	0.62	-	49,49,49,49	0
57	MG	BA	3067	1/1	0.94	0.29	-	35,35,35,35	0
57	MG	AA	1610	1/1	0.92	0.33	-	45,45,45,45	0
57	MG	BA	3256	1/1	0.91	0.19	-	56,56,56,56	0
57	MG	BA	3088	1/1	0.95	0.26	-	36,36,36,36	0
57	MG	AA	1643	1/1	0.93	0.39	-	56,56,56,56	0
57	MG	AA	1661	1/1	0.93	0.25	-	49,49,49,49	0
57	MG	BO	201	1/1	0.96	0.17	-	41,41,41,41	0
57	MG	AA	1676	1/1	0.92	0.41	-	52,52,52,52	0
57	MG	BA	3297	1/1	0.77	0.30	-	49,49,49,49	0
57	MG	AA	1615	1/1	0.97	0.29	-	40,40,40,40	0
57	MG	AA	1624	1/1	0.94	0.44	-	51,51,51,51	0
57	MG	AA	1620	1/1	0.96	0.16	-	52,52,52,52	0
57	MG	BA	3336	1/1	0.78	0.30	-	86,86,86,86	0
57	MG	BA	3081	1/1	0.96	0.39	-	35,35,35,35	0
57	MG	BA	3339	1/1	0.96	0.14	-	76,76,76,76	0
57	MG	AA	1696	1/1	0.87	0.24	-	89,89,89,89	0
57	MG	BA	3207	1/1	0.82	0.36	-	54,54,54,54	0
57	MG	BA	3285	1/1	0.84	0.26	-	75,75,75,75	0
57	MG	BA	3029	1/1	0.97	0.39	-	28,28,28,28	0
57	MG	BA	3246	1/1	0.87	0.27	-	48,48,48,48	0
57	MG	BA	3197	1/1	0.90	0.16	-	38,38,38,38	0
57	MG	AA	1653	1/1	0.96	0.17	-	41,41,41,41	0
57	MG	BA	3126	1/1	0.97	0.26	-	31,31,31,31	0
57	MG	BA	3331	1/1	0.80	0.32	-	64,64,64,64	0
57	MG	BA	3325	1/1	0.93	0.36	-	59,59,59,59	0
57	MG	BA	3033	1/1	0.99	0.42	-	25,25,25,25	0
57	MG	BA	3290	1/1	0.94	0.10	-	56,56,56,56	0
57	MG	BA	3210	1/1	0.60	0.39	-	73,73,73,73	0
57	MG	AA	1687	1/1	0.70	0.81	-	81,81,81,81	0
57	MG	AA	1651	1/1	0.89	0.31	-	51,51,51,51	0
57	MG	AA	1638	1/1	0.92	0.20	-	55,55,55,55	0
57	MG	AA	1674	1/1	0.92	0.13	-	55,55,55,55	0
57	MG	BA	3170	1/1	0.84	0.38	-	52,52,52,52	0
57	MG	BA	3146	1/1	0.88	0.33	-	40,40,40,40	0
57	MG	BA	3328	1/1	0.85	0.13	-	71,71,71,71	0
57	MG	BA	3164	1/1	0.91	0.14	-	45,45,45,45	0
57	MG	BA	3281	1/1	0.83	0.64	-	73,73,73,73	0
57	MG	BA	3340	1/1	0.95	0.51	-	61,61,61,61	0
57	MG	BA	3318	1/1	0.91	0.32	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3202	1/1	0.70	0.35	-	57,57,57,57	0
57	MG	BA	3250	1/1	0.94	0.64	-	66,66,66,66	0
57	MG	BA	3311	1/1	0.77	0.22	-	48,48,48,48	0
57	MG	AA	1625	1/1	0.92	0.22	-	40,40,40,40	0
57	MG	BA	3030	1/1	0.92	0.27	-	38,38,38,38	0
57	MG	BA	3064	1/1	0.94	0.21	-	24,24,24,24	0
57	MG	BA	3216	1/1	0.73	0.49	-	63,63,63,63	0
57	MG	BA	3025	1/1	0.92	0.31	-	32,32,32,32	0
57	MG	AA	1645	1/1	0.94	0.44	-	62,62,62,62	0
57	MG	BA	3349	1/1	0.69	0.33	-	79,79,79,79	0
57	MG	AA	1675	1/1	0.87	0.18	-	57,57,57,57	0
57	MG	AA	1678	1/1	0.82	0.53	-	65,65,65,65	0
57	MG	BA	3291	1/1	0.81	0.50	-	58,58,58,58	0
57	MG	AW	601	1/1	0.43	0.15	-	36,36,36,36	0
57	MG	AA	1605	1/1	0.95	0.24	-	38,38,38,38	0
57	MG	BA	3251	1/1	0.95	0.24	-	49,49,49,49	0
57	MG	BD	303	1/1	0.80	0.20	-	57,57,57,57	0
57	MG	AA	1658	1/1	0.77	0.47	-	61,61,61,61	0
57	MG	BA	3157	1/1	0.95	0.50	-	46,46,46,46	0
57	MG	BA	3344	1/1	0.91	0.14	-	71,71,71,71	0
57	MG	BA	3329	1/1	0.94	0.23	-	58,58,58,58	0
57	MG	AA	1700	1/1	0.84	0.34	-	65,65,65,65	0
57	MG	AA	1654	1/1	0.81	0.30	-	58,58,58,58	0
57	MG	BA	3071	1/1	0.96	0.39	-	35,35,35,35	0
57	MG	BA	3352	1/1	0.91	0.29	-	61,61,61,61	0
57	MG	BA	3346	1/1	0.83	0.55	-	83,83,83,83	0
57	MG	BA	3172	1/1	0.77	0.19	-	53,53,53,53	0
57	MG	BA	3302	1/1	0.81	0.53	-	68,68,68,68	0
57	MG	BA	3117	1/1	0.97	0.22	-	46,46,46,46	0
57	MG	BA	3314	1/1	0.87	0.42	-	56,56,56,56	0
57	MG	BC	301	1/1	0.82	0.38	-	53,53,53,53	0
57	MG	BA	3259	1/1	0.87	0.10	-	69,69,69,69	0
57	MG	BB	204	1/1	0.93	0.12	-	53,53,53,53	0
57	MG	BA	3095	1/1	0.95	0.28	-	42,42,42,42	0
57	MG	BA	3119	1/1	0.98	0.26	-	29,29,29,29	0
57	MG	BA	3287	1/1	0.93	0.23	-	83,83,83,83	0
57	MG	AA	1690	1/1	0.93	0.29	-	83,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.