



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 10:58 am BST

PDB ID : 4V7M
Title : The structures of Capreomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

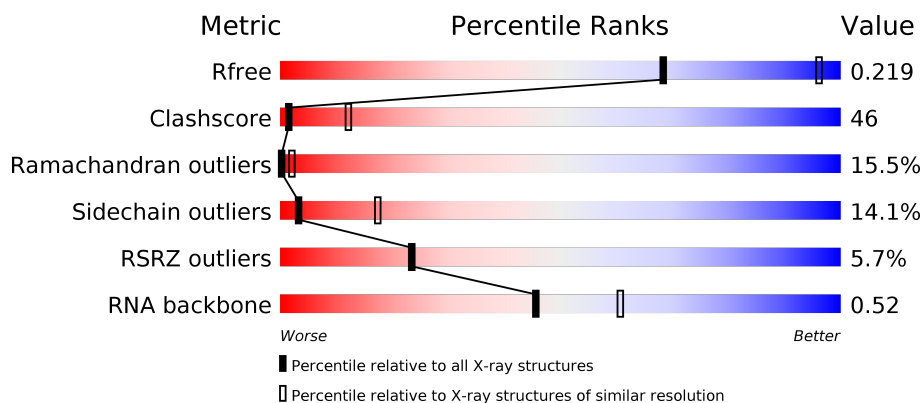
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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

Mol	Chain	Length	Quality of chain
1	AA	1508	 2% 22% 62% 13% ..
1	CA	1508	 2% 20% 63% 14% ..
2	AB	256	 4% 13% 61% 16% • 8%
2	CB	256	 7% 17% 58% 14% • 8%


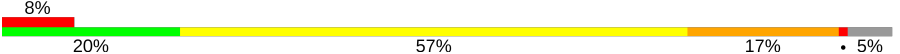
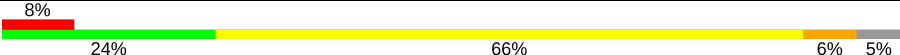
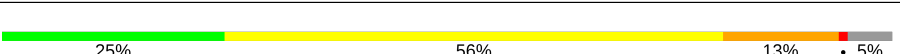
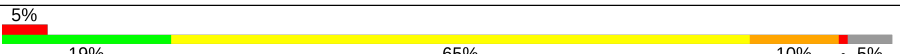
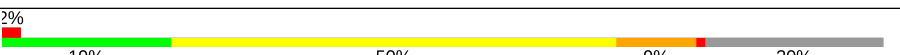
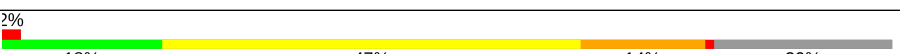
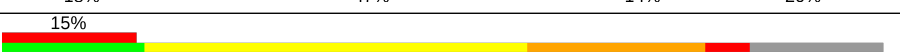
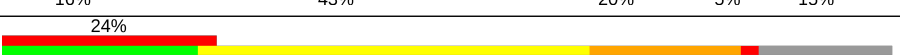
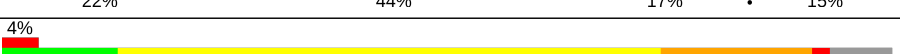
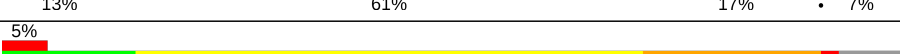
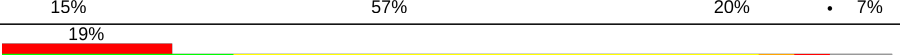

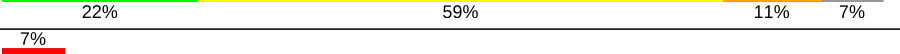


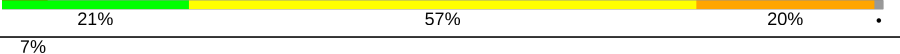
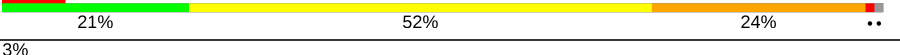
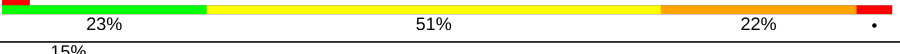
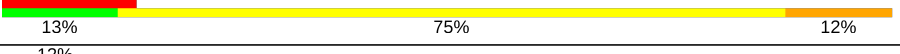
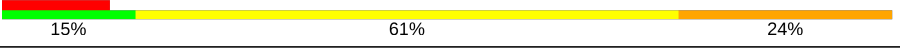
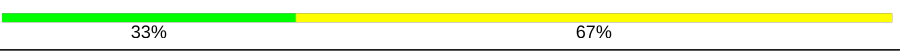

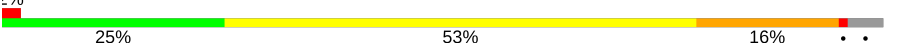
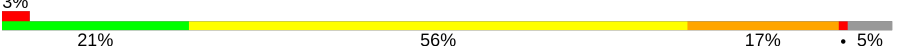
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	
28	BB	122	

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Mol	Chain	Length	Quality of chain
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	
40	DR	118	


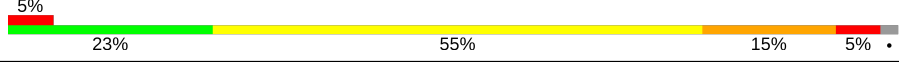
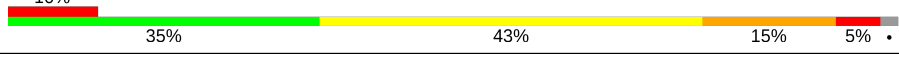

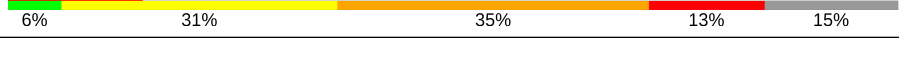
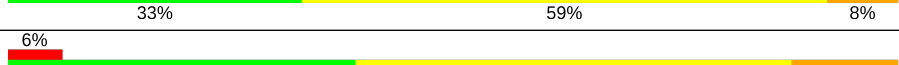
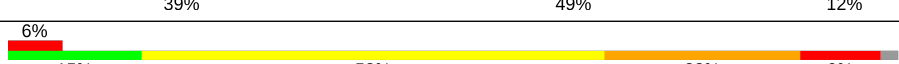
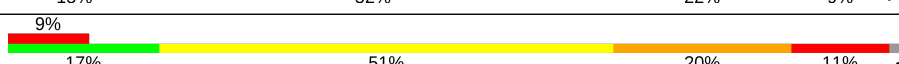
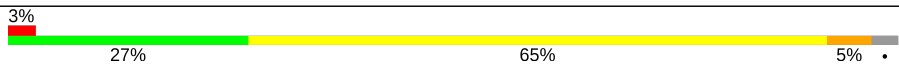
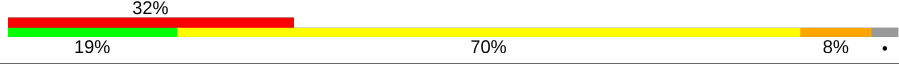
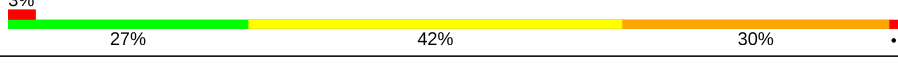

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Mol	Chain	Length	Quality of chain
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	
53	B4	71	

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Mol	Chain	Length	Quality of chain
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	
59	CX	77	

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
26	DPP	AZ	2	-	-	X	-
26	KBE	CZ	1	-	-	X	-
26	DPP	CZ	2	-	-	X	-
60	MG	AA	1630	-	-	-	X
60	MG	AA	1638	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1671	-	-	-	X
60	MG	AW	103	-	-	-	X
60	MG	BA	3140	-	-	-	X
60	MG	BA	3177	-	-	-	X
60	MG	BA	3215	-	-	-	X
60	MG	BA	3238	-	-	-	X
60	MG	BA	3294	-	-	-	X
60	MG	BA	3303	-	-	-	X
60	MG	BA	3316	-	-	-	X
60	MG	CA	1607	-	-	-	X
60	MG	CA	1609	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	1616	-	-	-	X
60	MG	CA	1633	-	-	-	X
60	MG	CA	1644	-	-	-	X
60	MG	CA	1674	-	-	-	X
60	MG	CA	1685	-	-	-	X
60	MG	CA	1700	-	-	-	X
60	MG	CA	1702	-	-	-	X
60	MG	CV	601	-	-	-	X
60	MG	DA	3042	-	-	-	X
60	MG	DA	3062	-	-	-	X
60	MG	DA	3066	-	-	-	X
60	MG	DA	3084	-	-	-	X
60	MG	DA	3086	-	-	-	X
60	MG	DA	3093	-	-	-	X
60	MG	DA	3104	-	-	-	X
60	MG	DA	3110	-	-	-	X
60	MG	DA	3111	-	-	-	X
60	MG	DA	3117	-	-	-	X
60	MG	DA	3136	-	-	-	X
60	MG	DA	3141	-	-	-	X
60	MG	DA	3148	-	-	-	X
60	MG	DA	3154	-	-	-	X
60	MG	DA	3155	-	-	-	X
60	MG	DA	3170	-	-	-	X
60	MG	DA	3171	-	-	-	X
60	MG	DA	3176	-	-	-	X
60	MG	DA	3184	-	-	-	X
60	MG	DA	3199	-	-	-	X
60	MG	DA	3203	-	-	-	X
60	MG	DA	3204	-	-	-	X
60	MG	DA	3217	-	-	-	X
60	MG	DA	3225	-	-	-	X
60	MG	DA	3228	-	-	-	X
60	MG	DB	202	-	-	-	X
60	MG	DF	301	-	-	-	X
60	MG	DO	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 293848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32132	14303	5953	10382	1494			
1	CA	1493	Total	C	N	O	P	0	0	0
			32098	14287	5956	10363	1492			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	206	Total	C	N	O	S	0	0	1
			1604	1011	314	278	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	154	Total	C	N	O	S	0	0	0
			1249	776	251	217	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1006	637	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1006	637	195	174				

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	122	Total	C	N	O	S	0	0	1
			965	597	200	166	2			
13	CM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

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

- Molecule 22 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			205	93	40	63	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			
23	CW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	CONFLICT	GB CP001790.1
AY	44	U	A	CONFLICT	GB CP001790.1
CY	33	G	C	CONFLICT	GB CP001790.1
CY	44	U	A	CONFLICT	GB CP001790.1

- Molecule 26 is a protein called capreomycin IA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			47	25	14	8			
26	CZ	6	Total	C	N	O	0	0	0
			47	25	14	8			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2789	Total	C	N	O	P	0	0	0
			60072	26734	11238	19312	2788			
27	DA	2775	Total	C	N	O	P	0	0	0
			59767	26598	11176	19219	2774			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
30	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	206	Total	C	N	O	S	0	0	1
			1607	1024	301	280	2			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	161	Total	C	N	O	S	0	0	0
			1233	783	227	222	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
39	DQ	138	Total	C	N	O	S	0	0	0
			1094	697	205	185	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	88	Total	C	N	O	S	0	0	1
			672	432	131	105	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
51	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			
53	D4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	48	Total	C	N	O	S	0	0	1
			402	249	83	66	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
56	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
57	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CX	46	G	A	CONFLICT	GB CP001637.1

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	334	Total	Mg	0	0
			334	334		
60	CA	102	Total	Mg	0	0
			102	102		
60	DF	1	Total	Mg	0	0
			1	1		
60	CV	1	Total	Mg	0	0
			1	1		
60	BE	3	Total	Mg	0	0
			3	3		
60	AW	4	Total	Mg	0	0
			4	4		
60	BP	2	Total	Mg	0	0
			2	2		
60	AX	9	Total	Mg	0	0
			9	9		
60	B5	1	Total	Mg	0	0
			1	1		
60	BB	5	Total	Mg	0	0
			5	5		
60	DO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BF	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	CK	1	Total 1	Mg 1	0	0
60	D7	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0
60	AA	114	Total 114	Mg 114	0	0
60	DD	2	Total 2	Mg 2	0	0
60	D0	1	Total 1	Mg 1	0	0
60	BG	1	Total 1	Mg 1	0	0
60	BR	1	Total 1	Mg 1	0	0
60	DA	239	Total 239	Mg 239	0	0
60	AG	1	Total 1	Mg 1	0	0
60	DE	1	Total 1	Mg 1	0	0
60	CW	4	Total 4	Mg 4	0	0
60	D5	1	Total 1	Mg 1	0	0
60	BD	1	Total 1	Mg 1	0	0
60	B0	3	Total 3	Mg 3	0	0
60	CE	1	Total 1	Mg 1	0	0
60	DB	3	Total 3	Mg 3	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

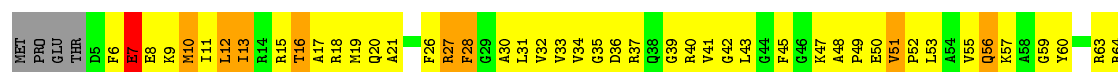
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B5	1	Total 1	Zn 1	0	0
61	B4	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0
61	D5	1	Total 1	Zn 1	0	0
61	D4	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0

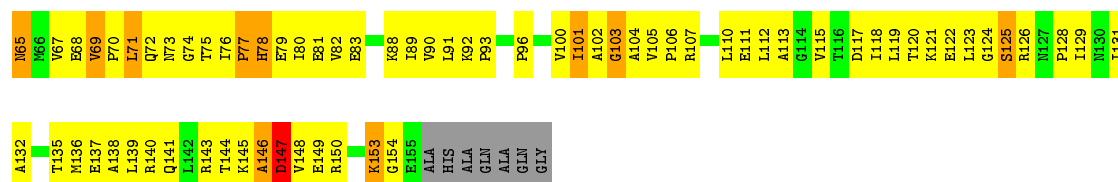


A935	C868	A794	G730	G662	G597	A532	A453	G388	G326	G258	U189E	A130	C653	U
C936	G869	C795	G731	A663	U598	A533	C457	A389	A327	G259	U189F	C131	G64	U
A937	U870	C796	C732	G664	C599	U534	C458	C390	C328	G260	G189G	G	U65	G
A938	U871	C797	A733	A665	G600	A535	G460	G391	A329	U261	G189H	A134	G66	U
G939	G874	G798	G734	G666	G601	C536	A461	A393	C330	A262	U189K	C135	G67	U5
C940	G875	G799	G735	G667	A602	G537	C470	G394	G331	A263	G189L	C136	G68	G6
C941	G876	G800	G736	G668	U603	G538	C471	C395	G332	U264	G189M	C137	G69	G7
G942	G877	A802	G737	U669	G604	A539	A472	G396	G333	G265	U190	G	A8	A8
C943	C878	G803	U605	G670	U605	G540	G473	G397	C334	G266	G191	A140	C71	G9
G944	C879	U804	G739	G671	G606	G541	G474	C398	C335	C267	U192	A141	C72	G9
G945	C880	C805	U740	G672	A607	G542	G475	G399	C336	C268	U193	G142	C73	G9
A946	C881	C806	G741	A675	A608	C543	G476	G402	C337	C269	C194	A143	C76	U13
C947	C882	G807	G742	A676	G609	G544	A477	G403	C338	A270	A195	G144	C77	U14
C948	C883	G808	U612	U677	G610	C545	A478	C404	C339	C271	A196	G145	G	G15
A949	U884	C811	G613	U678	G611	G546	C479	U404	U340	C272	A197	G146	G	G16
U950	G890	A814	A614	G679	G615	A547	C480	U405	U341	A273	G198	G147	G	U17
G951	U891	C815	C615	G680	G616	G548	A482	U406	C342	A274	G199	G148	U	C18
U952	C892	A816	C616	G681	G617	G549	G483	G407	U343	G275	G200	A149	U	C19
G953	C893	C817	G743	G682	U619	G550	G484	A408	A344	G276	C201	C150	U	U20
G954	C894	C818	G744	G683	A620	U551	G485	A409	A345	C277	U202	A151	U	G21
U955	C895	G819	G745	G684	A621	U552	C488	G410	G347	G278	U203	A152	U	G22
C956	C896	A820	G746	G685	A622	U553	C489	A411	G348	A279	U204	C153	C	C23
U957	C897	U820	U686	U686	G623	C554	G490	A412	A349	C280	G216	C154	U	
A958	C898	G821	G754	A687	G624	C555	G491	G413	A350	G281	C217	C155	C	A26
C959	C899	C822	G755	G688	C625	G556	G492	A414	G351	G282	G220	G156	G92	G27
U960	A900	C824	C756	C689	G626	G557	G493	A415	C352	G283	C221	G	G93	G28
U961	G901	G825	U757	G690	U627	G558	A495	A416	A353	G284	U222	G159	U96	G29
C962	G902	C826	G758	G691	G628	U559	A496	G417	G354	G285	U223	A161	G97	U30
G963	C903	U827	U759	U692	G629	U560	U498	C418	C355	G289	U224	A162	G98	G31
A964	C904	A828	G760	G693	G630	U561	G499	U421	A356	C295	C225	C163	U99	A32
U965	U905	G829	G761	A694	G631	C562	G500	G422	U359	C296	G226	A164	A101	A33
A966	C906	G830	G762	A695	A632	U563	G501	G423	U360	U296	G227	C165	G102	C34
C967	A907	C832	G763	A696	C633	C564	G502	G424	A360	G297	U228	G166	G103	G35
U968	A908	U833	G764	G703	C634	U569	G503	G425	G361	A298	U229	G167	G104	C36
A969	A909	C834	C765	A702	G635	G570	A504	G426	G362	G299	G230	G168	G105	U37
C970	C910	U835	U766	G703	U636	U571	A505	G427	A363	A300	G231	G169	G106	G38
G971	U911	G836	G767	A706	U637	A572	C507	U428	C366	G301	G232	U170	G107	G39
C972	C912	C837	G768	C707	G638	A573	C508	G429	U367	G302	C233	A171	G108	C40
G973	G913	U838	C770	C708	G639	U574	A509	A430	U368	A303	C234	G	G109	G41
A974	A914	U839	G771	G709	A640	G575	A510	A431	U369	U304	C235	C174	C110	G42
U975	A915	C840	U772	G710	G643	G576	C511	A432	C370	G305	G236	C175	G111	G43
G976	C916	U841	G773	G711	C644	G577	C512	C433	C371	G309	G237	C176	G112	U45
A977	G917	C849	G774	A712	G645	G578	C513	U434	C372	G310	U238	C177	G113	G46
U978	A918	U850	G775	G713	C646	U579	C514	C435	A373	C311	U239	C178	G114	C47
C979	A919	G851	U776	G714	U647	U580	G515	C436	A374	C312	A243	A179	G115	G48
U980	U920	C852	G777	A715	C648	U581	U516	U437	U375	A313	U244	G181	A116	U49
G981	C921	G853	C779	A716	A649	U582	G517	G438	G376	C314	C245	U182	G119	A50
U982	A923	C854	G717	G718	G650	A583	C518	A439	G377	A315	A246	G183	A120	G52
A983	C924	G855	U781	G719	C651	C586	G521	G	G378	G316	G247	G184	C121	G53
C984	G925	C856	A782	C720	U652	G587	C522	C443	C379	G317	A250	A185	G122	A53
G985	U926	C857	G783	G721	A653	U590	A523	C444	G380	G318	G251	C186	C123	C54
A986	C927	G858	C784	A722	G654	G591	G524	G445	C381	G319	U252	C187	G124	A55
U991	G928	A859	G785	A723	A655	U592	C525	G446	A382	C320	U253	G188	U125	U56
G992	C929	A860	G786	U723	C656	G593	C526	G447	A383	A321	G254	C189	G126	G57
C993	C930	C861	G787	G724	G657	G594	G527	A448	G384	C322	G255	C189A	G127	C58
A994	G931	C862	U790	G725	G658	G595	C530	C449	C385	U923	U256	C189B	G128	A59
C995	C932	G863	G791	A728	U659	G596	G530	G	C386	G324	U129	C189C	U129	A60
A996	G934	G867	U793	A729	G	C596	U531	A452	U387	A325	G257	C189D	G129A	G61

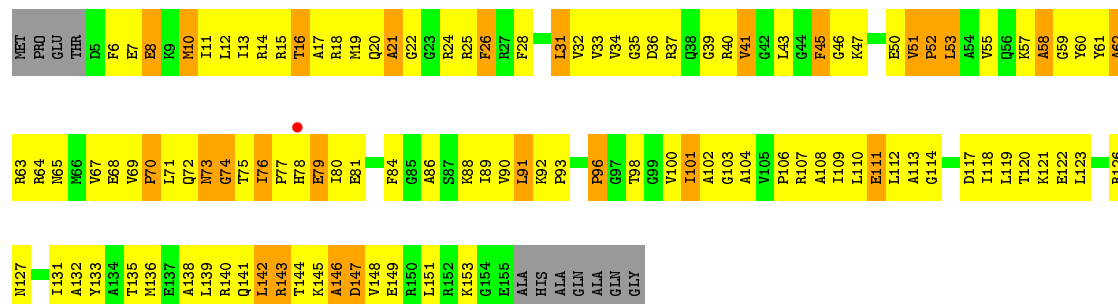




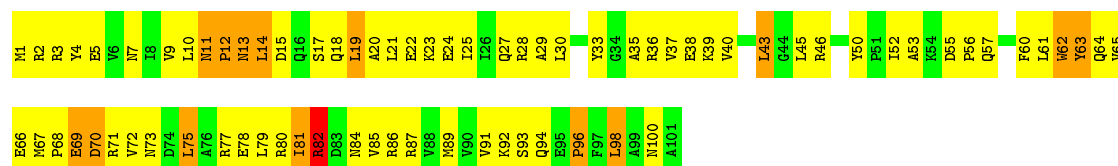




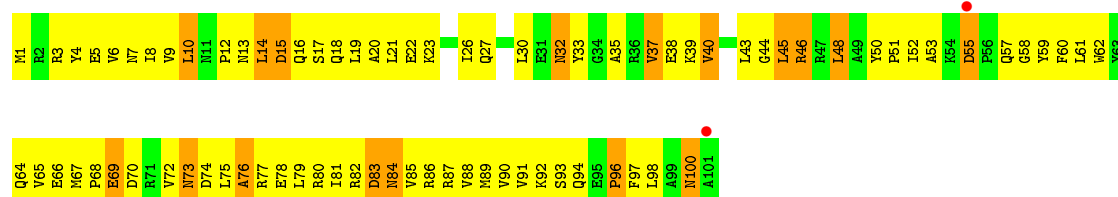
• Molecule 5: 30S ribosomal protein S5



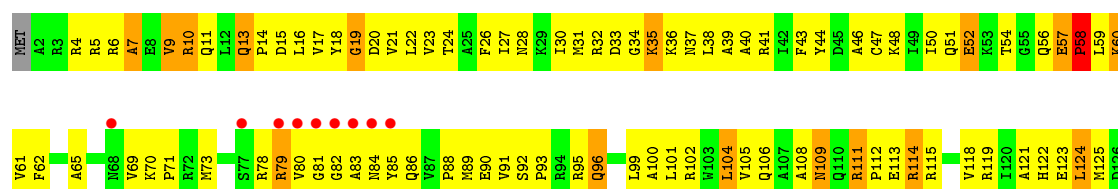
• Molecule 6: 30S ribosomal protein S6

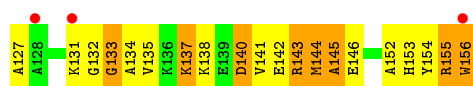


• Molecule 6: 30S ribosomal protein S6

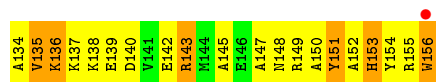
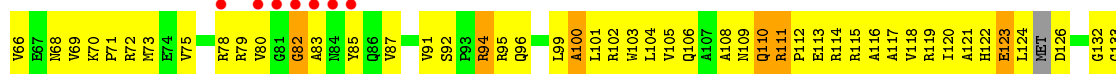


• Molecule 7: 30S ribosomal protein S7





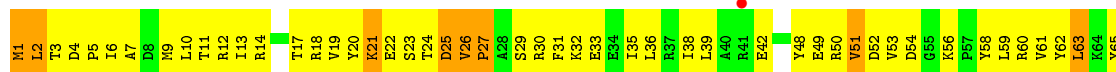
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

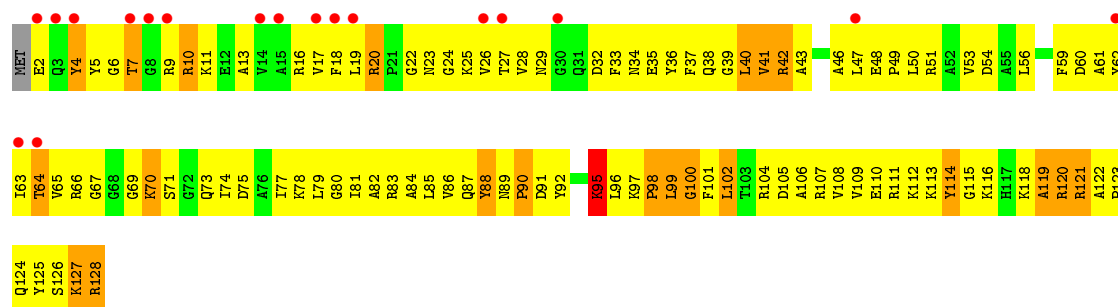


- Molecule 8: 30S ribosomal protein S8

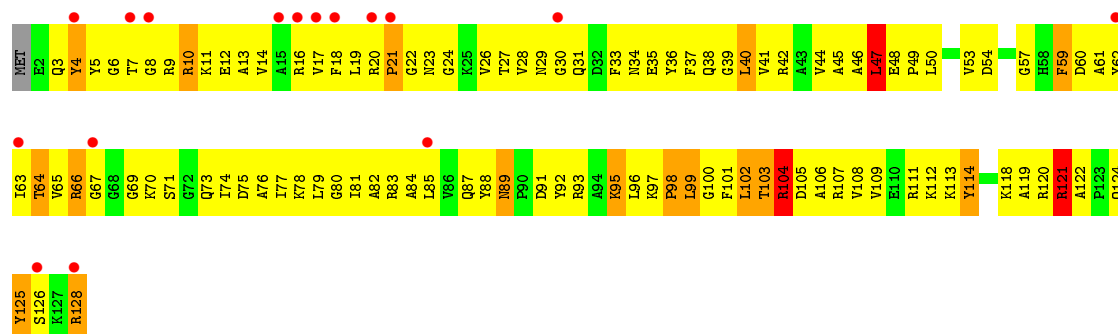


- Molecule 9: 30S ribosomal protein S9

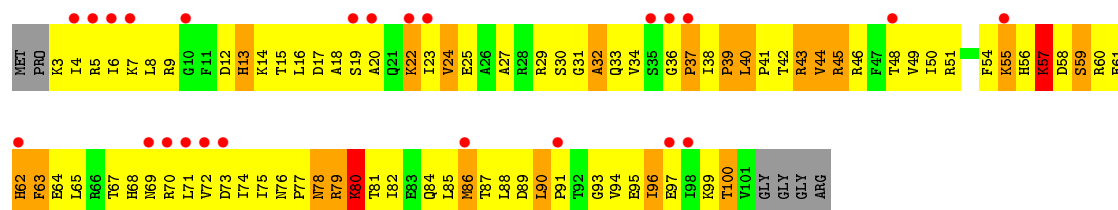
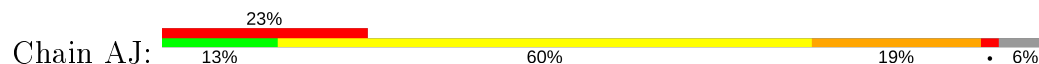




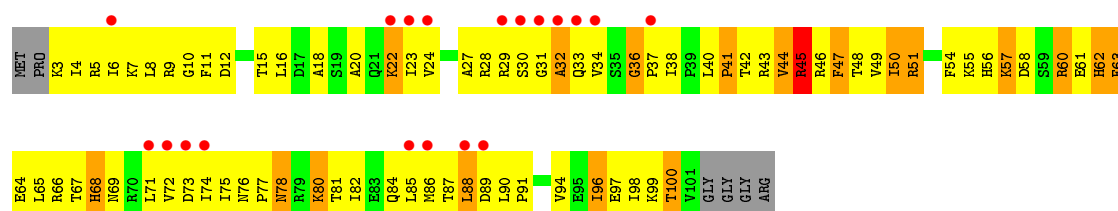
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

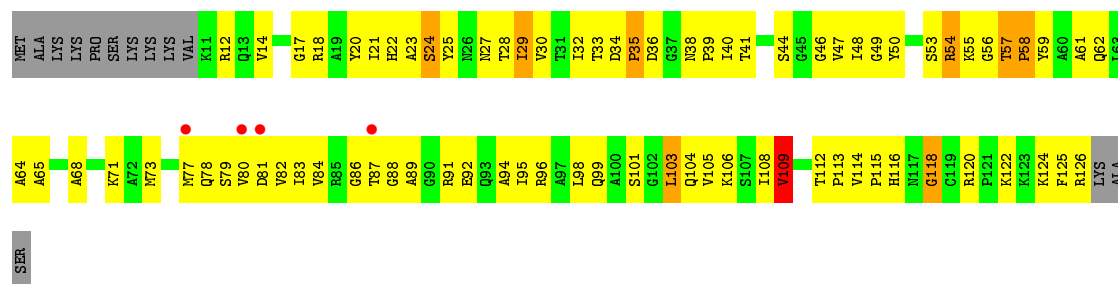


• Molecule 10: 30S ribosomal protein S10

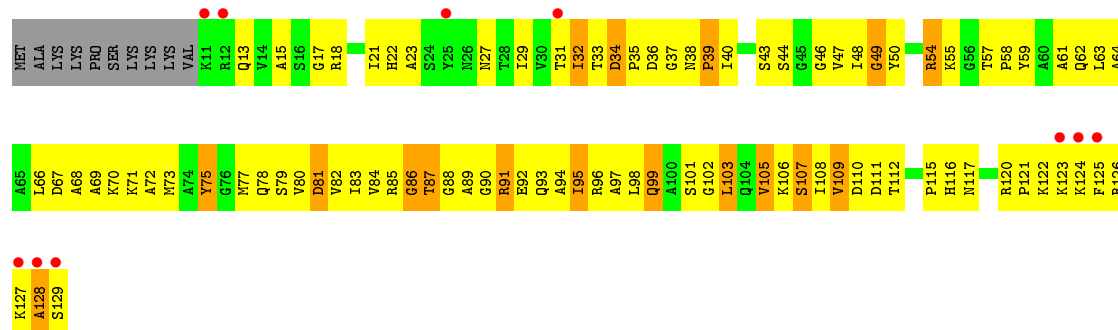


• Molecule 11: 30S ribosomal protein S11

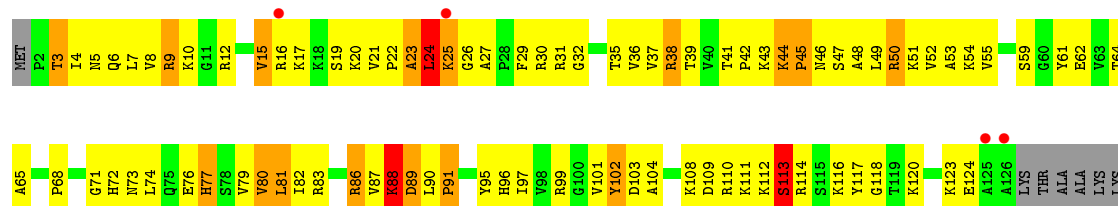




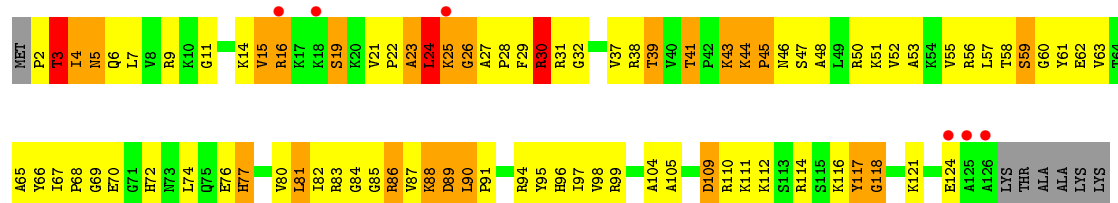
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

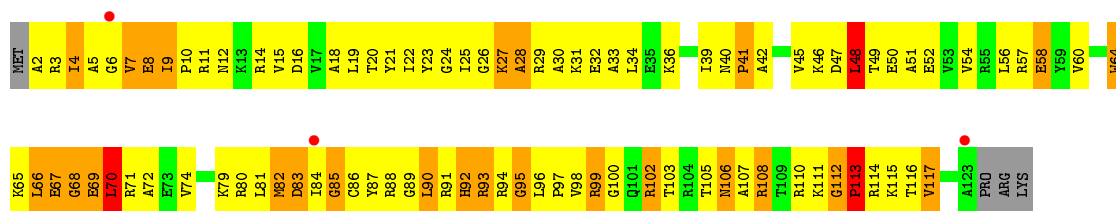


- Molecule 12: 30S ribosomal protein S12

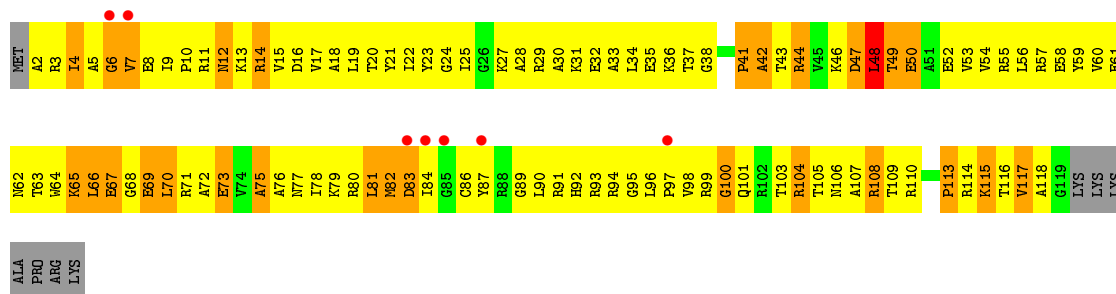
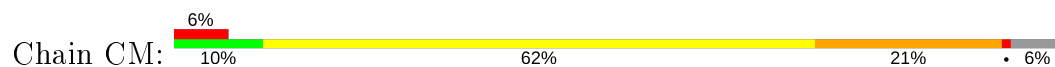


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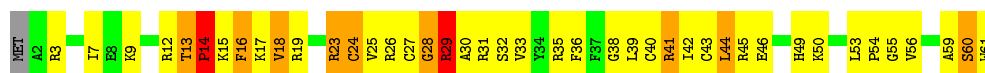




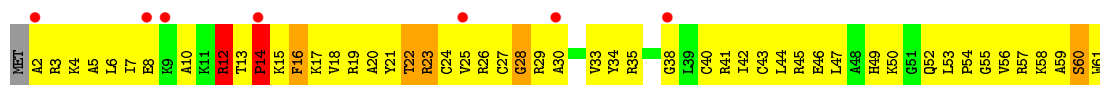
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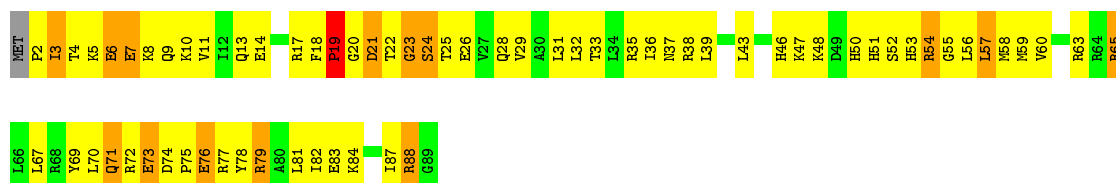
• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14

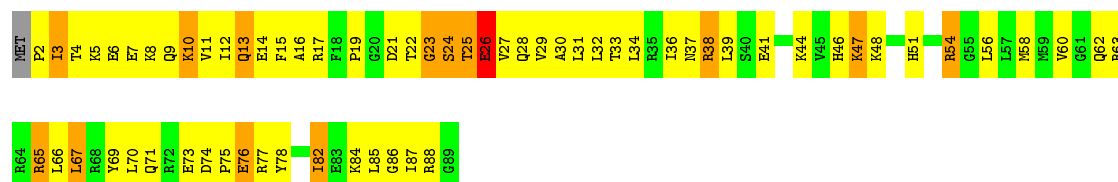


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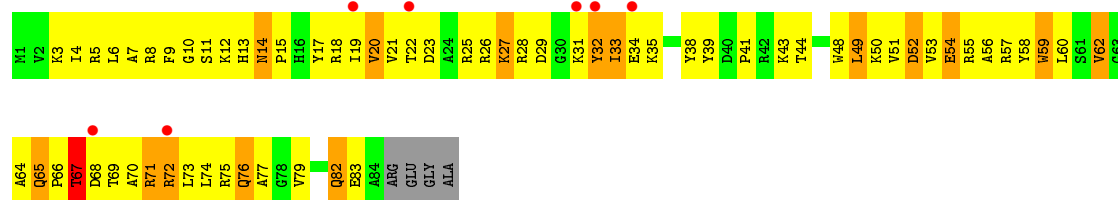


• Molecule 15: 30S ribosomal protein S15

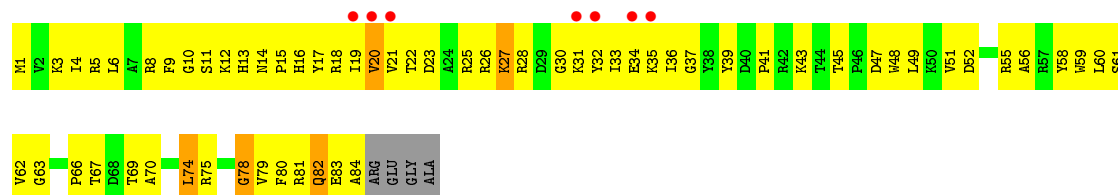




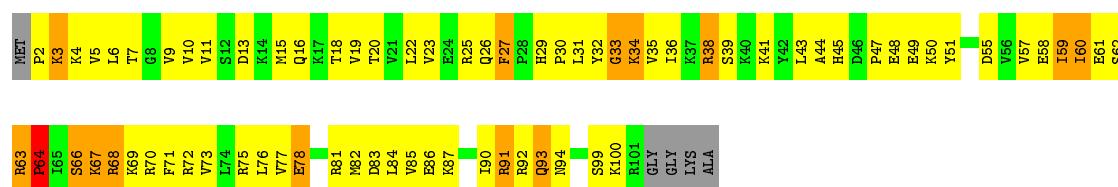
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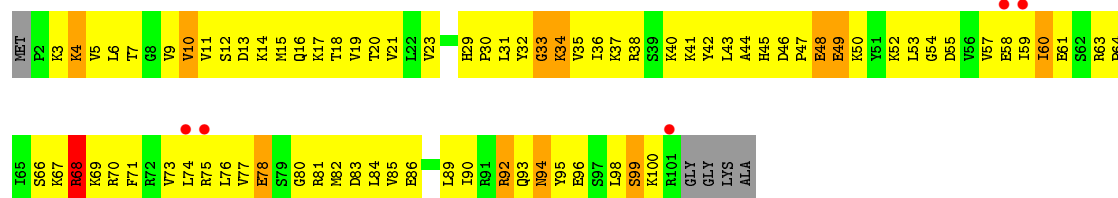
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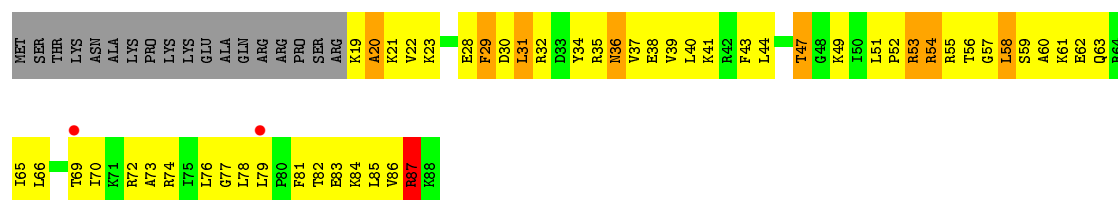
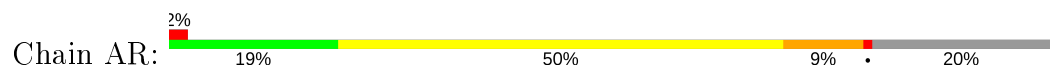
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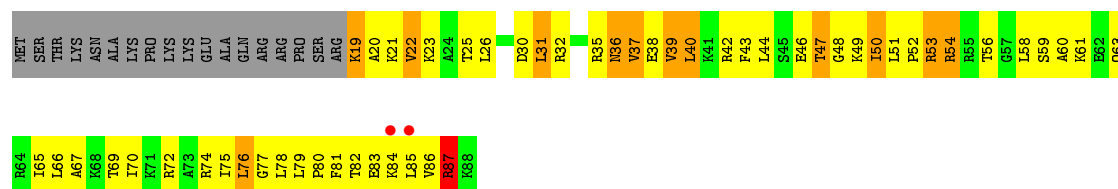
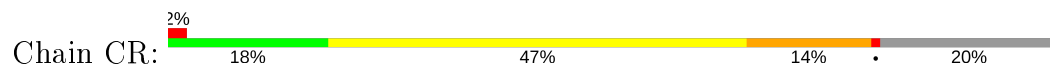
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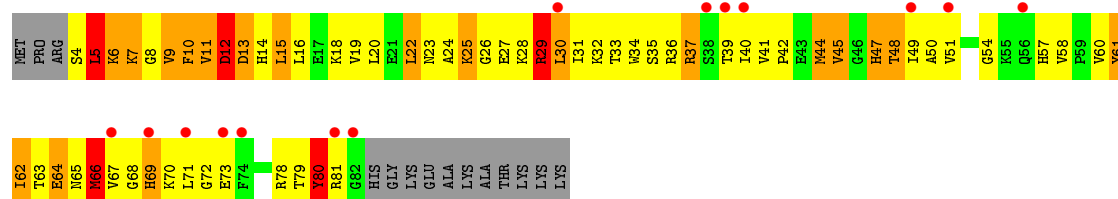
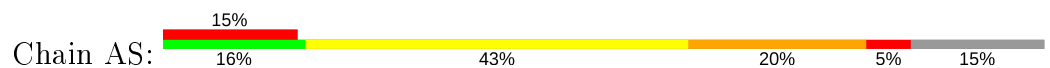
• Molecule 18: 30S ribosomal protein S18



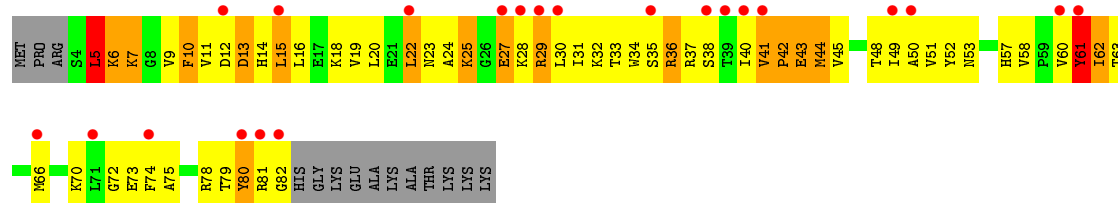
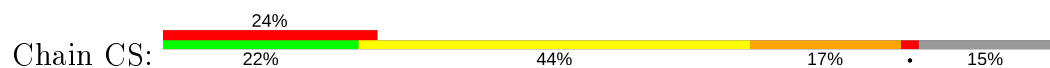
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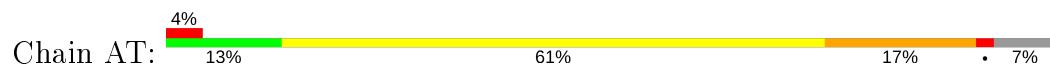
• Molecule 19: 30S ribosomal protein S19

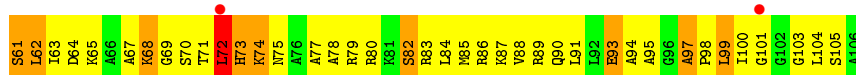


• Molecule 19: 30S ribosomal protein S19

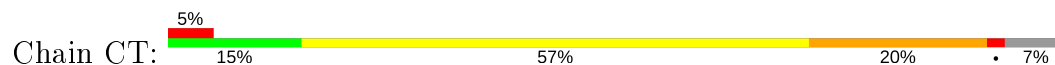


• Molecule 20: 30S ribosomal protein S20

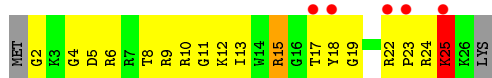




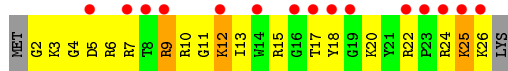
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



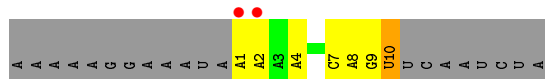
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

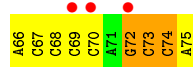
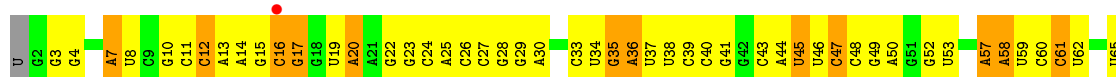


- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

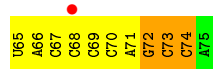
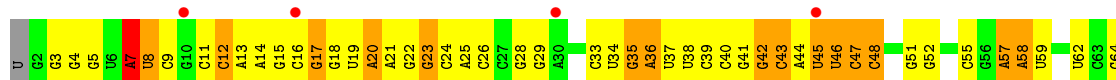


- Molecule 23: tRNA-Gln





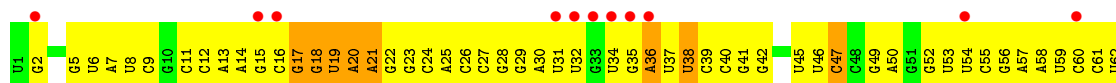
• Molecule 23: tRNA-Gln



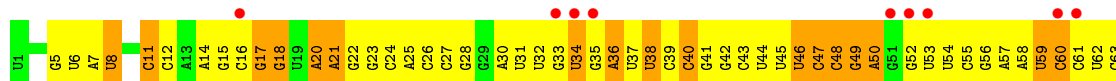
• Molecule 24: tRNA-Met



• Molecule 25: tRNA-Gln



• Molecule 25: tRNA-Gln



• Molecule 26: capreomycin 1A



71
A2
73
74
A5
S6

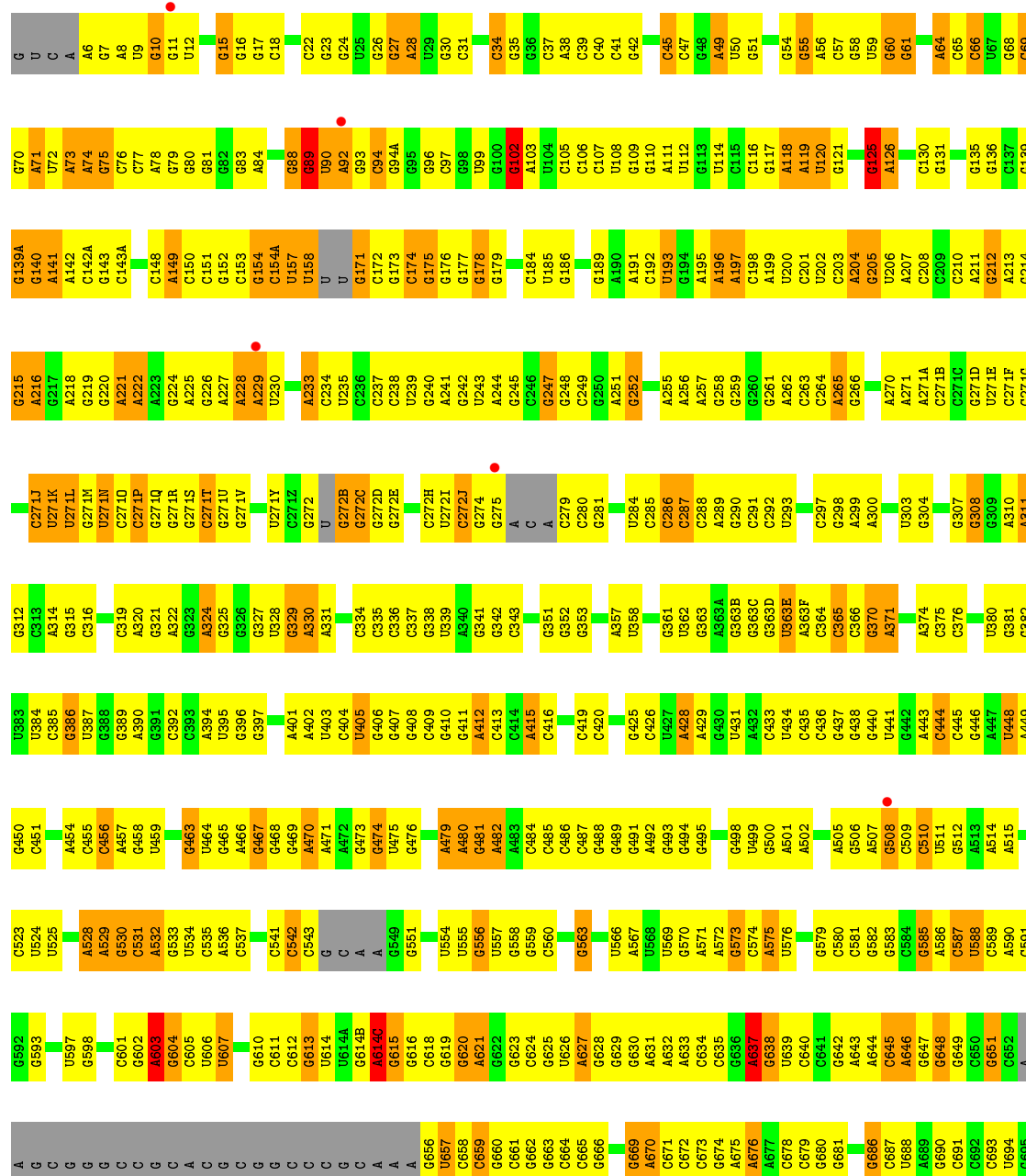
• Molecule 26: capreomycin IA

Chain CZ: 33% 67%

71
A2
73
74
A5
S6

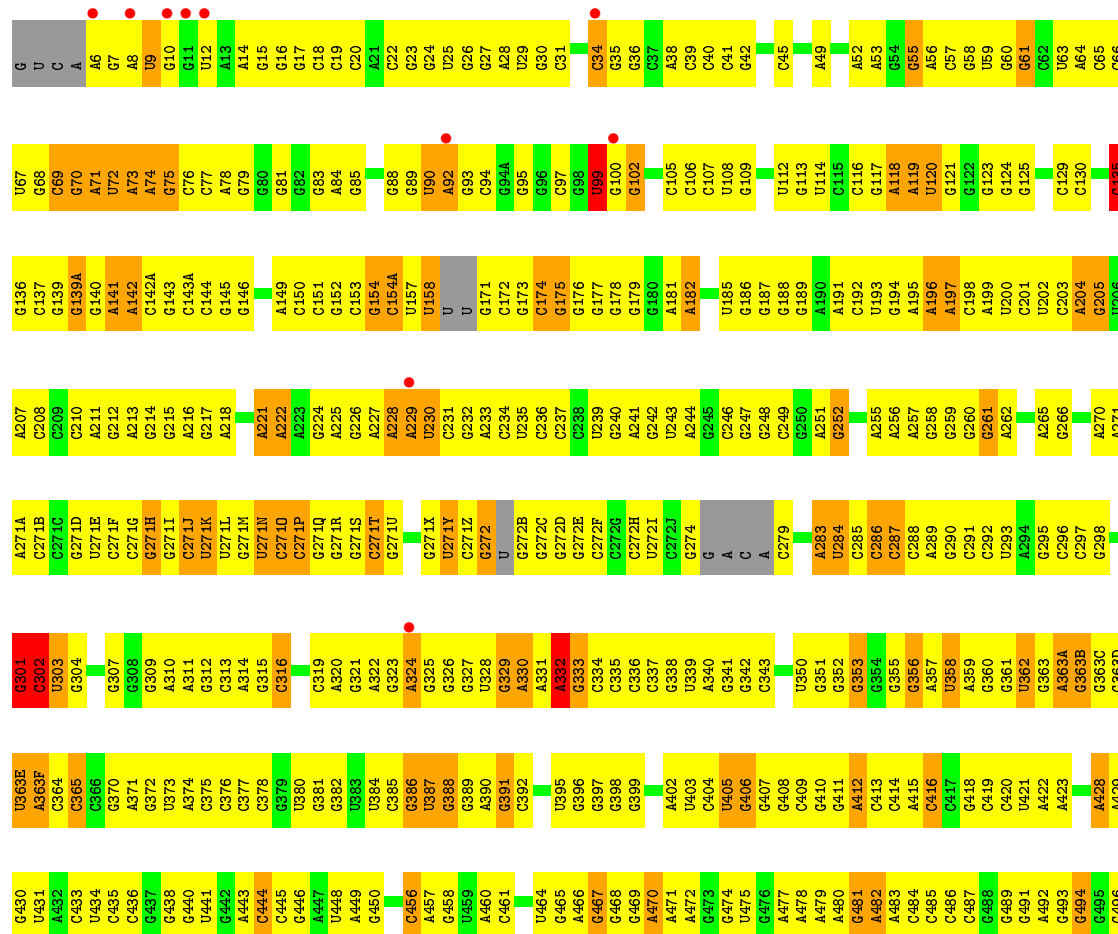
• Molecule 27: 23S ribosomal RNA

Chain BA: 2% 25% 53% 16%



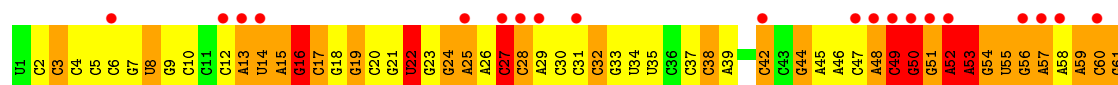
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G1565	C1502	C1370	A1302	G1222	A1156	U	U1033	C965	C902	C838	U773	C698
G1568	U1503	G1441	G1303	G1223	G1161	G	U1034	U969	C903	U839	U774	A699
A1569	G1504	G1442	C1304	C1224	G1162	A	U1035	C970	G904	C840	G775	G700
A1570	C1505	C1374	C1305	G1225	G1163	A	G1036	C971	U905	A841	G776	
A1571	C1506	C1375	C1306	G1230	G1164	U		C972	G906	C842	A777	G704
A1572	G1443	C1376	A1307	G1231	G1165	A	G1039	A973	U907	C843	A778	A705
G1573	G1444	G1377	G1308	G1238	U1166	G	A1040	A974	C908	C844	A779	A706
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G1510	A1449	G1448	U1313	G1241	G1171	U	A1045	G978	C914	C850	A784	G711
G1511	G1450	G1449	C1314	G1245	G	G	A1046		C915	G851	G785	G712
U1512	C1385	A1384		A1246	A	U	A1047	A983	G916	G852	G786	G713
C1513	C1386	U1385	G1319	A1247	U	U1108	A1048	A984	A917	G853	A787	U714
U1514	C1387	C1387	G1320	G1248	G	C1109	C1049	C985		C854	A788	
G1515	U1453	G1388	A1321	U1249	A	G1110	A1050	C986	G921	C855	A789	C719
C1516	G1455	G1389	A1322	G1250	G1178	A1111	C1051	C987	U922	C856	C790	C720
G1517	U1390	U1390	U1323	C1251	C1179	G	C1052	A988	C923	C857	A792	C721
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G1519	G1394	G1389	G1325	A1253	C1181	G	A1054	A990	C925	U859	A794	U724
U1520	U1395	U1395	U1326		G1184	U1115	G1055	C991	A926	U860	C795	G725
U1523	A1395	U1396	C1327	G1256	G1185	C1116	G	C992	G927	A861	C796	G726
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C1531	A1471	G1409	A1336	C1270	G1193	U	U	U937	U871	A805	G805	G741
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U	C1474	A1412	G1338	A1272	G1195	A		G939	G873	G808	G807	G743
A	G1475	G1413		U1273	C1196	G		A941	C874	G809	A819	G744
C	G1476	G1416	A1342	A1274	G1197	U1130		C1006	G875	U810		U747
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C1546	G1425	G1425	A1353	A1285	G1208	U1142	C	C951	C887	C888		
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C1548	A1427	A1427	A1355	U1288	A1210	A1143	U	A953	A890	A890	U826	U762
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A1618	G1491	G1429	G1358	C1290	G1212	C1145	U	C955	C893	G763	A764	A764
C1551	G1492	C1430	A1359	C1291	A1213	U	A	G956	C894	U828	G765	G765
C1493	U1431	U1431	A1360	U1292	A1213	C1147	A	A957	C895	C894	A829	A829
A1494	C1432	C1432	A1361	C1293	G1216		A	U958	U895	G830	C766	C766
A1495	U1433	U1433	C1363		C1217	C1150	G	A959	A896	G831	U767	U767
A1496	A1434	A1434	G1364	C1297	G1218	G1151	A	A960	C897	G832	G768	G768
U1497	G1435	A1365	A1365	C1298	G1219	C1152	G	C961	C898	A1027	G769	G769
A1554	G1436	G1436		G1299	A1220	C1153	U	G962	A899		A835	G770
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C1556												
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G1621												
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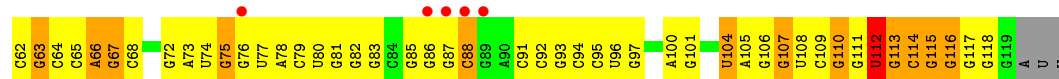
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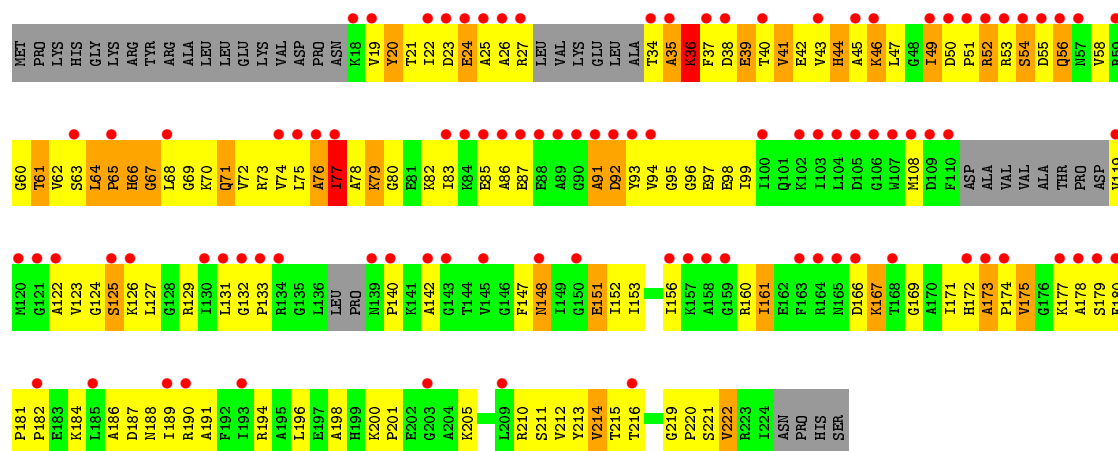


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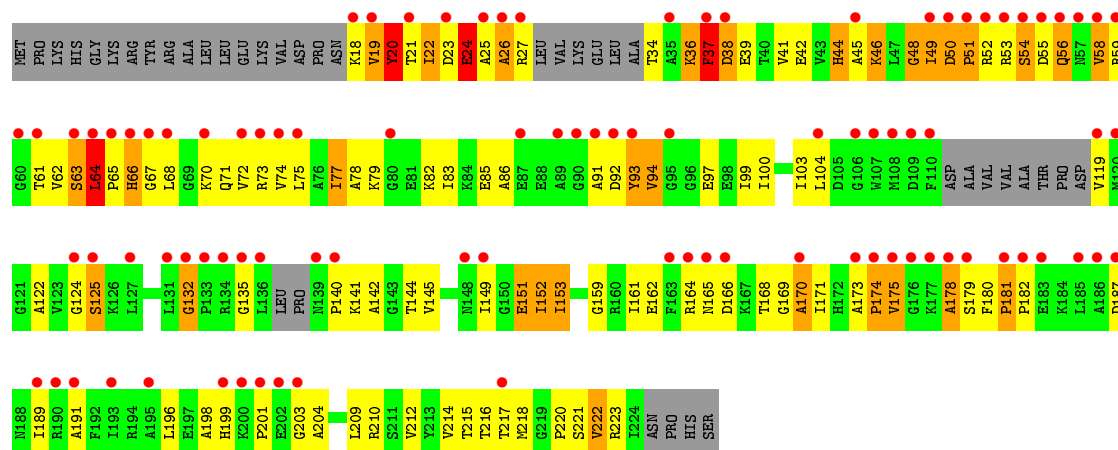




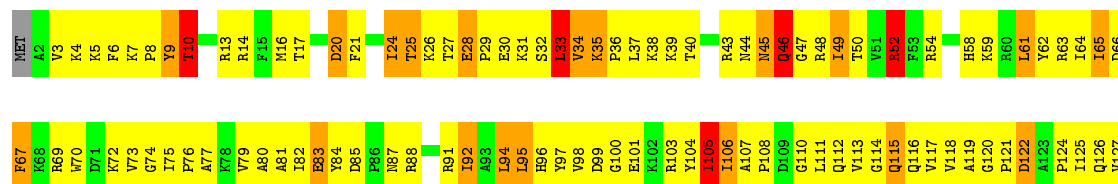
• Molecule 29: 50S ribosomal protein L1

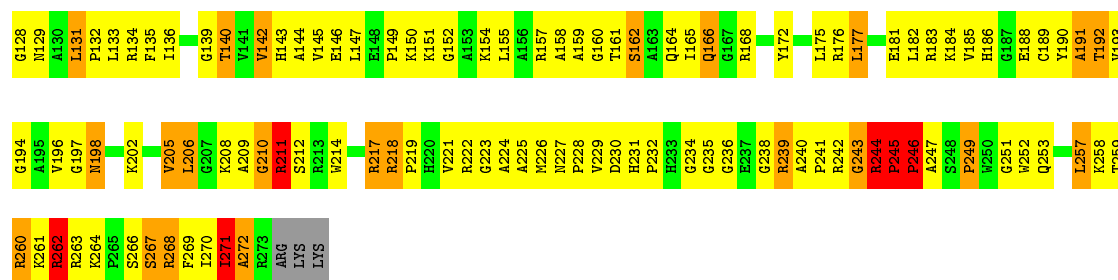


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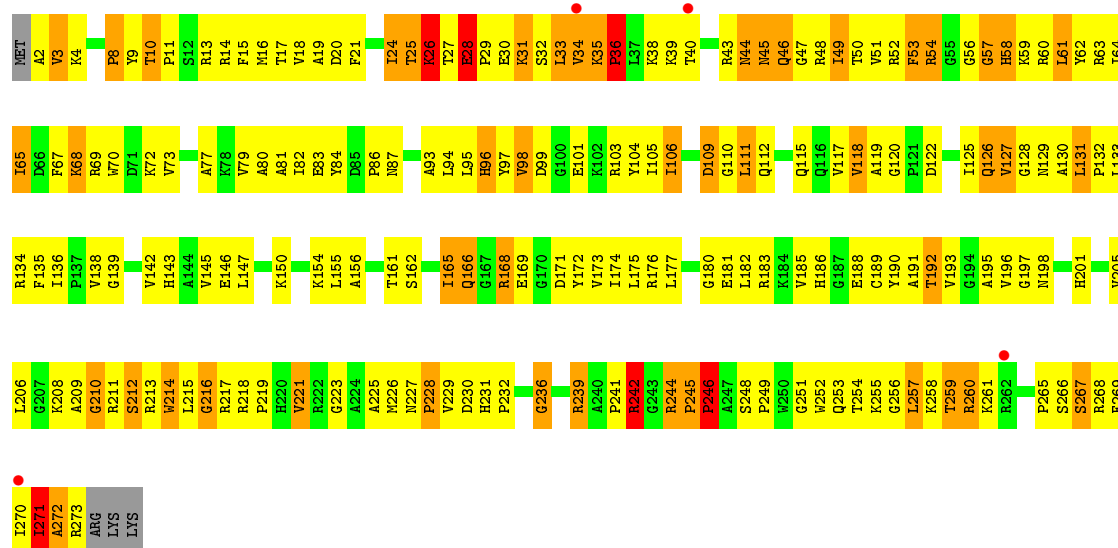


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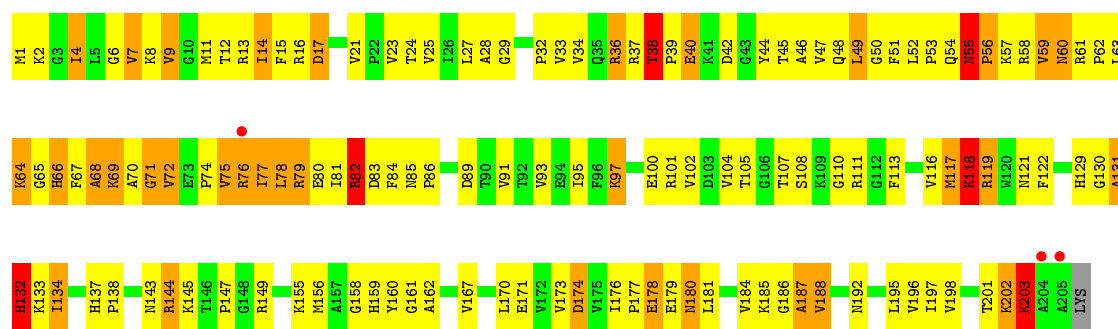




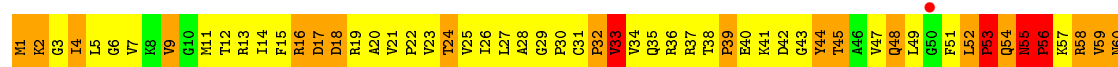
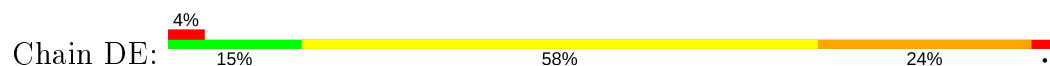
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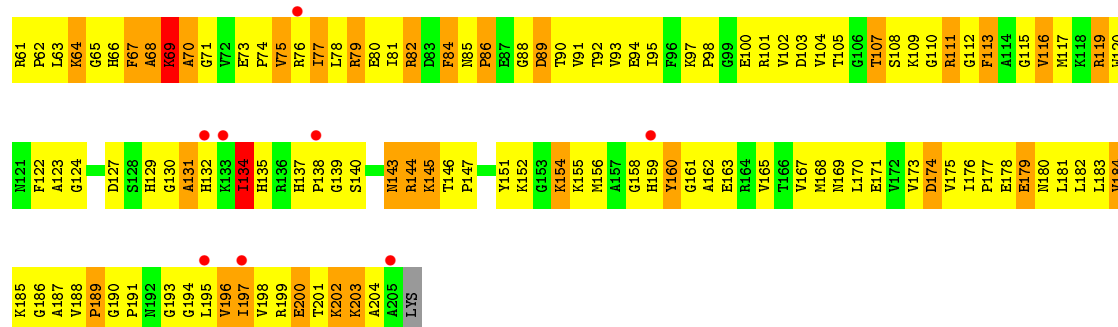


• Molecule 31: 50S ribosomal protein L3

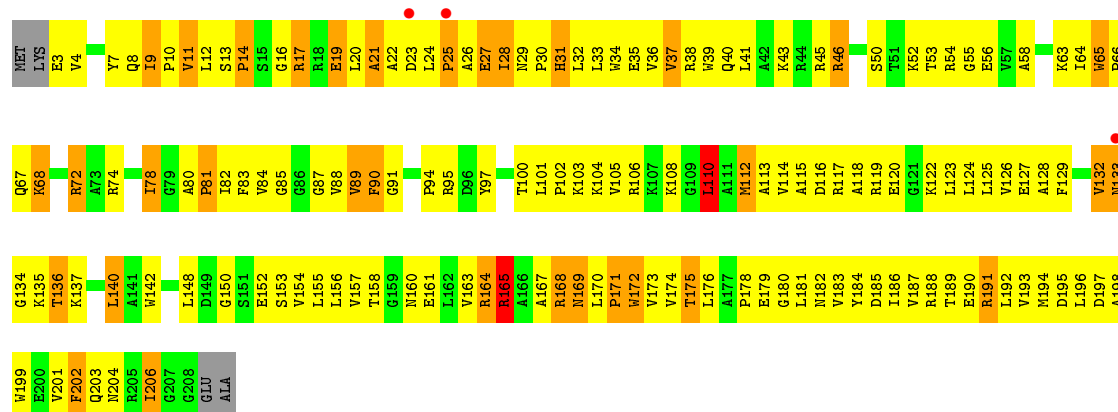


• Molecule 31: 50S ribosomal protein L3

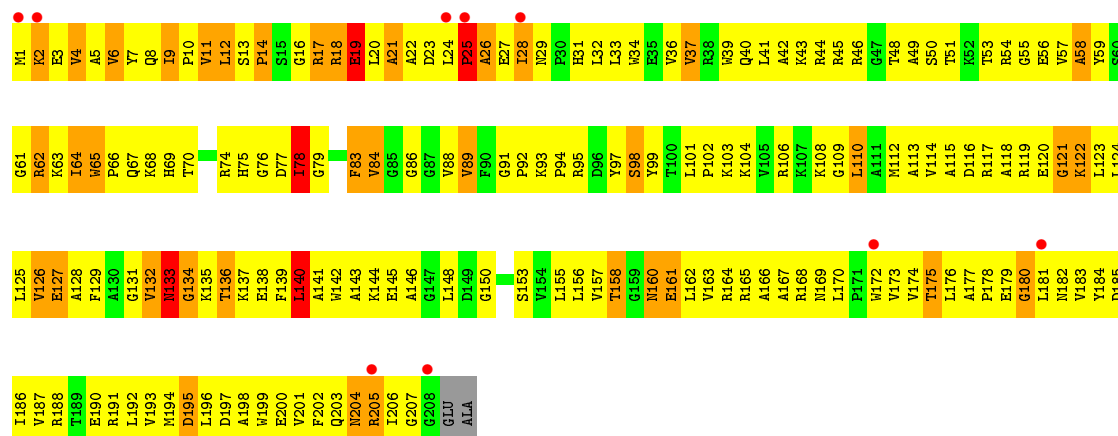




• Molecule 32: 50S ribosomal protein L4

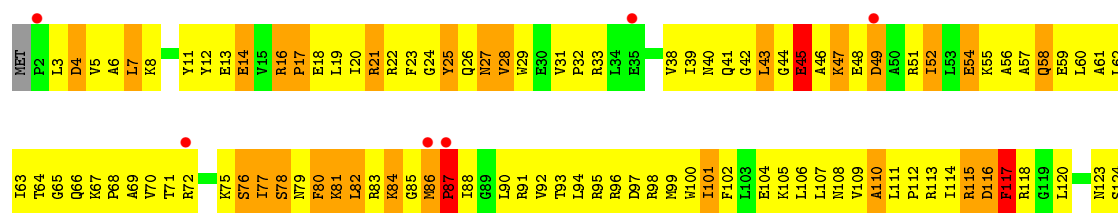


• Molecule 32: 50S ribosomal protein L4

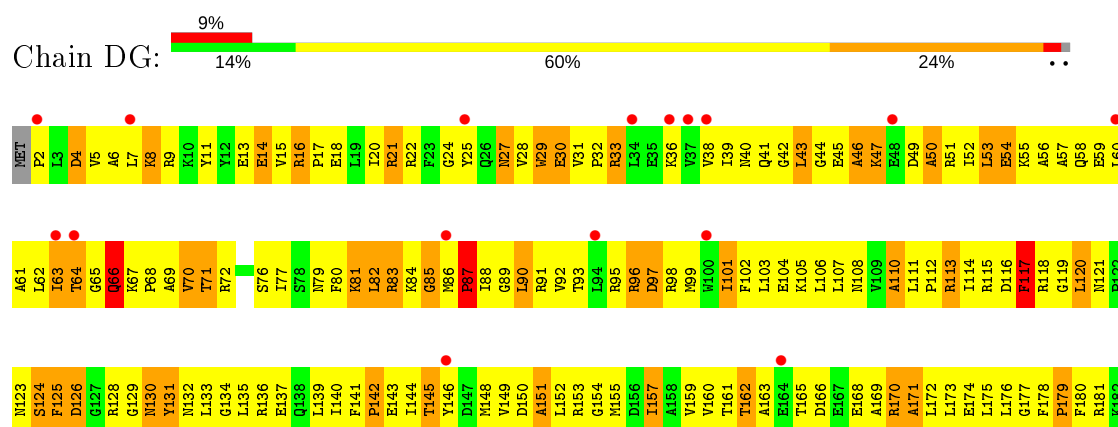


• Molecule 33: 50S ribosomal protein L5

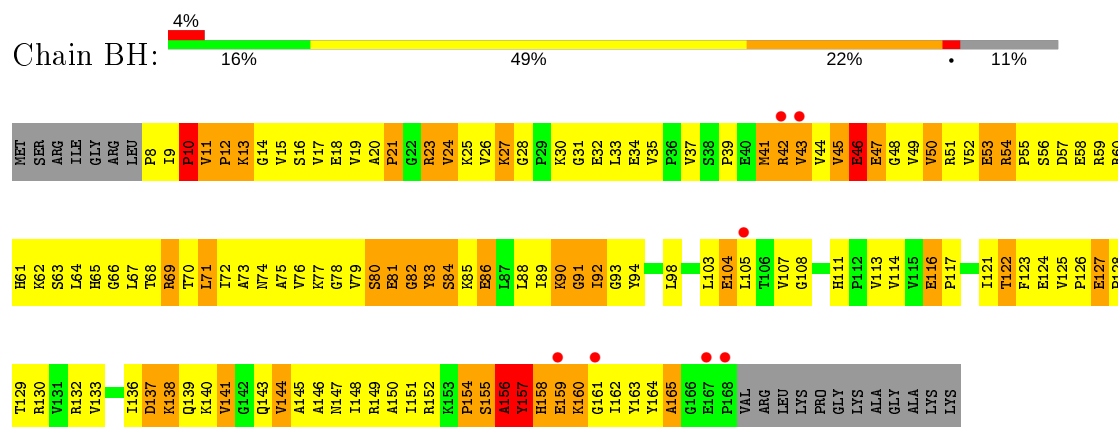




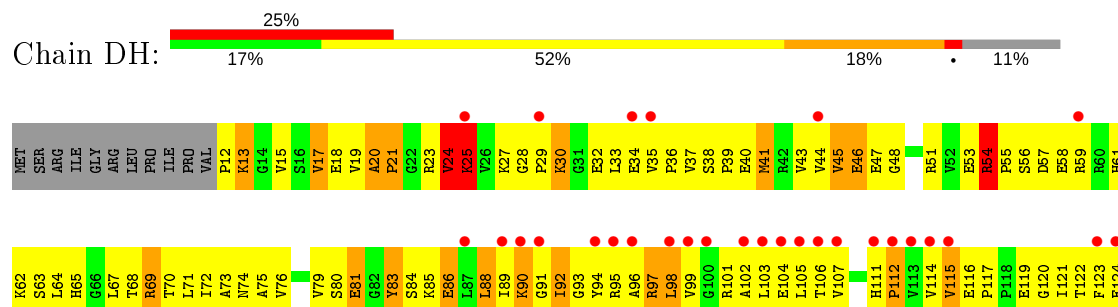
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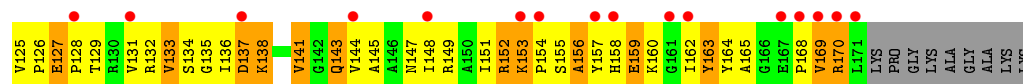


• Molecule 34: 50S ribosomal protein L6

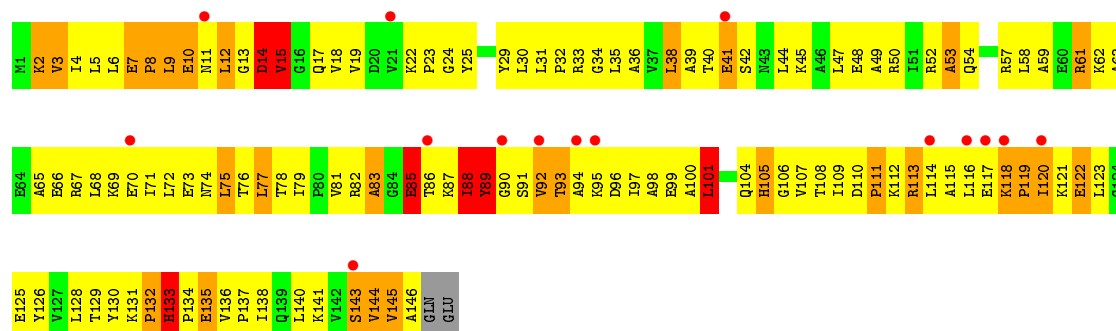
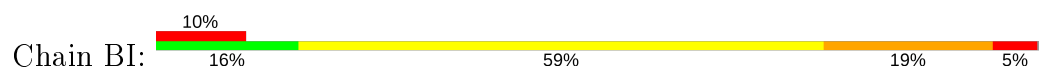


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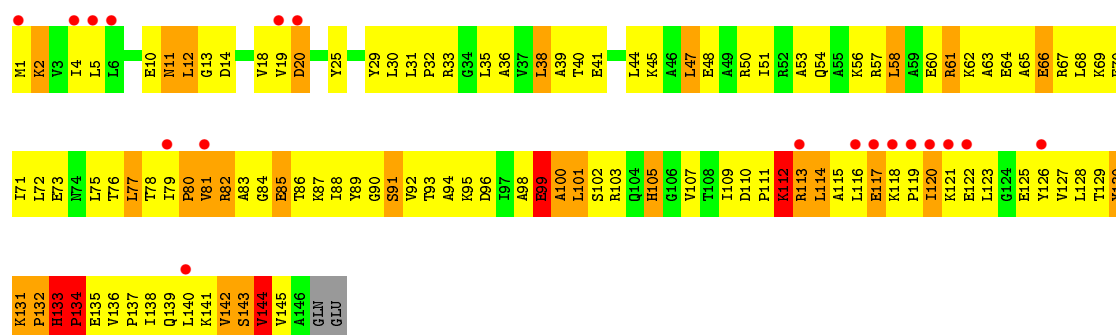




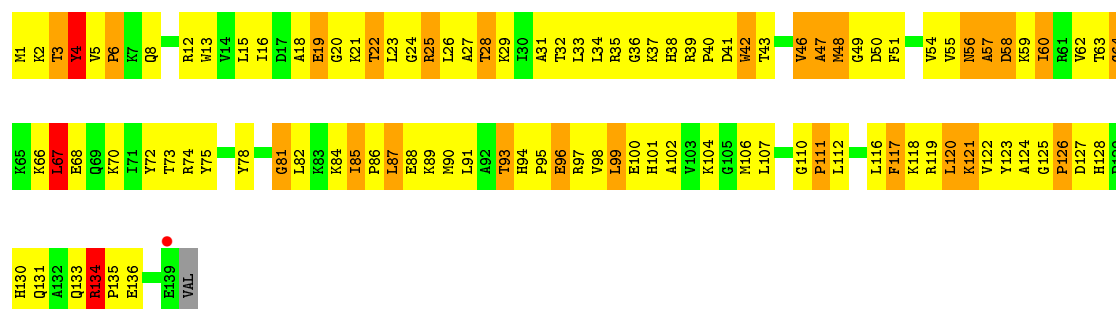
• Molecule 35: 50S ribosomal protein L9



• Molecule 35: 50S ribosomal protein L9

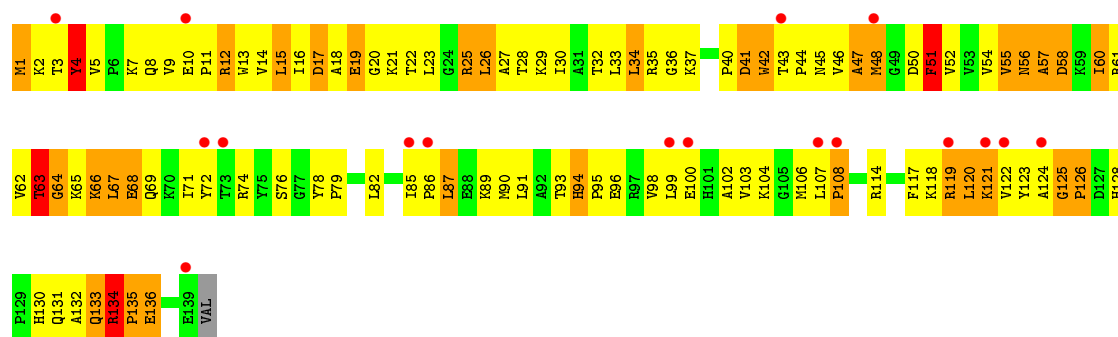


• Molecule 36: 50S ribosomal protein L13



• Molecule 36: 50S ribosomal protein L13

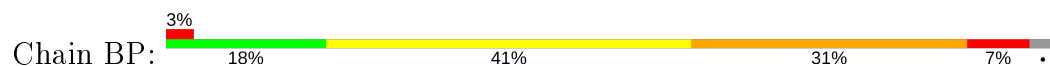




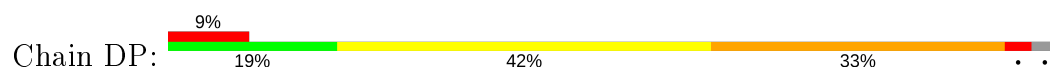
- Molecule 37: 50S ribosomal protein L14

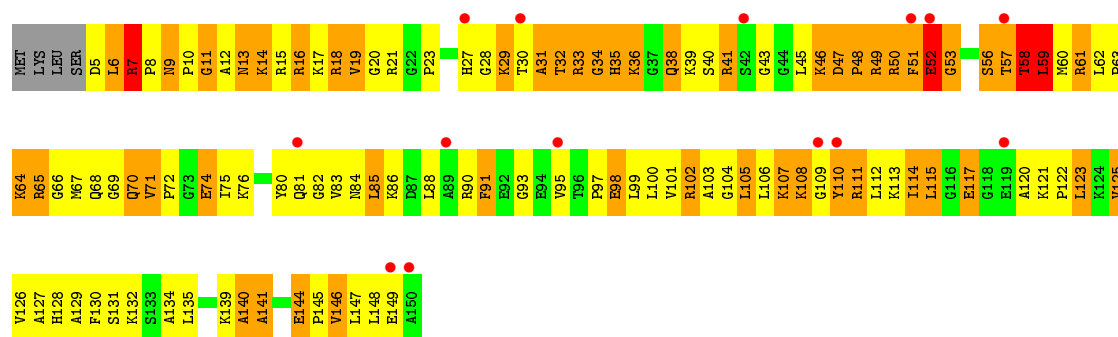
- Molecule 37: 50S ribosomal protein L14

- Molecule 38: 50S ribosomal protein L15

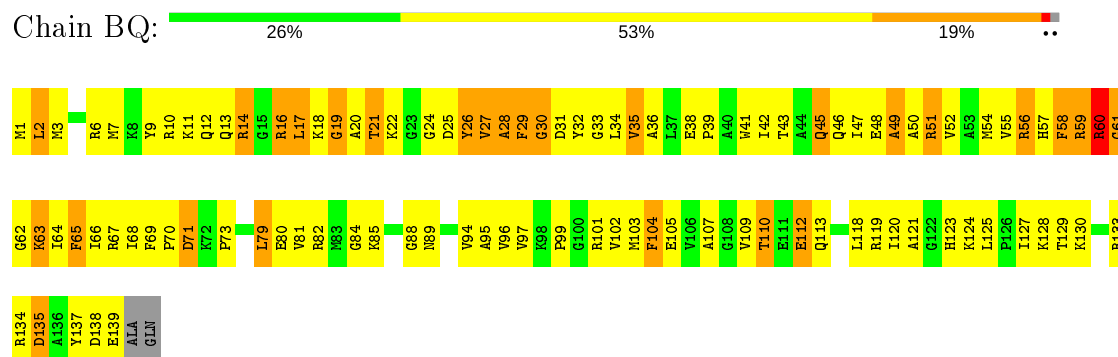


- Molecule 38: 50S ribosomal protein L15

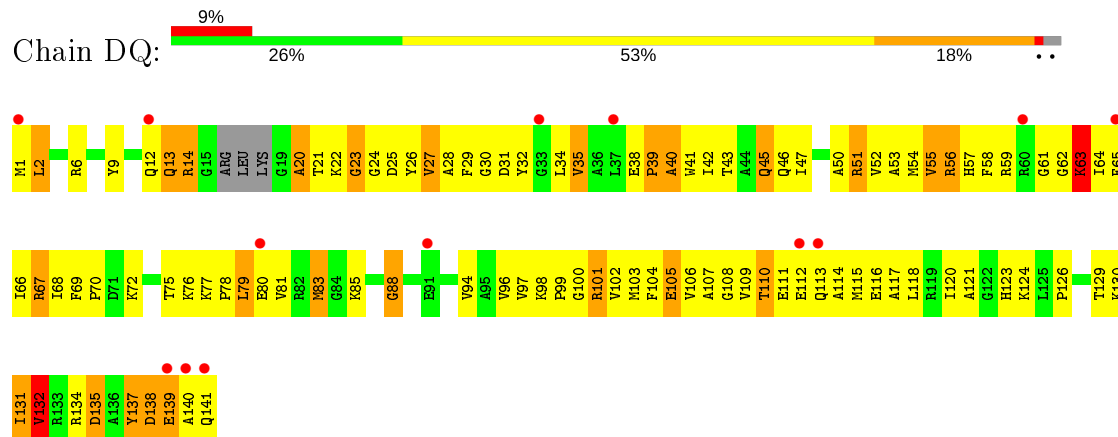




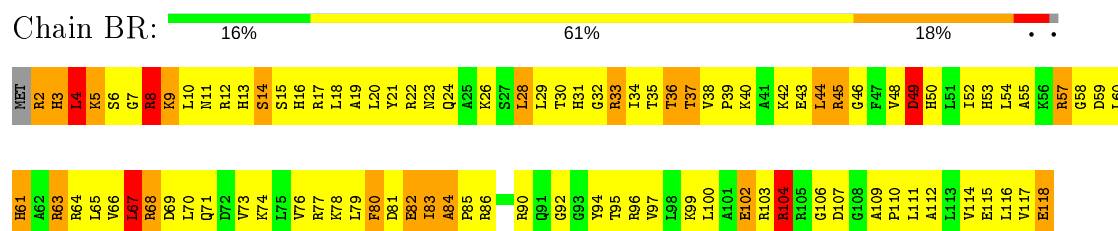
- Molecule 39: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L16

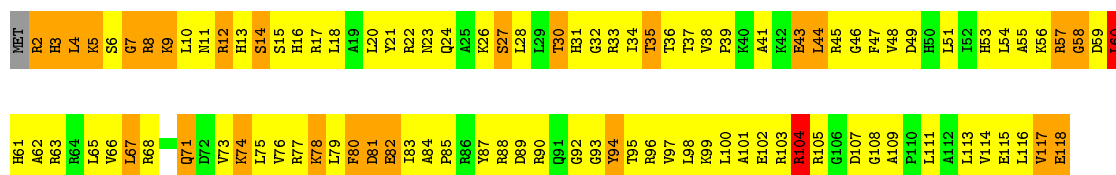


- Molecule 40: 50S ribosomal protein L17



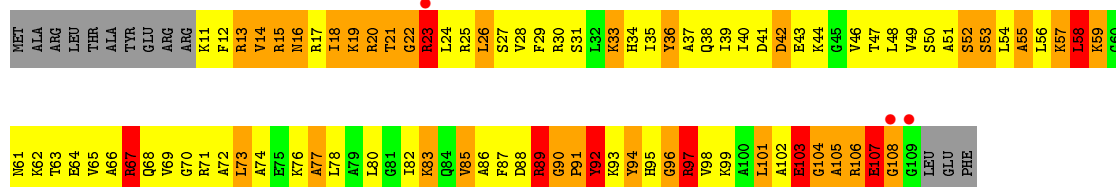
- Molecule 40: 50S ribosomal protein L17

Chain DR: 




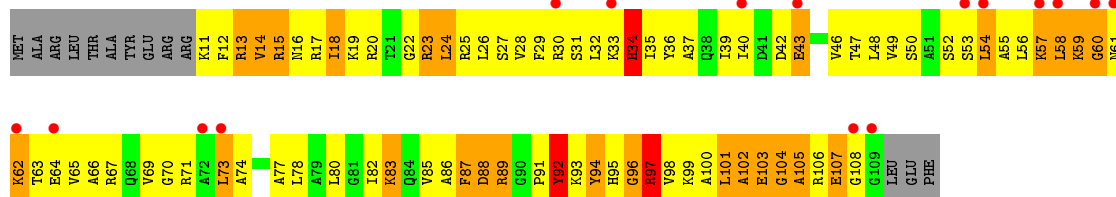
• Molecule 41: 50S ribosomal protein L18

Chain BS: 




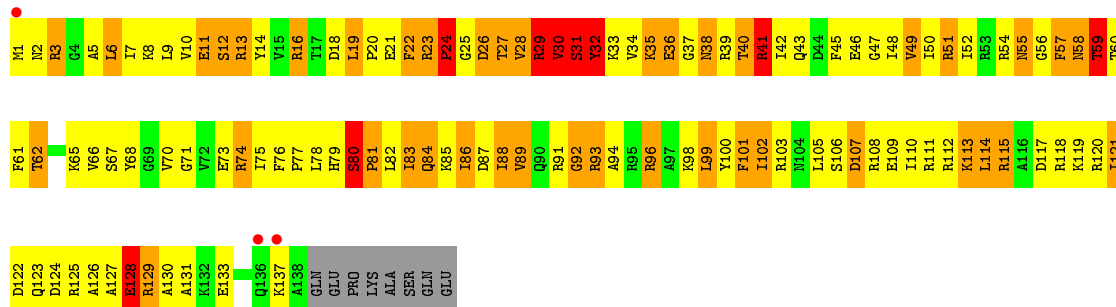
• Molecule 41: 50S ribosomal protein L18

Chain DS: 



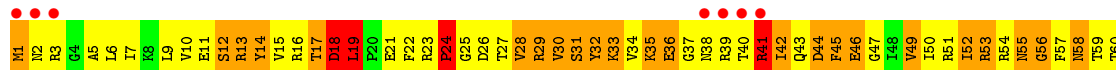
• Molecule 42: 50S ribosomal protein L19

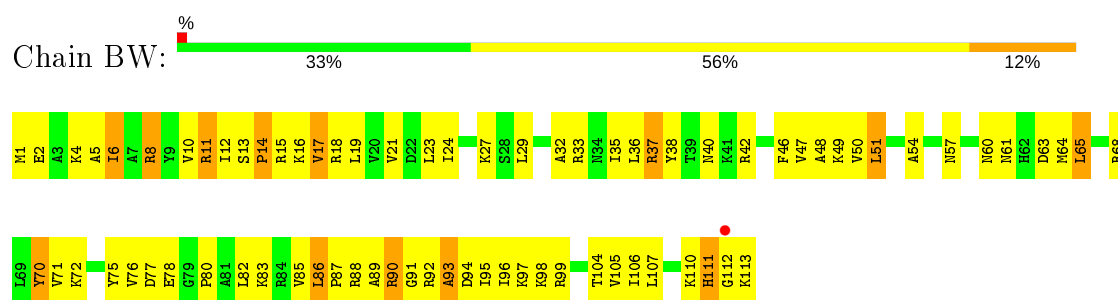
Chain BT: 



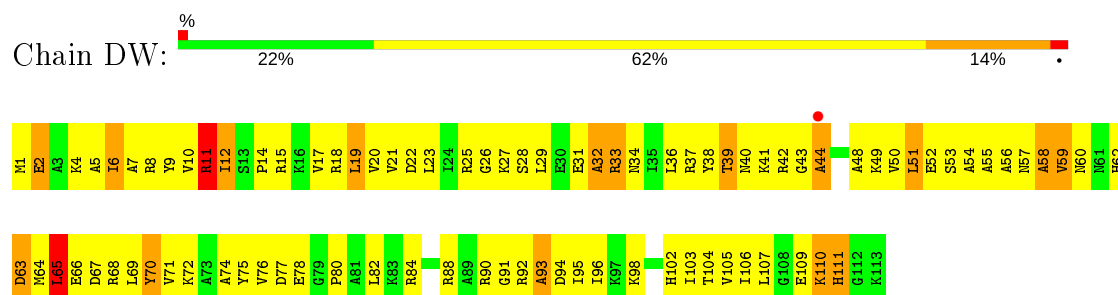
• Molecule 42: 50S ribosomal protein L19

Chain DT: 

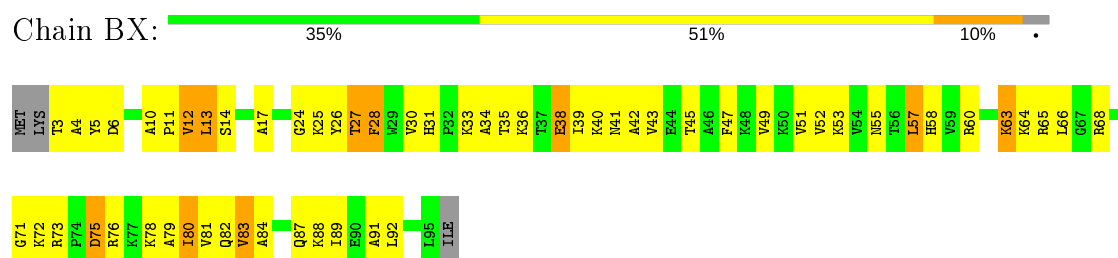




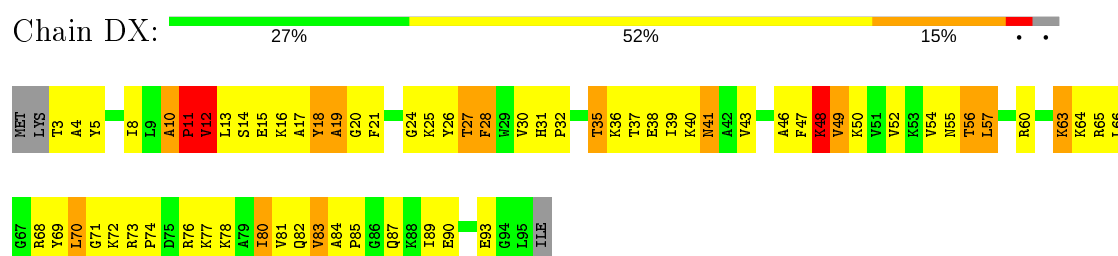
- Molecule 45: 50S ribosomal protein L22



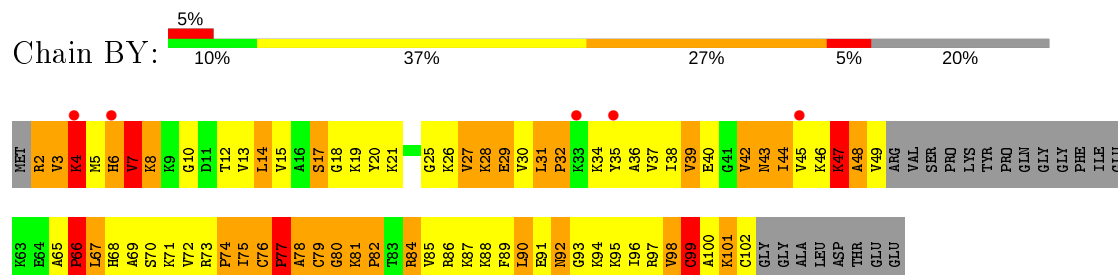
- Molecule 46: 50S ribosomal protein L23



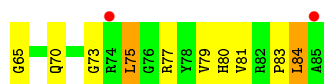
- Molecule 46: 50S ribosomal protein L23



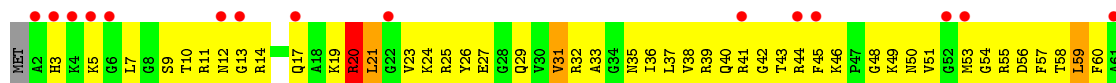
- Molecule 47: 50S ribosomal protein L24



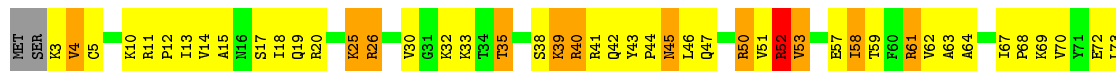
- | MET |
|-----|
| A2 |
| H3 |
| K4 |
| K5 |
| G6 |
| L7 |
| T10 |
| R11 |
| N12 |
| G13 |
| R14 |
| D15 |
| S16 |
| Q17 |
| A18 |
| K19 |
| R20 |
| V23 |
| K24 |
| R25 |
| Y26 |
| E27 |
| G28 |
| Q29 |
| V30 |
| V31 |
| R32 |
| I36 |
| L37 |
| V38 |
| R39 |
| G42 |
| T43 |
| R44 |
| F45 |
| K46 |
| P47 |
| G48 |
| K49 |
| N50 |
| V51 |
| G52 |
| M53 |
| G54 |
| R55 |
| D56 |
| F57 |
| T58 |
| L59 |
| F60 |
| A61 |
| L62 |
| V63 |
| D64 |



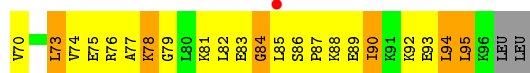
- Molecule 49: 50S ribosomal protein L27



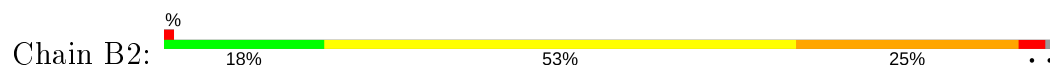
- Molecule 50: 50S ribosomal protein L28



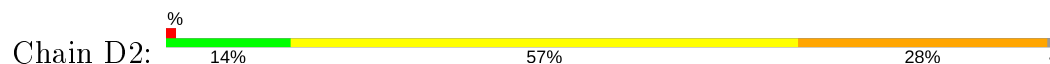
- Molecule 50: 50S ribosomal protein L28

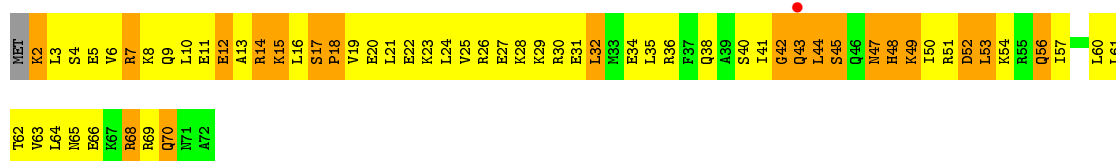


- Molecule 51: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L29

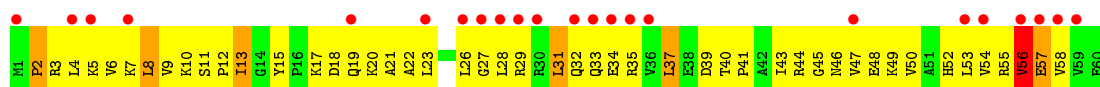




- Molecule 52: 50S ribosomal protein L30



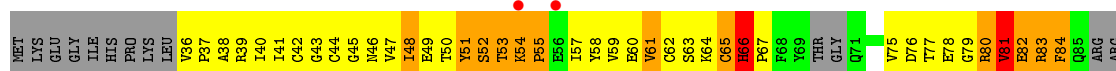
- Molecule 52: 50S ribosomal protein L30



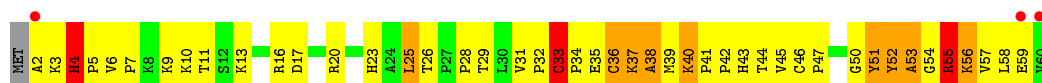
- Molecule 53: 50S ribosomal protein L31



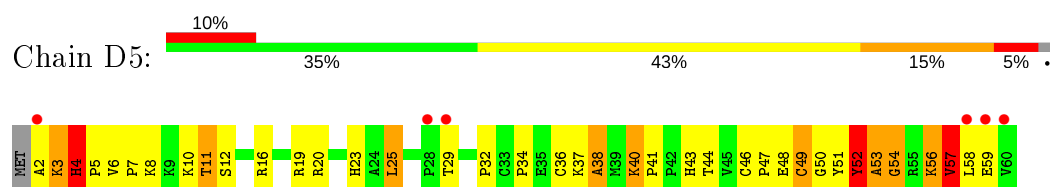
- Molecule 53: 50S ribosomal protein L31



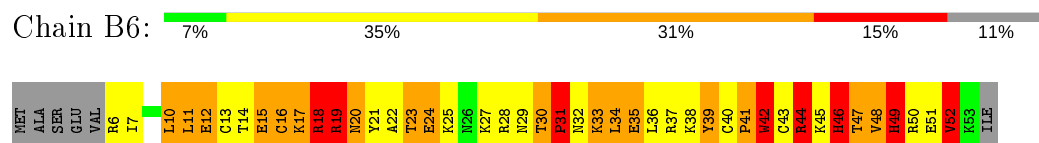
- Molecule 54: 50S ribosomal protein L32



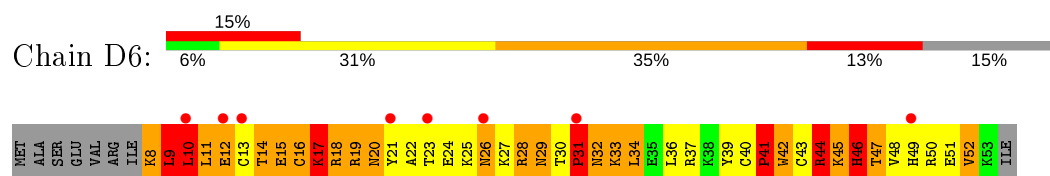
- Molecule 54: 50S ribosomal protein L32



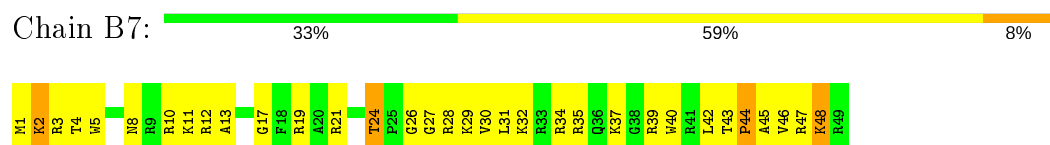
- Molecule 55: 50S ribosomal protein L33



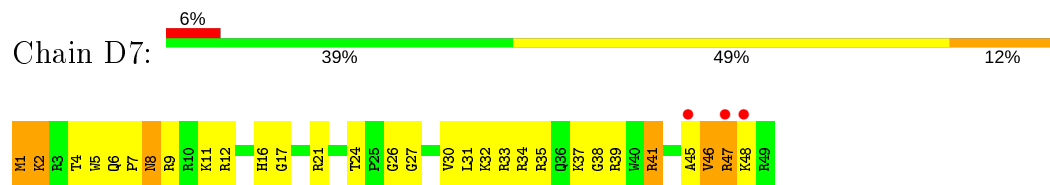
- Molecule 55: 50S ribosomal protein L33



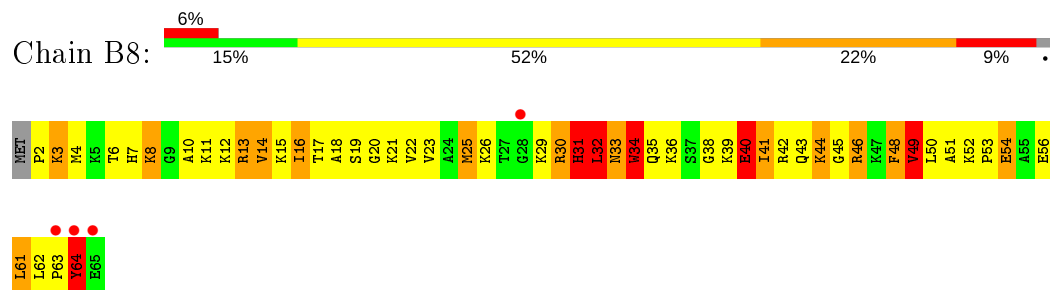
- Molecule 56: 50S ribosomal protein L34



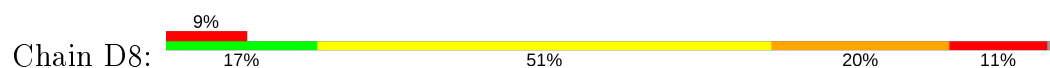
- Molecule 56: 50S ribosomal protein L34

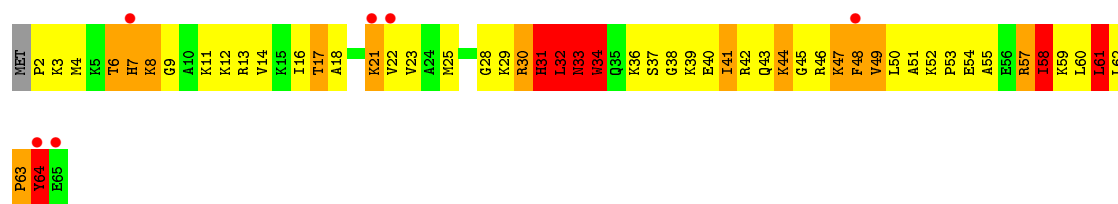


- Molecule 57: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L35

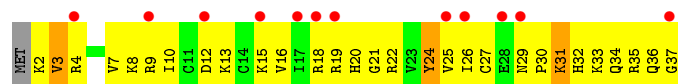




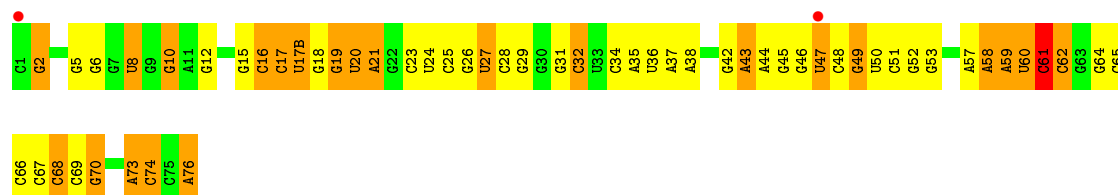
- Molecule 58: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L36



- Molecule 59: RNA (77-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 448.24Å 631.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.45 49.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.45) 82.3 (49.75-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.268 0.220 , 0.219	Depositor DCC
R_{free} test set	33507 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	293848	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: ZN, DPP, MG, KBE, UAL, MYN

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	0.48	0/35968	0.74	23/56136 (0.0%)
1	CA	0.50	9/35932 (0.0%)	0.75	27/56082 (0.0%)
2	AB	0.39	0/1936	0.68	0/2611
2	CB	0.37	0/1936	0.66	0/2611
3	AC	0.38	0/1637	0.65	0/2207
3	CC	0.37	0/1627	0.67	0/2192
4	AD	0.42	0/1733	0.71	0/2318
4	CD	0.44	0/1733	0.72	1/2318 (0.0%)
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.42	0/1163	0.68	0/1566
6	AF	0.44	0/856	0.75	1/1154 (0.1%)
6	CF	0.43	0/856	0.71	0/1154
7	AG	0.38	0/1276	0.61	0/1709
7	CG	0.39	0/1267	0.62	0/1696
8	AH	0.40	0/1136	0.72	0/1527
8	CH	0.38	0/1136	0.70	0/1527
9	AI	0.38	0/1024	0.68	0/1372
9	CI	0.36	0/1024	0.67	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.36	0/808	0.67	0/1087
11	AK	0.41	0/879	0.75	0/1187
11	CK	0.39	0/900	0.68	0/1213
12	AL	0.44	0/987	0.80	0/1322
12	CL	0.44	0/987	0.74	0/1322
13	AM	0.37	0/975	0.75	2/1305 (0.2%)
13	CM	0.36	0/947	0.72	0/1270
14	AN	0.41	0/501	0.69	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.39	0/745	0.64	0/992
15	CO	0.37	0/745	0.64	0/992
16	AP	0.40	0/717	0.70	0/965
16	CP	0.43	0/717	0.74	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.68	0/1119
18	AR	0.48	0/579	0.75	0/768
18	CR	0.41	0/579	0.72	0/768
19	AS	0.40	0/643	0.70	1/867 (0.1%)
19	CS	0.37	0/643	0.66	0/867
20	AT	0.38	0/765	0.72	1/1007 (0.1%)
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.42	0/213	0.60	0/279
21	CU	0.34	0/213	0.62	0/279
22	AV	0.48	0/230	0.65	0/357
22	CV	0.45	0/239	0.69	0/371
23	AW	0.47	0/1756	0.78	0/2734
23	CW	0.46	0/1756	0.75	2/2734 (0.1%)
24	AX	0.58	2/1831 (0.1%)	0.87	6/2853 (0.2%)
25	AY	0.37	0/1776	0.71	0/2766
25	CY	0.36	0/1776	0.71	0/2766
26	AZ	0.91	0/5	0.51	0/5
26	CZ	0.51	0/5	0.85	0/5
27	BA	0.61	3/67273 (0.0%)	0.79	62/105005 (0.1%)
27	DA	0.51	1/66930 (0.0%)	0.77	45/104469 (0.0%)
28	BB	0.57	0/2853	0.81	6/4451 (0.1%)
28	DB	0.79	6/2853 (0.2%)	0.95	13/4451 (0.3%)
29	BC	0.31	0/1145	0.60	0/1556
29	DC	0.30	0/1145	0.61	0/1556
30	BD	0.54	0/2155	0.86	3/2907 (0.1%)
30	DD	0.51	0/2155	0.82	2/2907 (0.1%)
31	BE	0.56	0/1597	0.87	2/2155 (0.1%)
31	DE	0.42	0/1597	0.75	0/2155
32	BF	0.50	0/1642	0.82	1/2225 (0.0%)
32	DF	0.42	0/1659	0.75	1/2246 (0.0%)
33	BG	0.44	0/1499	0.78	0/2016
33	DG	0.40	0/1499	0.72	0/2016
34	BH	0.59	0/1258	0.91	2/1703 (0.1%)
34	DH	0.33	0/1246	0.67	0/1684
35	BI	0.39	0/1147	0.74	0/1553
35	DI	0.37	0/1147	0.75	0/1553
36	BN	0.54	0/1132	0.91	2/1527 (0.1%)
36	DN	0.41	0/1132	0.77	1/1527 (0.1%)
37	BO	0.54	0/943	0.80	0/1269
37	DO	0.44	0/943	0.69	0/1269
38	BP	0.59	0/1131	1.16	5/1504 (0.3%)
38	DP	0.48	0/1131	1.00	5/1504 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BQ	0.53	0/1128	0.77	0/1508
39	DQ	0.42	0/1114	0.68	0/1488
40	BR	0.55	0/974	0.92	2/1302 (0.2%)
40	DR	0.43	0/974	0.81	0/1302
41	BS	0.55	0/779	0.97	2/1038 (0.2%)
41	DS	0.43	0/779	0.75	0/1038
42	BT	0.57	0/1156	0.96	5/1544 (0.3%)
42	DT	0.46	0/1156	0.83	1/1544 (0.1%)
43	BU	0.57	0/975	0.85	0/1297
43	DU	0.38	0/975	0.69	0/1297
44	BV	0.58	0/790	0.95	2/1057 (0.2%)
44	DV	0.41	0/790	0.72	0/1057
45	BW	0.53	0/907	0.77	0/1216
45	DW	0.41	0/907	0.72	0/1216
46	BX	0.51	0/740	0.78	0/995
46	DX	0.48	0/740	0.73	0/995
47	BY	0.61	0/680	0.93	1/904 (0.1%)
47	DY	0.46	0/789	0.82	1/1053 (0.1%)
48	BZ	0.41	0/1436	0.72	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.47	0/671	0.74	0/892
49	D0	0.41	0/671	0.67	0/892
50	B1	0.49	0/739	0.76	1/983 (0.1%)
50	D1	0.43	0/739	0.76	0/983
51	B2	0.45	0/600	0.74	0/793
51	D2	0.39	0/600	0.67	0/793
52	B3	0.48	0/473	0.76	0/636
52	D3	0.34	0/473	0.63	0/636
53	B4	0.43	0/349	0.71	0/474
53	D4	0.39	0/349	0.64	0/474
54	B5	0.62	0/473	1.04	2/639 (0.3%)
54	D5	0.50	0/473	0.82	0/639
55	B6	0.72	0/409	1.07	0/548
55	D6	0.70	0/397	1.12	4/531 (0.8%)
56	B7	0.55	0/427	0.80	0/563
56	D7	0.48	0/427	0.73	0/563
57	B8	0.63	0/516	1.02	2/681 (0.3%)
57	D8	0.51	0/516	0.87	1/681 (0.1%)
58	B9	0.53	0/302	0.80	0/397
58	D9	0.39	0/302	0.70	0/397
59	CX	0.47	0/1832	0.75	1/2855 (0.0%)
All	All	0.51	21/318243 (0.0%)	0.77	239/475835 (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
1	AA	0	35
1	CA	1	31
19	AS	0	1
23	AW	0	1
23	CW	0	1
24	AX	0	1
27	BA	4	96
27	DA	0	63
28	BB	0	3
28	DB	0	6
42	BT	0	1
59	CX	0	2
All	All	5	241

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	46	A	C6-N6	-11.79	1.24	1.33
1	CA	101	A	C6-N6	-8.09	1.27	1.33
1	CA	1458	G	C5-C6	-7.73	1.34	1.42
1	CA	70	G	C5-C6	-7.36	1.34	1.42
1	CA	1446	U	N1-C2	-7.30	1.31	1.38

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	46	A	C5-C6-N1	-12.54	111.43	117.70
28	DB	53	A	O5'-P-OP2	11.96	125.06	110.70
24	AX	46	A	C6-N1-C2	10.83	125.10	118.60
24	AX	46	A	N1-C2-N3	-10.72	123.94	129.30
27	BA	1992	G	C2'-C3'-O3'	10.30	132.16	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	BA	1378	A	C3'
27	BA	1799	G	C3'
27	BA	1992	G	C3'

Continued on next page...

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Mol	Chain	Res	Type	Atom
27	BA	2497	A	C3'
1	CA	533	A	C3'

5 of 241 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	181	G	Sidechain
1	AA	298	A	Sidechain
1	AA	37	U	Sidechain
1	AA	388	G	Sidechain
1	AA	490	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32132	0	16219	1429	0
1	CA	32098	0	16199	1614	0
2	AB	1901	0	1951	312	0
2	CB	1901	0	1951	269	0
3	AC	1613	0	1677	278	0
3	CC	1604	0	1670	270	0
4	AD	1703	0	1763	264	0
4	CD	1703	0	1763	197	0
5	AE	1147	0	1207	160	0
5	CE	1147	0	1207	172	0
6	AF	843	0	857	91	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	161	0
7	CG	1249	0	1286	155	0
8	AH	1116	0	1177	165	0
8	CH	1116	0	1177	143	0
9	AI	1006	0	1034	176	0
9	CI	1006	0	1034	201	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	175	0
11	AK	864	0	881	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	117	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	128	0
13	AM	965	0	1034	166	0
13	CM	937	0	995	162	0
14	AN	492	0	533	77	0
14	CN	492	0	533	108	0
15	AO	734	0	771	94	0
15	CO	734	0	771	99	0
16	AP	701	0	720	107	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	114	0
17	CQ	824	0	891	125	0
18	AR	574	0	644	87	0
18	CR	574	0	644	83	0
19	AS	630	0	652	126	0
19	CS	630	0	652	110	0
20	AT	763	0	861	134	0
20	CT	763	0	861	131	0
21	AU	209	0	221	26	0
21	CU	209	0	221	24	0
22	AV	205	0	106	7	0
22	CV	213	0	110	11	0
23	AW	1573	0	800	86	0
23	CW	1573	0	800	72	0
24	AX	1639	0	835	72	0
25	AY	1591	0	810	72	0
25	CY	1591	0	810	81	0
26	AZ	47	0	40	11	0
26	CZ	47	0	40	14	0
27	BA	60072	0	30294	2481	0
27	DA	59767	0	30140	2934	0
28	BB	2551	0	1295	107	0
28	DB	2551	0	1295	201	0
29	BC	1142	0	865	119	0
29	DC	1142	0	865	116	0
30	BD	2105	0	2182	345	0
30	DD	2105	0	2182	317	0
31	BE	1564	0	1629	250	0
31	DE	1564	0	1629	346	0
32	BF	1607	0	1652	226	0
32	DF	1624	0	1677	293	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BG	1474	0	1535	250	0
33	DG	1474	0	1535	310	0
34	BH	1233	0	1294	217	0
34	DH	1223	0	1282	184	0
35	BI	1132	0	1218	207	0
35	DI	1132	0	1218	223	0
36	BN	1105	0	1180	153	0
36	DN	1105	0	1180	195	0
37	BO	933	0	996	114	0
37	DO	933	0	996	145	0
38	BP	1114	0	1187	303	0
38	DP	1114	0	1187	329	0
39	BQ	1107	0	1166	179	0
39	DQ	1094	0	1141	150	0
40	BR	960	0	1021	148	0
40	DR	960	0	1021	182	0
41	BS	771	0	832	185	0
41	DS	771	0	832	188	0
42	BT	1142	0	1202	236	0
42	DT	1142	0	1202	303	0
43	BU	958	0	1014	151	0
43	DU	958	0	1015	187	0
44	BV	779	0	852	162	0
44	DV	779	0	852	141	0
45	BW	896	0	953	108	0
45	DW	896	0	953	135	0
46	BX	726	0	778	75	0
46	DX	726	0	778	87	0
47	BY	672	0	766	190	0
47	DY	776	0	870	211	0
48	BZ	1404	0	1432	215	0
48	DZ	1404	0	1432	266	0
49	B0	662	0	688	83	0
49	D0	662	0	688	92	0
50	B1	732	0	808	97	0
50	D1	732	0	808	98	0
51	B2	598	0	653	75	0
51	D2	598	0	653	95	0
52	B3	468	0	523	46	0
52	D3	468	0	523	71	0
53	B4	344	0	305	69	0
53	D4	344	0	305	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B5	459	0	476	80	0
54	D5	459	0	477	62	0
55	B6	402	0	413	109	0
55	D6	390	0	404	135	0
56	B7	419	0	467	46	0
56	D7	419	0	467	41	0
57	B8	508	0	576	130	0
57	D8	508	0	576	138	0
58	B9	299	0	323	34	0
58	D9	299	0	323	57	0
59	CX	1640	0	837	62	0
60	AA	114	0	0	0	0
60	AG	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	9	0	0	0	0
60	B0	3	0	0	0	0
60	B5	1	0	0	0	0
60	BA	334	0	0	0	0
60	BB	5	0	0	0	0
60	BD	1	0	0	0	0
60	BE	3	0	0	0	0
60	BF	1	0	0	0	0
60	BG	1	0	0	0	0
60	BP	2	0	0	0	0
60	BR	1	0	0	0	0
60	BU	2	0	0	0	0
60	BX	1	0	0	0	0
60	CA	102	0	0	0	0
60	CE	1	0	0	0	0
60	CK	1	0	0	0	0
60	CV	1	0	0	0	0
60	CW	4	0	0	0	0
60	D0	1	0	0	0	0
60	D5	1	0	0	0	0
60	D7	1	0	0	0	0
60	DA	239	0	0	0	0
60	DB	3	0	0	0	0
60	DD	2	0	0	0	0
60	DE	1	0	0	0	0
60	DF	1	0	0	0	0
60	DO	1	0	0	0	0
61	AD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B4	1	0	0	0	0
61	B5	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	D4	1	0	0	0	0
61	D5	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	293848	0	198788	22560	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 22560 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)
55:B6:15:GLU:CD	55:B6:18:ARG:HE	1.41	1.22
4:AD:19:LEU:HD11	4:AD:67:ILE:HG13	1.24	1.19
1:CA:1321:C:H3'	1:CA:1322:C:H5''	1.21	1.19
13:AM:90:LEU:HD23	13:AM:93:ARG:HG2	1.23	1.18
2:AB:166:ASP:HB3	2:AB:169:LYS:HB2	1.24	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	147 (63%)	57 (24%)	29 (12%)	0	4
2	CB	233/256 (91%)	144 (62%)	56 (24%)	33 (14%)	0	3
3	AC	205/239 (86%)	122 (60%)	53 (26%)	30 (15%)	0	2
3	CC	202/239 (84%)	116 (57%)	48 (24%)	38 (19%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	39 (19%)	29 (14%)	0	3
4	CD	206/209 (99%)	141 (68%)	39 (19%)	26 (13%)	0	4
5	AE	149/162 (92%)	98 (66%)	34 (23%)	17 (11%)	0	5
5	CE	149/162 (92%)	107 (72%)	27 (18%)	15 (10%)	0	6
6	AF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	7
6	CF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	11
7	AG	153/156 (98%)	108 (71%)	28 (18%)	17 (11%)	0	5
7	CG	150/156 (96%)	93 (62%)	39 (26%)	18 (12%)	0	4
8	AH	136/138 (99%)	87 (64%)	37 (27%)	12 (9%)	1	7
8	CH	136/138 (99%)	92 (68%)	37 (27%)	7 (5%)	2	17
9	AI	125/128 (98%)	86 (69%)	26 (21%)	13 (10%)	0	6
9	CI	125/128 (98%)	72 (58%)	43 (34%)	10 (8%)	1	9
10	AJ	97/105 (92%)	59 (61%)	27 (28%)	11 (11%)	0	5
10	CJ	97/105 (92%)	52 (54%)	34 (35%)	11 (11%)	0	5
11	AK	114/129 (88%)	82 (72%)	26 (23%)	6 (5%)	2	16
11	CK	117/129 (91%)	81 (69%)	25 (21%)	11 (9%)	0	7
12	AL	123/132 (93%)	78 (63%)	29 (24%)	16 (13%)	0	3
12	CL	123/132 (93%)	82 (67%)	19 (15%)	22 (18%)	0	1
13	AM	120/126 (95%)	69 (58%)	28 (23%)	23 (19%)	0	1
13	CM	116/126 (92%)	66 (57%)	24 (21%)	26 (22%)	0	1
14	AN	58/61 (95%)	33 (57%)	17 (29%)	8 (14%)	0	3
14	CN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	4
15	AO	86/89 (97%)	61 (71%)	16 (19%)	9 (10%)	0	5
15	CO	86/89 (97%)	62 (72%)	15 (17%)	9 (10%)	0	5
16	AP	82/88 (93%)	54 (66%)	19 (23%)	9 (11%)	0	5
16	CP	82/88 (93%)	56 (68%)	24 (29%)	2 (2%)	6	34
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	7
17	CQ	98/105 (93%)	64 (65%)	23 (24%)	11 (11%)	0	5
18	AR	68/88 (77%)	48 (71%)	14 (21%)	6 (9%)	1	7
18	CR	68/88 (77%)	50 (74%)	11 (16%)	7 (10%)	0	6
19	AS	77/93 (83%)	46 (60%)	13 (17%)	18 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	49 (64%)	18 (23%)	10 (13%)	0	3
20	AT	97/106 (92%)	57 (59%)	25 (26%)	15 (16%)	0	2
20	CT	97/106 (92%)	64 (66%)	18 (19%)	15 (16%)	0	2
21	AU	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	2	21
21	CU	23/27 (85%)	19 (83%)	1 (4%)	3 (13%)	0	3
29	BC	183/229 (80%)	67 (37%)	66 (36%)	50 (27%)	0	0
29	DC	183/229 (80%)	62 (34%)	69 (38%)	52 (28%)	0	0
30	BD	270/276 (98%)	175 (65%)	54 (20%)	41 (15%)	0	2
30	DD	270/276 (98%)	180 (67%)	51 (19%)	39 (14%)	0	2
31	BE	203/206 (98%)	133 (66%)	38 (19%)	32 (16%)	0	2
31	DE	203/206 (98%)	115 (57%)	49 (24%)	39 (19%)	0	1
32	BF	204/210 (97%)	141 (69%)	40 (20%)	23 (11%)	0	5
32	DF	206/210 (98%)	126 (61%)	44 (21%)	36 (18%)	0	1
33	BG	179/182 (98%)	114 (64%)	31 (17%)	34 (19%)	0	1
33	DG	179/182 (98%)	98 (55%)	53 (30%)	28 (16%)	0	2
34	BH	159/180 (88%)	92 (58%)	31 (20%)	36 (23%)	0	1
34	DH	158/180 (88%)	96 (61%)	30 (19%)	32 (20%)	0	1
35	BI	144/148 (97%)	72 (50%)	37 (26%)	35 (24%)	0	0
35	DI	144/148 (97%)	73 (51%)	48 (33%)	23 (16%)	0	2
36	BN	137/140 (98%)	98 (72%)	23 (17%)	16 (12%)	0	4
36	DN	137/140 (98%)	83 (61%)	30 (22%)	24 (18%)	0	1
37	BO	120/122 (98%)	95 (79%)	19 (16%)	6 (5%)	2	18
37	DO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	5
38	BP	144/150 (96%)	68 (47%)	33 (23%)	43 (30%)	0	0
38	DP	144/150 (96%)	69 (48%)	38 (26%)	37 (26%)	0	0
39	BQ	137/141 (97%)	99 (72%)	25 (18%)	13 (10%)	0	7
39	DQ	134/141 (95%)	86 (64%)	28 (21%)	20 (15%)	0	2
40	BR	115/118 (98%)	73 (64%)	24 (21%)	18 (16%)	0	2
40	DR	115/118 (98%)	69 (60%)	29 (25%)	17 (15%)	0	2
41	BS	97/112 (87%)	46 (47%)	25 (26%)	26 (27%)	0	0
41	DS	97/112 (87%)	44 (45%)	28 (29%)	25 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BT	136/146 (93%)	81 (60%)	25 (18%)	30 (22%)	0	1
42	DT	136/146 (93%)	71 (52%)	28 (21%)	37 (27%)	0	0
43	BU	115/118 (98%)	79 (69%)	27 (24%)	9 (8%)	1	9
43	DU	115/118 (98%)	63 (55%)	36 (31%)	16 (14%)	0	3
44	BV	99/101 (98%)	59 (60%)	18 (18%)	22 (22%)	0	1
44	DV	99/101 (98%)	56 (57%)	25 (25%)	18 (18%)	0	1
45	BW	111/113 (98%)	86 (78%)	20 (18%)	5 (4%)	2	20
45	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	4
46	BX	91/96 (95%)	71 (78%)	19 (21%)	1 (1%)	14	50
46	DX	91/96 (95%)	63 (69%)	16 (18%)	12 (13%)	0	3
47	BY	84/110 (76%)	30 (36%)	25 (30%)	29 (34%)	0	0
47	DY	99/110 (90%)	36 (36%)	27 (27%)	36 (36%)	0	0
48	BZ	175/206 (85%)	94 (54%)	46 (26%)	35 (20%)	0	1
48	DZ	175/206 (85%)	85 (49%)	52 (30%)	38 (22%)	0	1
49	B0	82/85 (96%)	66 (80%)	11 (13%)	5 (6%)	1	13
49	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	18
50	B1	92/98 (94%)	72 (78%)	13 (14%)	7 (8%)	1	9
50	D1	92/98 (94%)	70 (76%)	11 (12%)	11 (12%)	0	4
51	B2	69/72 (96%)	43 (62%)	13 (19%)	13 (19%)	0	1
51	D2	69/72 (96%)	41 (59%)	16 (23%)	12 (17%)	0	2
52	B3	58/60 (97%)	49 (84%)	4 (7%)	5 (9%)	1	8
52	D3	58/60 (97%)	46 (79%)	6 (10%)	6 (10%)	0	6
53	B4	45/71 (63%)	18 (40%)	10 (22%)	17 (38%)	0	0
53	D4	45/71 (63%)	19 (42%)	11 (24%)	15 (33%)	0	0
54	B5	57/60 (95%)	41 (72%)	8 (14%)	8 (14%)	0	3
54	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	4
55	B6	46/54 (85%)	18 (39%)	9 (20%)	19 (41%)	0	0
55	D6	44/54 (82%)	15 (34%)	12 (27%)	17 (39%)	0	0
56	B7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13
56	D7	47/49 (96%)	40 (85%)	5 (11%)	2 (4%)	2	21
57	B8	62/65 (95%)	30 (48%)	19 (31%)	13 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	D8	62/65 (95%)	33 (53%)	17 (27%)	12 (19%)	0	1
58	B9	34/37 (92%)	27 (79%)	5 (15%)	2 (6%)	1	14
58	D9	34/37 (92%)	24 (71%)	7 (21%)	3 (9%)	1	7
All	All	11692/12586 (93%)	7260 (62%)	2616 (22%)	1816 (16%)	0	2

5 of 1816 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	122	PHE
2	AB	128	GLU
2	AB	154	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	177 (88%)	25 (12%)	4	22
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	22
3	AC	160/188 (85%)	144 (90%)	16 (10%)	7	31
3	CC	159/188 (85%)	142 (89%)	17 (11%)	6	28
4	AD	180/181 (99%)	159 (88%)	21 (12%)	5	24
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	31
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	29
5	CE	115/123 (94%)	99 (86%)	16 (14%)	3	18
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	36
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	22
7	AG	126/127 (99%)	109 (86%)	17 (14%)	4	19
7	CG	125/127 (98%)	115 (92%)	10 (8%)	12	40
8	AH	119/119 (100%)	106 (89%)	13 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	105 (88%)	14 (12%)	5	23
9	AI	97/99 (98%)	85 (88%)	12 (12%)	4	22
9	CI	97/99 (98%)	82 (84%)	15 (16%)	2	14
10	AJ	88/92 (96%)	73 (83%)	15 (17%)	2	10
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	21
11	AK	88/99 (89%)	82 (93%)	6 (7%)	16	47
11	CK	90/99 (91%)	83 (92%)	7 (8%)	12	41
12	AL	104/109 (95%)	92 (88%)	12 (12%)	5	24
12	CL	104/109 (95%)	92 (88%)	12 (12%)	5	24
13	AM	97/101 (96%)	84 (87%)	13 (13%)	4	19
13	CM	94/101 (93%)	82 (87%)	12 (13%)	4	20
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	22
14	CN	49/50 (98%)	47 (96%)	2 (4%)	30	62
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	30
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	20
16	AP	72/74 (97%)	62 (86%)	10 (14%)	3	18
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	32
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	38
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
18	AR	61/77 (79%)	57 (93%)	4 (7%)	16	48
18	CR	61/77 (79%)	53 (87%)	8 (13%)	4	20
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	5
19	CS	69/80 (86%)	55 (80%)	14 (20%)	1	5
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	CT	76/82 (93%)	66 (87%)	10 (13%)	4	19
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	29
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	29
26	AZ	1/1 (100%)	1 (100%)	0	100	100
26	CZ	1/1 (100%)	1 (100%)	0	100	100
29	BC	61/181 (34%)	55 (90%)	6 (10%)	8	31
29	DC	61/181 (34%)	52 (85%)	9 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	213/218 (98%)	184 (86%)	29 (14%)	3	18
30	DD	213/218 (98%)	183 (86%)	30 (14%)	3	17
31	BE	165/166 (99%)	142 (86%)	23 (14%)	3	18
31	DE	165/166 (99%)	133 (81%)	32 (19%)	1	6
32	BF	163/166 (98%)	142 (87%)	21 (13%)	4	20
32	DF	165/166 (99%)	143 (87%)	22 (13%)	4	19
33	BG	155/156 (99%)	136 (88%)	19 (12%)	4	22
33	DG	155/156 (99%)	133 (86%)	22 (14%)	3	17
34	BH	134/148 (90%)	116 (87%)	18 (13%)	4	19
34	DH	132/148 (89%)	119 (90%)	13 (10%)	8	31
35	BI	122/124 (98%)	107 (88%)	15 (12%)	4	22
35	DI	122/124 (98%)	104 (85%)	18 (15%)	3	16
36	BN	117/119 (98%)	94 (80%)	23 (20%)	1	6
36	DN	117/119 (98%)	98 (84%)	19 (16%)	2	12
37	BO	100/100 (100%)	84 (84%)	16 (16%)	2	13
37	DO	100/100 (100%)	88 (88%)	12 (12%)	5	23
38	BP	112/116 (97%)	86 (77%)	26 (23%)	1	3
38	DP	112/116 (97%)	90 (80%)	22 (20%)	1	6
39	BQ	110/111 (99%)	89 (81%)	21 (19%)	1	6
39	DQ	108/111 (97%)	96 (89%)	12 (11%)	6	26
40	BR	100/101 (99%)	83 (83%)	17 (17%)	2	10
40	DR	100/101 (99%)	84 (84%)	16 (16%)	2	13
41	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
41	DS	77/88 (88%)	67 (87%)	10 (13%)	4	20
42	BT	120/127 (94%)	88 (73%)	32 (27%)	0	2
42	DT	120/127 (94%)	87 (72%)	33 (28%)	0	2
43	BU	92/94 (98%)	78 (85%)	14 (15%)	3	15
43	DU	92/94 (98%)	82 (89%)	10 (11%)	6	27
44	BV	82/82 (100%)	64 (78%)	18 (22%)	1	4
44	DV	82/82 (100%)	65 (79%)	17 (21%)	1	5
45	BW	91/92 (99%)	78 (86%)	13 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DW	91/92 (99%)	84 (92%)	7 (8%)	13	42
46	BX	74/78 (95%)	63 (85%)	11 (15%)	3	16
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	4
47	BY	73/91 (80%)	59 (81%)	14 (19%)	1	6
47	DY	84/91 (92%)	69 (82%)	15 (18%)	2	8
48	BZ	155/179 (87%)	131 (84%)	24 (16%)	2	14
48	DZ	155/179 (87%)	138 (89%)	17 (11%)	6	27
49	B0	66/67 (98%)	60 (91%)	6 (9%)	9	35
49	D0	66/67 (98%)	58 (88%)	8 (12%)	5	22
50	B1	78/83 (94%)	65 (83%)	13 (17%)	2	11
50	D1	78/83 (94%)	72 (92%)	6 (8%)	13	42
51	B2	66/67 (98%)	52 (79%)	14 (21%)	1	4
51	D2	66/67 (98%)	58 (88%)	8 (12%)	5	22
52	B3	51/52 (98%)	44 (86%)	7 (14%)	3	18
52	D3	51/52 (98%)	46 (90%)	5 (10%)	8	31
53	B4	34/63 (54%)	30 (88%)	4 (12%)	5	23
53	D4	34/63 (54%)	28 (82%)	6 (18%)	2	9
54	B5	51/52 (98%)	42 (82%)	9 (18%)	2	9
54	D5	51/52 (98%)	41 (80%)	10 (20%)	1	6
55	B6	44/52 (85%)	27 (61%)	17 (39%)	0	1
55	D6	44/52 (85%)	30 (68%)	14 (32%)	0	2
56	B7	41/42 (98%)	37 (90%)	4 (10%)	8	31
56	D7	41/42 (98%)	35 (85%)	6 (15%)	3	16
57	B8	53/55 (96%)	40 (76%)	13 (24%)	0	3
57	D8	53/55 (96%)	39 (74%)	14 (26%)	0	2
58	B9	33/34 (97%)	32 (97%)	1 (3%)	41	70
58	D9	33/34 (97%)	31 (94%)	2 (6%)	18	51
All	All	9644/10430 (92%)	8280 (86%)	1364 (14%)	3	17

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BZ	167	GLU

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Mol	Chain	Res	Type
4	CD	138	TYR
47	DY	42	VAL
50	B1	80	LEU
56	B7	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 345 such sidechains are listed below:

Mol	Chain	Res	Type
50	B1	45	ASN
3	CC	181	ASN
46	DX	41	ASN
51	B2	43	GLN
58	B9	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1508 (99%)	234 (15%)	56 (3%)
1	CA	1491/1508 (98%)	248 (16%)	61 (4%)
22	AV	9/30 (30%)	1 (11%)	0
22	CV	9/30 (30%)	2 (22%)	0
23	AW	73/75 (97%)	15 (20%)	3 (4%)
23	CW	73/75 (97%)	20 (27%)	3 (4%)
24	AX	76/77 (98%)	24 (31%)	4 (5%)
25	AY	74/75 (98%)	19 (25%)	0
25	CY	74/75 (98%)	20 (27%)	0
27	BA	2779/2915 (95%)	539 (19%)	96 (3%)
27	DA	2765/2915 (94%)	555 (20%)	114 (4%)
28	BB	118/122 (96%)	16 (13%)	3 (2%)
28	DB	118/122 (96%)	40 (33%)	5 (4%)
59	CX	76/77 (98%)	21 (27%)	2 (2%)
All	All	9228/9604 (96%)	1754 (19%)	347 (3%)

5 of 1754 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	28	G
1	AA	31	G
1	AA	32	A

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Mol	Chain	Res	Type
1	AA	39	G

5 of 347 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2778	A
1	CA	968	A
27	DA	2490	G
28	BB	66	A
1	CA	366	C

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

10 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	$\# Z > 2$
26	KBE	CZ	1	26	8,8,9	1.33	1 (12%)	7,8,10	2.24	2 (28%)
26	DPP	CZ	2	26	3,5,6	0.95	0	1,5,7	0.30	0
26	UAL	AZ	3	26	7,8,9	2.52	2 (28%)	5,9,11	1.80	1 (20%)
26	DPP	CZ	5	26	3,5,6	0.84	0	1,5,7	0.32	0
26	MYN	AZ	4	26	7,11,12	0.56	0	6,14,16	1.47	1 (16%)
26	DPP	AZ	2	26	3,5,6	0.64	0	1,5,7	0.55	0
26	MYN	CZ	4	26	7,11,12	0.83	0	6,14,16	1.49	1 (16%)
26	DPP	AZ	5	26	3,5,6	0.59	0	1,5,7	0.25	0
26	UAL	CZ	3	26	7,8,9	2.51	2 (28%)	5,9,11	1.47	1 (20%)
26	KBE	AZ	1	26	8,8,9	1.61	1 (12%)	7,8,10	2.61	2 (28%)

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
26	KBE	CZ	1	26	-	1/7/7/8	-
26	DPP	CZ	2	26	-	1/2/4/6	-
26	UAL	AZ	3	26	-	0/3/7/9	-
26	DPP	CZ	5	26	-	0/2/4/6	-
26	MYN	AZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	2	26	-	2/2/4/6	-
26	MYN	CZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	5	26	-	0/2/4/6	-
26	UAL	CZ	3	26	-	0/3/7/9	-
26	KBE	AZ	1	26	-	1/7/7/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CZ	3	UAL	C-CA	4.97	1.53	1.45
26	AZ	3	UAL	C-CA	4.67	1.52	1.45
26	AZ	3	UAL	C1-N1	-4.40	1.33	1.40
26	CZ	3	UAL	C1-N1	-4.13	1.33	1.40
26	AZ	1	KBE	CA-C	-4.10	1.39	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AZ	1	KBE	CB-CA-C	6.21	121.39	112.25
26	CZ	1	KBE	CB-CA-C	5.28	120.02	112.25
26	AZ	3	UAL	O-C-CA	-3.67	120.72	125.39
26	AZ	1	KBE	O-C-CA	-2.82	117.22	125.43
26	CZ	3	UAL	O-C-CA	-2.69	121.97	125.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	CZ	1	KBE	C-CA-CB-N
26	AZ	2	DPP	N-CA-CB-NG
26	AZ	1	KBE	C-CA-CB-N
26	AZ	2	DPP	C-CA-CB-NG
26	CZ	2	DPP	N-CA-CB-NG

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	CZ	1	KBE	10	0
26	CZ	2	DPP	4	0
26	AZ	3	UAL	3	0
26	AZ	4	MYN	3	0
26	AZ	2	DPP	4	0
26	CZ	4	MYN	1	0
26	CZ	3	UAL	2	0
26	AZ	1	KBE	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 850 ligands modelled in this entry, 850 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1495/1508 (99%)	-0.08	28 (1%) 66 64	32, 72, 154, 200	0
1	CA	1493/1508 (99%)	0.16	30 (2%) 65 63	38, 81, 158, 200	0
2	AB	235/256 (91%)	0.19	9 (3%) 40 39	69, 98, 133, 148	0
2	CB	235/256 (91%)	0.29	19 (8%) 12 14	74, 103, 147, 165	0
3	AC	207/239 (86%)	-0.05	1 (0%) 91 89	66, 86, 109, 114	0
3	CC	206/239 (86%)	0.26	15 (7%) 15 17	76, 98, 123, 136	0
4	AD	208/209 (99%)	0.21	6 (2%) 51 49	52, 73, 87, 92	0
4	CD	208/209 (99%)	0.10	1 (0%) 91 89	47, 68, 85, 89	0
5	AE	151/162 (93%)	-0.12	0 100 100	49, 67, 94, 107	0
5	CE	151/162 (93%)	0.09	1 (0%) 87 85	53, 75, 94, 100	0
6	AF	101/101 (100%)	-0.36	0 100 100	54, 69, 84, 98	0
6	CF	101/101 (100%)	-0.00	2 (1%) 65 63	49, 73, 83, 98	0
7	AG	155/156 (99%)	0.42	12 (7%) 13 16	62, 82, 107, 124	0
7	CG	154/156 (98%)	0.15	12 (7%) 13 15	69, 92, 116, 124	0
8	AH	138/138 (100%)	0.33	2 (1%) 75 72	54, 71, 82, 96	0
8	CH	138/138 (100%)	0.29	4 (2%) 51 49	55, 75, 87, 97	0
9	AI	127/128 (99%)	0.73	18 (14%) 2 4	57, 99, 123, 126	0
9	CI	127/128 (99%)	0.81	16 (12%) 3 5	72, 106, 123, 129	0
10	AJ	99/105 (94%)	1.08	24 (24%) 0 0	69, 108, 130, 130	0
10	CJ	99/105 (94%)	1.07	19 (19%) 1 1	79, 115, 136, 143	0
11	AK	116/129 (89%)	0.29	4 (3%) 45 43	53, 67, 89, 107	0
11	CK	119/129 (92%)	0.40	10 (8%) 11 13	56, 76, 99, 114	0
12	AL	125/132 (94%)	0.23	4 (3%) 47 46	49, 63, 80, 103	0
12	CL	125/132 (94%)	0.24	6 (4%) 30 30	51, 71, 83, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	122/126 (96%)	0.07	3 (2%) 57 54	63, 87, 97, 102	0
13	CM	118/126 (93%)	0.26	7 (5%) 22 23	77, 100, 114, 120	0
14	AN	60/61 (98%)	0.17	0 100 100	52, 77, 91, 97	0
14	CN	60/61 (98%)	1.01	7 (11%) 4 6	75, 92, 101, 105	0
15	AO	88/89 (98%)	-0.12	0 100 100	47, 65, 82, 93	0
15	CO	88/89 (98%)	-0.12	0 100 100	50, 70, 87, 92	0
16	AP	84/88 (95%)	0.65	7 (8%) 11 14	50, 68, 95, 109	0
16	CP	84/88 (95%)	0.54	7 (8%) 11 14	55, 66, 85, 109	0
17	AQ	100/105 (95%)	-0.19	0 100 100	53, 69, 84, 88	0
17	CQ	100/105 (95%)	0.24	5 (5%) 28 28	59, 73, 91, 94	0
18	AR	70/88 (79%)	0.45	2 (2%) 51 49	49, 68, 94, 100	0
18	CR	70/88 (79%)	-0.05	2 (2%) 51 49	56, 74, 99, 104	0
19	AS	79/93 (84%)	0.95	14 (17%) 1 2	63, 90, 110, 115	0
19	CS	79/93 (84%)	1.53	22 (27%) 0 0	91, 111, 132, 138	0
20	AT	99/106 (93%)	0.46	4 (4%) 38 36	54, 75, 104, 110	0
20	CT	99/106 (93%)	0.52	5 (5%) 28 27	63, 76, 111, 114	0
21	AU	25/27 (92%)	1.34	5 (20%) 1 1	74, 82, 90, 95	0
21	CU	25/27 (92%)	2.35	15 (60%) 0 0	72, 93, 105, 109	0
22	AV	10/30 (33%)	1.00	2 (20%) 1 1	51, 66, 125, 128	0
22	CV	10/30 (33%)	0.97	2 (20%) 1 1	65, 81, 134, 138	0
23	AW	74/75 (98%)	0.33	4 (5%) 25 26	49, 117, 149, 154	0
23	CW	74/75 (98%)	0.92	5 (6%) 17 19	79, 129, 148, 165	0
24	AX	77/77 (100%)	0.01	2 (2%) 56 53	35, 85, 115, 128	0
25	AY	75/75 (100%)	0.77	11 (14%) 2 3	62, 157, 189, 191	0
25	CY	75/75 (100%)	0.86	9 (12%) 4 6	76, 170, 192, 197	0
26	AZ	1/6 (16%)	-0.54	0 100 100	64, 64, 64, 64	0
26	CZ	1/6 (16%)	-0.04	0 100 100	91, 91, 91, 91	0
27	BA	2789/2915 (95%)	-0.19	54 (1%) 66 64	19, 44, 164, 200	0
27	DA	2775/2915 (95%)	0.48	77 (2%) 53 51	30, 72, 170, 200	0
28	BB	119/122 (97%)	-0.15	3 (2%) 57 54	36, 70, 127, 168	0
28	DB	119/122 (97%)	1.10	25 (21%) 1 1	109, 142, 170, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BC	191/229 (83%)	2.51	97 (50%) 0 0	103, 169, 180, 186	0
29	DC	191/229 (83%)	2.38	93 (48%) 0 0	125, 170, 183, 186	0
30	BD	272/276 (98%)	-0.28	0 100 100	18, 41, 61, 73	0
30	DD	272/276 (98%)	0.10	4 (1%) 73 71	31, 52, 69, 81	0
31	BE	205/206 (99%)	-0.24	3 (1%) 73 71	16, 42, 76, 94	0
31	DE	205/206 (99%)	0.51	9 (4%) 34 33	44, 80, 112, 119	0
32	BF	206/210 (98%)	-0.22	3 (1%) 73 71	17, 46, 110, 129	0
32	DF	208/210 (99%)	0.52	9 (4%) 35 34	40, 69, 120, 132	0
33	BG	181/182 (99%)	0.30	7 (3%) 39 38	49, 74, 102, 119	0
33	DG	181/182 (99%)	0.63	16 (8%) 10 12	75, 101, 117, 125	0
34	BH	161/180 (89%)	0.17	7 (4%) 35 34	39, 65, 81, 95	0
34	DH	160/180 (88%)	1.36	45 (28%) 0 0	106, 129, 153, 161	0
35	BI	146/148 (98%)	0.69	15 (10%) 6 9	57, 134, 150, 159	0
35	DI	146/148 (98%)	0.72	18 (12%) 4 6	62, 107, 139, 150	0
36	BN	139/140 (99%)	-0.08	1 (0%) 87 85	23, 43, 67, 73	0
36	DN	139/140 (99%)	0.90	17 (12%) 4 6	69, 86, 106, 108	0
37	BO	122/122 (100%)	-0.32	0 100 100	22, 44, 60, 67	0
37	DO	122/122 (100%)	0.32	3 (2%) 57 54	47, 72, 80, 86	0
38	BP	146/150 (97%)	0.16	5 (3%) 45 43	17, 60, 91, 121	0
38	DP	146/150 (97%)	0.98	14 (9%) 8 10	45, 82, 103, 126	0
39	BQ	139/141 (98%)	-0.11	0 100 100	29, 47, 70, 82	0
39	DQ	138/141 (97%)	0.83	13 (9%) 8 10	58, 88, 107, 136	0
40	BR	117/118 (99%)	-0.26	0 100 100	17, 37, 59, 66	0
40	DR	117/118 (99%)	0.34	0 100 100	39, 64, 81, 88	0
41	BS	99/112 (88%)	0.29	3 (3%) 50 48	40, 65, 82, 91	0
41	DS	99/112 (88%)	1.05	16 (16%) 1 2	71, 93, 106, 109	0
42	BT	138/146 (94%)	0.06	3 (2%) 62 59	27, 53, 108, 143	0
42	DT	138/146 (94%)	0.42	10 (7%) 15 17	64, 79, 136, 142	0
43	BU	117/118 (99%)	-0.31	0 100 100	20, 37, 59, 86	0
43	DU	117/118 (99%)	0.49	7 (5%) 21 22	48, 80, 111, 120	0
44	BV	101/101 (100%)	0.08	1 (0%) 82 79	18, 49, 68, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DV	101/101 (100%)	0.53	9 (8%) 9 12	54, 100, 114, 122	0
45	BW	113/113 (100%)	-0.20	1 (0%) 84 81	21, 34, 64, 102	0
45	DW	113/113 (100%)	0.45	1 (0%) 84 81	39, 61, 93, 118	0
46	BX	93/96 (96%)	-0.15	0 100 100	31, 45, 69, 76	0
46	DX	93/96 (96%)	0.45	0 100 100	39, 66, 79, 85	0
47	BY	88/110 (80%)	0.59	5 (5%) 23 23	41, 58, 79, 87	0
47	DY	101/110 (91%)	1.53	31 (30%) 0 0	62, 83, 144, 153	0
48	BZ	177/206 (85%)	1.03	36 (20%) 1 1	52, 85, 159, 164	0
48	DZ	177/206 (85%)	1.72	49 (27%) 0 0	93, 123, 178, 184	0
49	B0	84/85 (98%)	0.35	5 (5%) 21 22	27, 49, 71, 85	0
49	D0	84/85 (98%)	1.30	24 (28%) 0 0	66, 82, 96, 104	0
50	B1	94/98 (95%)	0.07	0 100 100	28, 49, 80, 91	0
50	D1	94/98 (95%)	0.65	6 (6%) 19 20	40, 62, 94, 101	0
51	B2	71/72 (98%)	-0.08	1 (1%) 75 72	37, 62, 93, 106	0
51	D2	71/72 (98%)	0.22	1 (1%) 75 72	59, 78, 98, 117	0
52	B3	60/60 (100%)	0.16	1 (1%) 70 67	27, 44, 69, 103	0
52	D3	60/60 (100%)	1.61	23 (38%) 0 0	70, 88, 111, 119	0
53	B4	49/71 (69%)	-0.24	2 (4%) 37 36	72, 97, 116, 119	0
53	D4	49/71 (69%)	0.11	2 (4%) 37 36	100, 115, 120, 121	0
54	B5	59/60 (98%)	-0.13	3 (5%) 28 27	21, 38, 93, 115	0
54	D5	59/60 (98%)	0.50	6 (10%) 6 9	46, 62, 116, 136	0
55	B6	48/54 (88%)	-0.07	0 100 100	29, 58, 71, 90	0
55	D6	46/54 (85%)	1.01	8 (17%) 1 2	50, 81, 91, 101	0
56	B7	49/49 (100%)	-0.15	0 100 100	20, 32, 77, 90	0
56	D7	49/49 (100%)	0.68	3 (6%) 21 22	36, 47, 84, 92	0
57	B8	64/65 (98%)	0.46	4 (6%) 20 20	26, 44, 62, 99	0
57	D8	64/65 (98%)	1.12	6 (9%) 8 10	51, 66, 85, 109	0
58	B9	36/37 (97%)	0.64	1 (2%) 53 51	15, 45, 57, 59	0
58	D9	36/37 (97%)	1.48	12 (33%) 0 0	79, 94, 99, 102	0
59	CX	77/77 (100%)	0.25	2 (2%) 56 53	63, 100, 127, 140	0
All	All	21180/22202 (95%)	0.30	1203 (5%) 23 23	15, 72, 152, 200	0

The worst 5 of 1203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BC	179	SER	15.0
29	DC	57	ASN	13.1
29	DC	179	SER	12.9
48	DZ	110	VAL	12.9
27	DA	2802	G	12.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	KBE	CZ	1	9/10	0.81	0.52	95,98,100,100	0
26	UAL	CZ	3	9/10	0.81	0.28	91,92,93,93	0
26	KBE	AZ	1	9/10	0.83	0.59	71,74,78,79	0
26	DPP	CZ	5	6/7	0.85	0.26	88,89,89,90	0
26	MYN	CZ	4	11/12	0.86	0.22	88,89,91,92	0
26	UAL	AZ	3	9/10	0.87	0.24	63,66,70,71	0
26	DPP	CZ	2	6/7	0.88	0.20	92,93,95,98	0
26	MYN	AZ	4	11/12	0.90	0.23	61,64,65,65	0
26	DPP	AZ	2	6/7	0.93	0.21	66,67,69,71	0
26	DPP	AZ	5	6/7	0.93	0.20	62,64,65,65	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	AA	1646	1/1	0.15	1.01	71,71,71,71	0
60	MG	DA	3188	1/1	0.15	0.27	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AW	103	1/1	0.19	0.64	72,72,72,72	0
60	MG	CW	103	1/1	0.30	0.34	73,73,73,73	0
60	MG	DA	3110	1/1	0.39	0.52	48,48,48,48	0
60	MG	CA	1641	1/1	0.46	0.29	66,66,66,66	0
60	MG	CA	1686	1/1	0.50	0.28	37,37,37,37	0
60	MG	DA	3209	1/1	0.51	0.36	5,5,5,5	0
60	MG	AA	1638	1/1	0.51	0.74	76,76,76,76	0
60	MG	AA	1637	1/1	0.53	0.30	44,44,44,44	0
60	MG	DA	3136	1/1	0.53	0.44	31,31,31,31	0
60	MG	DA	3175	1/1	0.53	0.26	72,72,72,72	0
60	MG	DA	3176	1/1	0.55	0.45	54,54,54,54	0
60	MG	DA	3149	1/1	0.55	0.37	39,39,39,39	0
60	MG	DA	3154	1/1	0.56	0.81	38,38,38,38	0
60	MG	DB	202	1/1	0.56	0.77	80,80,80,80	0
60	MG	DF	301	1/1	0.56	0.56	53,53,53,53	0
60	MG	DA	3199	1/1	0.56	0.44	35,35,35,35	0
60	MG	DA	3198	1/1	0.57	0.21	32,32,32,32	0
60	MG	DA	3086	1/1	0.57	0.83	58,58,58,58	0
60	MG	CA	1652	1/1	0.58	0.28	61,61,61,61	0
60	MG	CA	1644	1/1	0.58	0.64	67,67,67,67	0
60	MG	DA	3239	1/1	0.59	0.33	34,34,34,34	0
60	MG	BA	3171	1/1	0.59	0.20	36,36,36,36	0
60	MG	AA	1671	1/1	0.60	0.42	49,49,49,49	0
60	MG	CA	1700	1/1	0.60	0.40	36,36,36,36	0
60	MG	DO	201	1/1	0.60	0.52	65,65,65,65	0
60	MG	BA	3289	1/1	0.61	0.37	42,42,42,42	0
60	MG	AA	1640	1/1	0.62	0.25	70,70,70,70	0
60	MG	AA	1707	1/1	0.62	0.39	52,52,52,52	0
60	MG	CA	1633	1/1	0.63	0.46	62,62,62,62	0
60	MG	DA	3164	1/1	0.64	0.21	64,64,64,64	0
60	MG	BA	3085	1/1	0.64	0.39	70,70,70,70	0
60	MG	DA	3128	1/1	0.65	0.36	24,24,24,24	0
60	MG	DA	3127	1/1	0.65	0.32	20,20,20,20	0
60	MG	DA	3161	1/1	0.65	0.17	33,33,33,33	0
60	MG	AA	1630	1/1	0.66	0.68	62,62,62,62	0
60	MG	DA	3189	1/1	0.66	0.17	57,57,57,57	0
60	MG	D7	101	1/1	0.66	0.30	36,36,36,36	0
60	MG	DA	3201	1/1	0.67	0.33	36,36,36,36	0
60	MG	CA	1631	1/1	0.67	0.18	19,19,19,19	0
60	MG	DA	3116	1/1	0.67	0.39	47,47,47,47	0
60	MG	DA	3021	1/1	0.67	0.28	27,27,27,27	0
60	MG	CA	1638	1/1	0.68	0.39	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3117	1/1	0.68	0.46	49,49,49,49	0
60	MG	DA	3228	1/1	0.68	0.69	34,34,34,34	0
60	MG	BA	3215	1/1	0.68	0.71	60,60,60,60	0
60	MG	DA	3184	1/1	0.68	0.86	35,35,35,35	0
60	MG	CA	1607	1/1	0.68	0.51	29,29,29,29	0
60	MG	BA	3109	1/1	0.68	0.24	58,58,58,58	0
60	MG	DA	3159	1/1	0.69	0.39	32,32,32,32	0
60	MG	DA	3109	1/1	0.69	0.20	50,50,50,50	0
60	MG	CA	1649	1/1	0.69	0.31	54,54,54,54	0
60	MG	CW	104	1/1	0.69	0.16	57,57,57,57	0
60	MG	DA	3190	1/1	0.69	0.25	43,43,43,43	0
60	MG	BA	3329	1/1	0.69	0.16	45,45,45,45	0
60	MG	DA	3042	1/1	0.69	0.40	46,46,46,46	0
60	MG	DA	3225	1/1	0.69	0.41	39,39,39,39	0
60	MG	DA	3095	1/1	0.70	0.15	61,61,61,61	0
60	MG	DA	3217	1/1	0.70	0.56	27,27,27,27	0
60	MG	DA	3156	1/1	0.70	0.11	47,47,47,47	0
60	MG	AX	103	1/1	0.71	0.20	51,51,51,51	0
60	MG	DA	3060	1/1	0.71	0.35	23,23,23,23	0
60	MG	DA	3084	1/1	0.71	0.52	71,71,71,71	0
60	MG	CA	1685	1/1	0.71	0.48	59,59,59,59	0
60	MG	DA	3016	1/1	0.72	0.28	12,12,12,12	0
60	MG	DA	3142	1/1	0.72	0.25	37,37,37,37	0
60	MG	DA	3122	1/1	0.72	0.20	40,40,40,40	0
60	MG	AA	1682	1/1	0.72	0.13	48,48,48,48	0
60	MG	CA	1692	1/1	0.72	0.27	32,32,32,32	0
60	MG	DA	3092	1/1	0.73	0.30	17,17,17,17	0
60	MG	CV	601	1/1	0.73	0.46	16,16,16,16	0
60	MG	CA	1656	1/1	0.73	0.28	39,39,39,39	0
60	MG	DA	3125	1/1	0.73	0.19	49,49,49,49	0
60	MG	DA	3065	1/1	0.73	0.27	28,28,28,28	0
60	MG	DA	3171	1/1	0.73	0.44	52,52,52,52	0
60	MG	BA	3186	1/1	0.73	0.30	60,60,60,60	0
60	MG	DA	3157	1/1	0.73	0.24	58,58,58,58	0
60	MG	DA	3111	1/1	0.73	0.47	64,64,64,64	0
60	MG	DA	3124	1/1	0.73	0.39	36,36,36,36	0
60	MG	BA	3189	1/1	0.74	0.21	40,40,40,40	0
60	MG	CA	1640	1/1	0.74	0.27	41,41,41,41	0
60	MG	AA	1713	1/1	0.74	0.13	43,43,43,43	0
60	MG	BA	3079	1/1	0.74	0.31	7,7,7,7	0
60	MG	DA	3138	1/1	0.75	0.16	63,63,63,63	0
60	MG	AA	1626	1/1	0.75	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1609	1/1	0.75	0.52	50,50,50,50	0
60	MG	DA	3202	1/1	0.75	0.22	18,18,18,18	0
60	MG	DA	3166	1/1	0.75	0.39	36,36,36,36	0
60	MG	BA	3303	1/1	0.75	0.55	32,32,32,32	0
60	MG	BA	3210	1/1	0.76	0.29	33,33,33,33	0
60	MG	DA	3078	1/1	0.76	0.30	26,26,26,26	0
60	MG	BA	3316	1/1	0.76	0.44	35,35,35,35	0
60	MG	CA	1616	1/1	0.76	0.48	52,52,52,52	0
60	MG	DA	3204	1/1	0.76	0.48	67,67,67,67	0
60	MG	DA	3148	1/1	0.76	0.58	42,42,42,42	0
60	MG	BA	3294	1/1	0.76	0.71	90,90,90,90	0
60	MG	AA	1708	1/1	0.76	0.26	41,41,41,41	0
60	MG	DA	3155	1/1	0.76	0.56	31,31,31,31	0
60	MG	DA	3104	1/1	0.77	0.44	42,42,42,42	0
60	MG	CA	1674	1/1	0.77	0.46	55,55,55,55	0
60	MG	DA	3153	1/1	0.77	0.18	13,13,13,13	0
60	MG	DA	3041	1/1	0.77	0.31	1,1,1,1	0
60	MG	AX	104	1/1	0.77	0.21	57,57,57,57	0
60	MG	DA	3025	1/1	0.77	0.39	1,1,1,1	0
60	MG	CA	1673	1/1	0.78	0.25	15,15,15,15	0
60	MG	DA	3001	1/1	0.78	0.39	51,51,51,51	0
60	MG	DA	3062	1/1	0.78	0.42	8,8,8,8	0
60	MG	CA	1676	1/1	0.78	0.20	25,25,25,25	0
60	MG	DA	3141	1/1	0.78	0.63	36,36,36,36	0
60	MG	BA	3177	1/1	0.78	0.43	41,41,41,41	0
60	MG	DA	3170	1/1	0.78	0.51	33,33,33,33	0
60	MG	DA	3066	1/1	0.78	0.56	40,40,40,40	0
60	MG	DA	3097	1/1	0.78	0.25	51,51,51,51	0
60	MG	BA	3255	1/1	0.78	0.33	19,19,19,19	0
60	MG	DA	3165	1/1	0.79	0.27	14,14,14,14	0
60	MG	DA	3203	1/1	0.79	0.44	38,38,38,38	0
60	MG	BA	3284	1/1	0.79	0.23	21,21,21,21	0
60	MG	BA	3162	1/1	0.79	0.27	56,56,56,56	0
60	MG	AA	1702	1/1	0.79	0.34	41,41,41,41	0
60	MG	AA	1695	1/1	0.79	0.18	30,30,30,30	0
60	MG	DA	3019	1/1	0.79	0.29	6,6,6,6	0
60	MG	BA	3309	1/1	0.79	0.13	1,1,1,1	0
60	MG	CA	1702	1/1	0.79	0.43	27,27,27,27	0
60	MG	DA	3093	1/1	0.79	0.47	31,31,31,31	0
60	MG	DA	3216	1/1	0.80	0.20	24,24,24,24	0
60	MG	DA	3068	1/1	0.80	0.22	9,9,9,9	0
60	MG	BA	3144	1/1	0.80	0.30	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3140	1/1	0.80	0.34	24,24,24,24	0
60	MG	DA	3034	1/1	0.80	0.19	1,1,1,1	0
60	MG	AA	1672	1/1	0.80	0.24	53,53,53,53	0
60	MG	BA	3140	1/1	0.80	0.52	26,26,26,26	0
60	MG	DA	3040	1/1	0.80	0.39	19,19,19,19	0
60	MG	B0	102	1/1	0.80	0.40	40,40,40,40	0
60	MG	AA	1680	1/1	0.80	0.62	70,70,70,70	0
60	MG	BA	3238	1/1	0.80	0.41	29,29,29,29	0
60	MG	DA	3014	1/1	0.80	0.36	4,4,4,4	0
60	MG	DA	3131	1/1	0.81	0.87	63,63,63,63	0
60	MG	DA	3096	1/1	0.81	0.40	16,16,16,16	0
60	MG	DA	3130	1/1	0.81	0.43	27,27,27,27	0
60	MG	DA	3173	1/1	0.81	0.48	10,10,10,10	0
60	MG	DA	3098	1/1	0.81	0.35	27,27,27,27	0
60	MG	CA	1698	1/1	0.81	0.51	29,29,29,29	0
60	MG	BA	3241	1/1	0.81	1.36	80,80,80,80	0
60	MG	BA	3104	1/1	0.81	0.39	42,42,42,42	0
60	MG	DA	3074	1/1	0.81	0.62	48,48,48,48	0
60	MG	AA	1629	1/1	0.82	0.22	51,51,51,51	0
60	MG	DA	3145	1/1	0.82	0.49	35,35,35,35	0
60	MG	BA	3187	1/1	0.82	0.46	17,17,17,17	0
60	MG	DA	3118	1/1	0.82	0.34	22,22,22,22	0
60	MG	BA	3251	1/1	0.82	0.32	1,1,1,1	0
60	MG	DA	3129	1/1	0.82	0.23	20,20,20,20	0
60	MG	DA	3077	1/1	0.82	0.18	13,13,13,13	0
60	MG	BA	3077	1/1	0.82	0.24	1,1,1,1	0
60	MG	CA	1684	1/1	0.82	0.18	33,33,33,33	0
60	MG	DA	3053	1/1	0.82	0.55	32,32,32,32	0
60	MG	AA	1645	1/1	0.82	0.41	22,22,22,22	0
60	MG	DA	3052	1/1	0.82	0.22	14,14,14,14	0
60	MG	BA	3195	1/1	0.82	0.61	49,49,49,49	0
60	MG	BA	3114	1/1	0.82	0.21	14,14,14,14	0
60	MG	BA	3051	1/1	0.82	0.38	14,14,14,14	0
60	MG	AA	1697	1/1	0.82	0.20	27,27,27,27	0
60	MG	DB	203	1/1	0.82	0.11	54,54,54,54	0
60	MG	CA	1658	1/1	0.82	0.27	30,30,30,30	0
60	MG	BA	3034	1/1	0.82	0.40	1,1,1,1	0
60	MG	CA	1637	1/1	0.82	0.73	57,57,57,57	0
60	MG	DA	3227	1/1	0.83	0.26	36,36,36,36	0
60	MG	AA	1620	1/1	0.83	0.42	31,31,31,31	0
60	MG	BA	3204	1/1	0.83	0.33	25,25,25,25	0
60	MG	AA	1648	1/1	0.83	0.45	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3094	1/1	0.83	0.25	11,11,11,11	0
60	MG	BA	3015	1/1	0.83	0.14	5,5,5,5	0
60	MG	DA	3115	1/1	0.83	0.29	36,36,36,36	0
60	MG	BX	101	1/1	0.83	0.23	31,31,31,31	0
60	MG	DA	3218	1/1	0.83	0.55	50,50,50,50	0
60	MG	BA	3170	1/1	0.83	0.38	55,55,55,55	0
60	MG	DA	3194	1/1	0.83	0.43	44,44,44,44	0
60	MG	DA	3162	1/1	0.83	0.43	44,44,44,44	0
60	MG	BA	3185	1/1	0.83	0.10	3,3,3,3	0
60	MG	CA	1677	1/1	0.83	0.39	51,51,51,51	0
60	MG	DA	3231	1/1	0.83	0.69	49,49,49,49	0
60	MG	BA	3142	1/1	0.83	0.36	30,30,30,30	0
60	MG	AA	1643	1/1	0.84	0.31	29,29,29,29	0
60	MG	DA	3179	1/1	0.84	0.15	19,19,19,19	0
60	MG	AA	1601	1/1	0.84	0.29	47,47,47,47	0
60	MG	DA	3094	1/1	0.84	0.47	16,16,16,16	0
60	MG	DA	3223	1/1	0.84	0.33	13,13,13,13	0
60	MG	DA	3080	1/1	0.84	0.49	36,36,36,36	0
60	MG	DA	3091	1/1	0.84	0.29	55,55,55,55	0
60	MG	DA	3083	1/1	0.84	0.56	35,35,35,35	0
60	MG	BA	3280	1/1	0.84	0.18	7,7,7,7	0
60	MG	DA	3232	1/1	0.84	0.14	3,3,3,3	0
60	MG	DA	3102	1/1	0.84	0.35	1,1,1,1	0
60	MG	AA	1670	1/1	0.84	0.30	54,54,54,54	0
60	MG	DA	3085	1/1	0.84	0.51	1,1,1,1	0
60	MG	BA	3184	1/1	0.84	0.62	40,40,40,40	0
60	MG	DA	3178	1/1	0.84	0.22	22,22,22,22	0
60	MG	BA	3191	1/1	0.84	0.33	6,6,6,6	0
60	MG	DA	3212	1/1	0.84	0.19	4,4,4,4	0
60	MG	AG	201	1/1	0.84	0.21	42,42,42,42	0
60	MG	DA	3215	1/1	0.84	0.28	23,23,23,23	0
60	MG	BA	3059	1/1	0.84	0.50	25,25,25,25	0
60	MG	DA	3235	1/1	0.84	0.44	61,61,61,61	0
60	MG	DA	3043	1/1	0.84	0.26	9,9,9,9	0
60	MG	DA	3137	1/1	0.84	0.72	39,39,39,39	0
60	MG	DA	3039	1/1	0.84	0.18	53,53,53,53	0
60	MG	DA	3123	1/1	0.85	0.42	40,40,40,40	0
60	MG	DA	3185	1/1	0.85	0.62	10,10,10,10	0
60	MG	BA	3042	1/1	0.85	0.23	1,1,1,1	0
60	MG	BA	3310	1/1	0.85	0.28	38,38,38,38	0
60	MG	BA	3271	1/1	0.85	0.14	28,28,28,28	0
60	MG	AA	1644	1/1	0.85	0.40	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3192	1/1	0.85	0.18	10,10,10,10	0
60	MG	DA	3193	1/1	0.85	0.28	29,29,29,29	0
60	MG	DA	3031	1/1	0.85	0.14	9,9,9,9	0
60	MG	BA	3331	1/1	0.85	0.69	35,35,35,35	0
60	MG	BA	3312	1/1	0.85	0.25	22,22,22,22	0
60	MG	DA	3208	1/1	0.85	0.15	12,12,12,12	0
60	MG	DA	3048	1/1	0.85	0.31	23,23,23,23	0
60	MG	DA	3013	1/1	0.85	0.39	30,30,30,30	0
60	MG	BA	3165	1/1	0.85	0.15	48,48,48,48	0
60	MG	CW	101	1/1	0.85	0.12	55,55,55,55	0
60	MG	DA	3120	1/1	0.85	0.38	3,3,3,3	0
60	MG	BA	3318	1/1	0.85	0.24	20,20,20,20	0
60	MG	DA	3220	1/1	0.85	0.45	30,30,30,30	0
60	MG	CA	1694	1/1	0.85	0.71	51,51,51,51	0
60	MG	DA	3237	1/1	0.85	0.36	10,10,10,10	0
60	MG	DA	3126	1/1	0.85	0.34	7,7,7,7	0
60	MG	CA	1624	1/1	0.86	0.58	40,40,40,40	0
60	MG	BA	3222	1/1	0.86	0.29	26,26,26,26	0
60	MG	CA	1603	1/1	0.86	0.23	38,38,38,38	0
60	MG	DA	3172	1/1	0.86	0.33	6,6,6,6	0
60	MG	DA	3205	1/1	0.86	0.36	2,2,2,2	0
60	MG	AW	101	1/1	0.86	0.30	48,48,48,48	0
60	MG	DA	3226	1/1	0.86	0.10	30,30,30,30	0
60	MG	DA	3210	1/1	0.86	0.28	2,2,2,2	0
60	MG	BA	3265	1/1	0.86	0.38	13,13,13,13	0
60	MG	BA	3103	1/1	0.86	0.26	1,1,1,1	0
60	MG	DA	3139	1/1	0.86	0.39	1,1,1,1	0
60	MG	AA	1709	1/1	0.86	0.35	36,36,36,36	0
60	MG	CA	1683	1/1	0.86	0.53	53,53,53,53	0
60	MG	DA	3200	1/1	0.86	0.50	42,42,42,42	0
60	MG	AA	1701	1/1	0.86	0.31	11,11,11,11	0
60	MG	CA	1653	1/1	0.86	0.23	36,36,36,36	0
60	MG	BA	3190	1/1	0.86	0.12	39,39,39,39	0
60	MG	DA	3213	1/1	0.86	0.21	31,31,31,31	0
60	MG	DA	3133	1/1	0.86	0.18	16,16,16,16	0
60	MG	BA	3302	1/1	0.86	0.17	11,11,11,11	0
60	MG	BA	3295	1/1	0.87	0.29	41,41,41,41	0
60	MG	D0	101	1/1	0.87	0.29	12,12,12,12	0
60	MG	AA	1683	1/1	0.87	0.14	16,16,16,16	0
60	MG	D5	101	1/1	0.87	0.19	10,10,10,10	0
60	MG	AA	1633	1/1	0.87	0.24	8,8,8,8	0
60	MG	AX	108	1/1	0.87	0.38	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3290	1/1	0.87	0.44	24,24,24,24	0
60	MG	CA	1636	1/1	0.87	0.24	26,26,26,26	0
60	MG	DA	3214	1/1	0.87	0.37	21,21,21,21	0
60	MG	BA	3084	1/1	0.87	0.22	27,27,27,27	0
60	MG	DE	301	1/1	0.87	0.23	1,1,1,1	0
60	MG	AA	1686	1/1	0.87	0.29	34,34,34,34	0
60	MG	BA	3319	1/1	0.87	0.32	31,31,31,31	0
60	MG	DA	3073	1/1	0.87	0.29	58,58,58,58	0
60	MG	DA	3057	1/1	0.87	0.13	32,32,32,32	0
60	MG	DA	3054	1/1	0.87	0.33	21,21,21,21	0
60	MG	BA	3064	1/1	0.87	0.70	45,45,45,45	0
60	MG	CA	1696	1/1	0.87	0.18	91,91,91,91	0
60	MG	BA	3274	1/1	0.87	0.19	21,21,21,21	0
60	MG	CA	1665	1/1	0.87	0.30	33,33,33,33	0
60	MG	BA	3001	1/1	0.87	0.26	43,43,43,43	0
60	MG	AA	1657	1/1	0.87	0.45	37,37,37,37	0
60	MG	BA	3203	1/1	0.87	0.20	17,17,17,17	0
60	MG	BA	3243	1/1	0.87	0.52	45,45,45,45	0
60	MG	DA	3211	1/1	0.87	0.24	23,23,23,23	0
60	MG	CA	1627	1/1	0.88	0.23	9,9,9,9	0
60	MG	DA	3011	1/1	0.88	0.18	4,4,4,4	0
60	MG	DA	3026	1/1	0.88	0.26	4,4,4,4	0
60	MG	CA	1642	1/1	0.88	0.10	28,28,28,28	0
60	MG	BA	3205	1/1	0.88	0.36	30,30,30,30	0
60	MG	CA	1601	1/1	0.88	0.24	1,1,1,1	0
60	MG	BA	3333	1/1	0.88	0.35	1,1,1,1	0
60	MG	AA	1614	1/1	0.88	0.20	22,22,22,22	0
60	MG	DA	3027	1/1	0.88	0.92	38,38,38,38	0
60	MG	BA	3095	1/1	0.88	0.72	47,47,47,47	0
60	MG	DA	3003	1/1	0.88	0.27	17,17,17,17	0
60	MG	AA	1625	1/1	0.88	0.25	21,21,21,21	0
60	MG	AA	1604	1/1	0.88	0.27	14,14,14,14	0
60	MG	CA	1623	1/1	0.88	0.52	33,33,33,33	0
60	MG	BA	3141	1/1	0.88	0.30	17,17,17,17	0
60	MG	BA	3293	1/1	0.88	0.55	45,45,45,45	0
60	MG	AA	1651	1/1	0.88	0.51	53,53,53,53	0
60	MG	DA	3020	1/1	0.88	0.46	40,40,40,40	0
60	MG	BA	3160	1/1	0.88	0.43	29,29,29,29	0
60	MG	AX	101	1/1	0.88	0.15	41,41,41,41	0
60	MG	AA	1711	1/1	0.88	0.17	15,15,15,15	0
60	MG	CA	1613	1/1	0.88	0.47	36,36,36,36	0
60	MG	AA	1664	1/1	0.88	0.29	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3007	1/1	0.88	0.30	1,1,1,1	0
60	MG	AA	1622	1/1	0.88	0.32	12,12,12,12	0
60	MG	CA	1668	1/1	0.88	0.32	30,30,30,30	0
60	MG	DA	3089	1/1	0.88	0.21	27,27,27,27	0
60	MG	BA	3122	1/1	0.88	0.33	12,12,12,12	0
60	MG	AA	1608	1/1	0.88	0.46	22,22,22,22	0
60	MG	AA	1685	1/1	0.88	0.27	69,69,69,69	0
60	MG	DB	201	1/1	0.88	0.68	51,51,51,51	0
60	MG	DA	3181	1/1	0.88	0.51	50,50,50,50	0
60	MG	DA	3167	1/1	0.88	0.26	36,36,36,36	0
60	MG	BA	3192	1/1	0.88	0.45	31,31,31,31	0
60	MG	BA	3260	1/1	0.88	0.96	65,65,65,65	0
61	ZN	B5	102	1/1	0.89	0.09	51,51,51,51	0
60	MG	AA	1673	1/1	0.89	0.18	39,39,39,39	0
60	MG	BA	3272	1/1	0.89	0.23	15,15,15,15	0
60	MG	CA	1632	1/1	0.89	0.35	6,6,6,6	0
60	MG	AA	1660	1/1	0.89	0.42	49,49,49,49	0
60	MG	BA	3240	1/1	0.89	0.39	75,75,75,75	0
60	MG	DA	3219	1/1	0.89	0.22	19,19,19,19	0
60	MG	BA	3148	1/1	0.89	0.15	1,1,1,1	0
60	MG	AA	1605	1/1	0.89	0.20	35,35,35,35	0
60	MG	DA	3058	1/1	0.89	0.22	1,1,1,1	0
60	MG	BA	3174	1/1	0.89	0.09	7,7,7,7	0
60	MG	BA	3173	1/1	0.89	0.19	50,50,50,50	0
60	MG	DA	3168	1/1	0.89	0.65	55,55,55,55	0
60	MG	BA	3313	1/1	0.89	0.45	45,45,45,45	0
60	MG	DA	3222	1/1	0.89	0.29	24,24,24,24	0
60	MG	AA	1688	1/1	0.89	0.12	49,49,49,49	0
60	MG	CA	1646	1/1	0.89	0.21	1,1,1,1	0
60	MG	BA	3298	1/1	0.89	0.32	13,13,13,13	0
60	MG	BA	3270	1/1	0.89	0.25	32,32,32,32	0
60	MG	DA	3186	1/1	0.89	0.23	53,53,53,53	0
60	MG	CA	1621	1/1	0.89	0.44	30,30,30,30	0
60	MG	DA	3229	1/1	0.89	0.26	20,20,20,20	0
60	MG	DA	3195	1/1	0.89	0.38	18,18,18,18	0
60	MG	CA	1647	1/1	0.89	0.31	44,44,44,44	0
60	MG	DA	3047	1/1	0.89	0.45	29,29,29,29	0
60	MG	BA	3138	1/1	0.89	0.20	1,1,1,1	0
60	MG	CA	1611	1/1	0.89	0.37	66,66,66,66	0
60	MG	BA	3056	1/1	0.89	0.19	1,1,1,1	0
60	MG	DA	3177	1/1	0.89	0.30	13,13,13,13	0
60	MG	CA	1682	1/1	0.89	0.62	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3107	1/1	0.89	0.41	37,37,37,37	0
60	MG	AA	1677	1/1	0.90	0.24	30,30,30,30	0
60	MG	CA	1612	1/1	0.90	0.42	35,35,35,35	0
60	MG	BA	3275	1/1	0.90	0.19	7,7,7,7	0
60	MG	CA	1606	1/1	0.90	0.64	45,45,45,45	0
60	MG	AA	1616	1/1	0.90	0.25	32,32,32,32	0
60	MG	BA	3197	1/1	0.90	0.21	24,24,24,24	0
60	MG	BA	3113	1/1	0.90	0.22	1,1,1,1	0
60	MG	AA	1704	1/1	0.90	0.19	13,13,13,13	0
60	MG	BA	3230	1/1	0.90	0.27	19,19,19,19	0
60	MG	BA	3227	1/1	0.90	0.37	33,33,33,33	0
60	MG	BA	3279	1/1	0.90	0.23	29,29,29,29	0
60	MG	CA	1678	1/1	0.90	0.53	25,25,25,25	0
60	MG	BA	3224	1/1	0.90	0.12	20,20,20,20	0
60	MG	B0	101	1/1	0.90	0.24	4,4,4,4	0
60	MG	AA	1621	1/1	0.90	0.66	28,28,28,28	0
60	MG	BA	3082	1/1	0.90	0.24	44,44,44,44	0
60	MG	BA	3194	1/1	0.90	0.57	54,54,54,54	0
60	MG	CW	102	1/1	0.90	0.15	40,40,40,40	0
60	MG	BA	3282	1/1	0.90	0.33	20,20,20,20	0
60	MG	DA	3005	1/1	0.90	0.31	28,28,28,28	0
60	MG	BA	3120	1/1	0.90	0.52	87,87,87,87	0
60	MG	DA	3049	1/1	0.90	0.27	36,36,36,36	0
60	MG	AA	1679	1/1	0.90	0.15	36,36,36,36	0
60	MG	DA	3023	1/1	0.90	0.10	14,14,14,14	0
60	MG	DD	302	1/1	0.90	0.22	6,6,6,6	0
60	MG	DA	3015	1/1	0.90	0.16	1,1,1,1	0
60	MG	DA	3050	1/1	0.90	0.26	38,38,38,38	0
60	MG	DA	3134	1/1	0.90	0.26	59,59,59,59	0
61	ZN	D4	101	1/1	0.90	0.05	113,113,113,113	0
60	MG	BA	3201	1/1	0.90	0.69	53,53,53,53	0
60	MG	DA	3144	1/1	0.90	0.29	53,53,53,53	0
60	MG	DA	3064	1/1	0.90	0.48	12,12,12,12	0
61	ZN	D5	102	1/1	0.90	0.09	75,75,75,75	0
60	MG	BA	3198	1/1	0.90	0.19	5,5,5,5	0
60	MG	AA	1607	1/1	0.90	0.72	51,51,51,51	0
60	MG	BA	3175	1/1	0.90	0.20	26,26,26,26	0
60	MG	DA	3143	1/1	0.90	0.62	54,54,54,54	0
60	MG	BA	3325	1/1	0.90	0.13	19,19,19,19	0
60	MG	CA	1634	1/1	0.90	0.19	16,16,16,16	0
60	MG	DA	3233	1/1	0.90	0.21	1,1,1,1	0
60	MG	BA	3207	1/1	0.90	0.22	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3183	1/1	0.90	0.30	9,9,9,9	0
60	MG	CA	1670	1/1	0.90	0.27	26,26,26,26	0
60	MG	BA	3301	1/1	0.90	0.31	16,16,16,16	0
60	MG	CA	1660	1/1	0.91	0.16	21,21,21,21	0
60	MG	AA	1642	1/1	0.91	0.41	41,41,41,41	0
60	MG	BA	3026	1/1	0.91	0.30	7,7,7,7	0
60	MG	AA	1610	1/1	0.91	0.16	36,36,36,36	0
60	MG	BA	3010	1/1	0.91	0.25	2,2,2,2	0
60	MG	AX	102	1/1	0.91	0.16	57,57,57,57	0
60	MG	DA	3103	1/1	0.91	0.62	26,26,26,26	0
60	MG	BA	3258	1/1	0.91	0.23	32,32,32,32	0
60	MG	DA	3169	1/1	0.91	0.36	16,16,16,16	0
61	ZN	D9	101	1/1	0.91	0.07	93,93,93,93	0
60	MG	CK	201	1/1	0.91	0.09	19,19,19,19	0
60	MG	CA	1654	1/1	0.91	0.20	44,44,44,44	0
60	MG	BA	3106	1/1	0.91	0.30	3,3,3,3	0
60	MG	DA	3012	1/1	0.91	0.33	1,1,1,1	0
60	MG	DA	3088	1/1	0.91	0.29	22,22,22,22	0
60	MG	AA	1699	1/1	0.91	0.19	21,21,21,21	0
60	MG	DA	3174	1/1	0.91	0.32	6,6,6,6	0
60	MG	BA	3311	1/1	0.91	0.42	40,40,40,40	0
60	MG	BA	3226	1/1	0.91	0.23	39,39,39,39	0
60	MG	BA	3229	1/1	0.91	0.40	49,49,49,49	0
60	MG	CA	1669	1/1	0.91	0.12	16,16,16,16	0
60	MG	BA	3283	1/1	0.91	0.60	38,38,38,38	0
60	MG	CA	1667	1/1	0.91	0.25	5,5,5,5	0
61	ZN	B4	101	1/1	0.91	0.05	89,89,89,89	0
60	MG	BA	3172	1/1	0.91	0.17	18,18,18,18	0
60	MG	DA	3075	1/1	0.91	0.50	1,1,1,1	0
60	MG	CA	1691	1/1	0.91	0.27	21,21,21,21	0
60	MG	DA	3160	1/1	0.91	0.36	27,27,27,27	0
60	MG	BA	3196	1/1	0.91	0.31	21,21,21,21	0
60	MG	DA	3158	1/1	0.91	0.54	49,49,49,49	0
60	MG	BA	3314	1/1	0.91	0.17	35,35,35,35	0
60	MG	BA	3097	1/1	0.91	0.32	44,44,44,44	0
60	MG	AW	102	1/1	0.91	0.13	36,36,36,36	0
60	MG	BA	3003	1/1	0.91	0.25	64,64,64,64	0
60	MG	DA	3221	1/1	0.91	0.50	52,52,52,52	0
60	MG	DA	3135	1/1	0.91	0.45	11,11,11,11	0
60	MG	BA	3163	1/1	0.91	0.09	12,12,12,12	0
60	MG	BA	3101	1/1	0.91	0.41	31,31,31,31	0
60	MG	DA	3079	1/1	0.91	0.34	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3119	1/1	0.91	0.33	5,5,5,5	0
60	MG	DA	3206	1/1	0.92	0.33	12,12,12,12	0
60	MG	BA	3179	1/1	0.92	0.26	17,17,17,17	0
60	MG	DA	3056	1/1	0.92	0.16	2,2,2,2	0
60	MG	BA	3118	1/1	0.92	0.83	46,46,46,46	0
60	MG	BA	3219	1/1	0.92	0.19	15,15,15,15	0
60	MG	BA	3223	1/1	0.92	0.35	42,42,42,42	0
60	MG	CA	1614	1/1	0.92	0.94	50,50,50,50	0
60	MG	AA	1700	1/1	0.92	0.30	74,74,74,74	0
60	MG	BA	3213	1/1	0.92	0.48	49,49,49,49	0
60	MG	DA	3197	1/1	0.92	0.46	21,21,21,21	0
60	MG	BA	3300	1/1	0.92	0.18	22,22,22,22	0
60	MG	DA	3002	1/1	0.92	0.15	9,9,9,9	0
60	MG	AA	1681	1/1	0.92	0.24	58,58,58,58	0
60	MG	DA	3063	1/1	0.92	0.21	24,24,24,24	0
60	MG	AA	1653	1/1	0.92	0.21	38,38,38,38	0
60	MG	BA	3159	1/1	0.92	0.20	20,20,20,20	0
60	MG	BA	3261	1/1	0.92	0.31	16,16,16,16	0
60	MG	BA	3307	1/1	0.92	0.24	19,19,19,19	0
60	MG	AW	104	1/1	0.92	0.25	31,31,31,31	0
60	MG	BA	3214	1/1	0.92	0.17	54,54,54,54	0
60	MG	AA	1665	1/1	0.92	0.15	31,31,31,31	0
60	MG	DA	3196	1/1	0.92	0.20	1,1,1,1	0
60	MG	BA	3266	1/1	0.92	0.30	12,12,12,12	0
60	MG	BA	3276	1/1	0.92	0.37	16,16,16,16	0
60	MG	CA	1675	1/1	0.92	0.34	31,31,31,31	0
60	MG	B0	103	1/1	0.92	0.23	22,22,22,22	0
60	MG	AA	1627	1/1	0.92	0.24	22,22,22,22	0
60	MG	DA	3146	1/1	0.92	0.30	17,17,17,17	0
60	MG	BB	201	1/1	0.92	0.24	46,46,46,46	0
60	MG	BA	3277	1/1	0.92	0.39	1,1,1,1	0
60	MG	BA	3264	1/1	0.92	0.28	32,32,32,32	0
60	MG	DA	3150	1/1	0.92	0.23	28,28,28,28	0
60	MG	DA	3114	1/1	0.92	0.12	34,34,34,34	0
60	MG	BA	3149	1/1	0.92	0.34	14,14,14,14	0
60	MG	DA	3082	1/1	0.92	0.24	15,15,15,15	0
60	MG	BA	3246	1/1	0.92	0.26	1,1,1,1	0
60	MG	BA	3074	1/1	0.92	0.18	4,4,4,4	0
60	MG	AX	105	1/1	0.93	0.08	12,12,12,12	0
60	MG	BA	3228	1/1	0.93	0.63	52,52,52,52	0
60	MG	CA	1657	1/1	0.93	0.56	23,23,23,23	0
60	MG	AA	1617	1/1	0.93	0.44	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3096	1/1	0.93	0.39	34,34,34,34	0
60	MG	BA	3211	1/1	0.93	0.33	36,36,36,36	0
60	MG	CA	1679	1/1	0.93	0.16	43,43,43,43	0
60	MG	BA	3168	1/1	0.93	0.34	60,60,60,60	0
60	MG	DA	3024	1/1	0.93	0.35	5,5,5,5	0
60	MG	AX	106	1/1	0.93	0.28	25,25,25,25	0
60	MG	CA	1602	1/1	0.93	0.31	26,26,26,26	0
60	MG	BA	3269	1/1	0.93	0.40	12,12,12,12	0
60	MG	BA	3154	1/1	0.93	0.11	16,16,16,16	0
60	MG	BA	3111	1/1	0.93	0.19	1,1,1,1	0
60	MG	BA	3022	1/1	0.93	0.15	19,19,19,19	0
60	MG	DA	3028	1/1	0.93	0.20	1,1,1,1	0
60	MG	DA	3059	1/1	0.93	0.27	6,6,6,6	0
60	MG	CA	1701	1/1	0.93	0.18	53,53,53,53	0
60	MG	DA	3090	1/1	0.93	0.28	21,21,21,21	0
60	MG	DA	3182	1/1	0.93	0.34	23,23,23,23	0
60	MG	DA	3072	1/1	0.93	0.32	8,8,8,8	0
60	MG	CA	1695	1/1	0.93	0.14	40,40,40,40	0
60	MG	CA	1693	1/1	0.93	0.23	20,20,20,20	0
60	MG	BA	3287	1/1	0.93	0.12	7,7,7,7	0
60	MG	DA	3032	1/1	0.93	0.14	1,1,1,1	0
60	MG	BA	3304	1/1	0.93	0.21	36,36,36,36	0
60	MG	BA	3050	1/1	0.93	0.30	1,1,1,1	0
60	MG	BA	3291	1/1	0.93	0.21	14,14,14,14	0
60	MG	BA	3250	1/1	0.93	0.32	12,12,12,12	0
60	MG	BA	3263	1/1	0.93	0.19	47,47,47,47	0
60	MG	CA	1672	1/1	0.93	0.18	21,21,21,21	0
60	MG	DA	3207	1/1	0.93	0.16	1,1,1,1	0
60	MG	AA	1631	1/1	0.93	0.39	12,12,12,12	0
60	MG	BA	3161	1/1	0.93	0.50	24,24,24,24	0
60	MG	BA	3334	1/1	0.93	0.20	1,1,1,1	0
60	MG	AA	1632	1/1	0.93	0.42	48,48,48,48	0
60	MG	CA	1689	1/1	0.93	0.15	7,7,7,7	0
60	MG	CA	1610	1/1	0.93	0.25	48,48,48,48	0
60	MG	BA	3047	1/1	0.93	0.14	1,1,1,1	0
60	MG	BA	3061	1/1	0.93	0.20	17,17,17,17	0
60	MG	DA	3030	1/1	0.93	0.14	8,8,8,8	0
60	MG	BA	3092	1/1	0.93	0.41	3,3,3,3	0
60	MG	DA	3006	1/1	0.93	0.35	4,4,4,4	0
60	MG	DA	3224	1/1	0.93	0.11	18,18,18,18	0
60	MG	AA	1652	1/1	0.93	0.38	28,28,28,28	0
60	MG	BA	3328	1/1	0.93	0.27	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1635	1/1	0.93	0.20	23,23,23,23	0
60	MG	DA	3236	1/1	0.93	0.28	39,39,39,39	0
60	MG	BA	3006	1/1	0.93	0.38	37,37,37,37	0
60	MG	BA	3036	1/1	0.93	0.56	8,8,8,8	0
60	MG	BA	3181	1/1	0.93	0.36	16,16,16,16	0
60	MG	BA	3121	1/1	0.93	0.50	23,23,23,23	0
60	MG	BA	3158	1/1	0.93	0.52	35,35,35,35	0
60	MG	DA	3009	1/1	0.93	0.18	12,12,12,12	0
60	MG	BA	3066	1/1	0.93	0.19	1,1,1,1	0
60	MG	BA	3286	1/1	0.93	0.49	18,18,18,18	0
60	MG	BA	3131	1/1	0.93	0.35	1,1,1,1	0
60	MG	BU	202	1/1	0.94	0.21	1,1,1,1	0
60	MG	BA	3035	1/1	0.94	0.19	1,1,1,1	0
60	MG	BA	3249	1/1	0.94	0.55	13,13,13,13	0
60	MG	BA	3107	1/1	0.94	0.47	65,65,65,65	0
60	MG	BA	3225	1/1	0.94	0.27	9,9,9,9	0
60	MG	BA	3292	1/1	0.94	0.31	27,27,27,27	0
60	MG	BA	3281	1/1	0.94	0.26	21,21,21,21	0
60	MG	BA	3130	1/1	0.94	0.41	1,1,1,1	0
60	MG	BB	203	1/1	0.94	0.25	35,35,35,35	0
60	MG	DA	3029	1/1	0.94	0.43	1,1,1,1	0
60	MG	CA	1639	1/1	0.94	0.31	16,16,16,16	0
60	MG	BA	3297	1/1	0.94	0.16	42,42,42,42	0
60	MG	DA	3152	1/1	0.94	0.32	8,8,8,8	0
60	MG	BA	3128	1/1	0.94	0.19	16,16,16,16	0
60	MG	BA	3078	1/1	0.94	0.33	1,1,1,1	0
60	MG	BA	3236	1/1	0.94	0.36	11,11,11,11	0
60	MG	DA	3147	1/1	0.94	0.20	26,26,26,26	0
60	MG	CA	1671	1/1	0.94	0.14	24,24,24,24	0
60	MG	CA	1645	1/1	0.94	0.78	56,56,56,56	0
60	MG	AA	1694	1/1	0.94	0.29	5,5,5,5	0
60	MG	DA	3081	1/1	0.94	0.34	3,3,3,3	0
60	MG	CA	1697	1/1	0.94	0.27	27,27,27,27	0
60	MG	CA	1618	1/1	0.94	0.16	14,14,14,14	0
60	MG	BA	3060	1/1	0.94	0.27	4,4,4,4	0
60	MG	CA	1626	1/1	0.94	0.42	31,31,31,31	0
60	MG	BA	3007	1/1	0.94	0.28	1,1,1,1	0
60	MG	BA	3105	1/1	0.94	0.17	8,8,8,8	0
60	MG	BA	3155	1/1	0.94	0.35	14,14,14,14	0
60	MG	BA	3299	1/1	0.94	0.18	13,13,13,13	0
60	MG	DA	3022	1/1	0.94	0.28	11,11,11,11	0
60	MG	DA	3069	1/1	0.94	0.66	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3036	1/1	0.94	0.27	5,5,5,5	0
60	MG	BA	3218	1/1	0.94	0.12	9,9,9,9	0
60	MG	BA	3025	1/1	0.94	0.34	31,31,31,31	0
60	MG	BA	3285	1/1	0.94	0.12	1,1,1,1	0
60	MG	CA	1655	1/1	0.94	0.31	29,29,29,29	0
60	MG	DA	3108	1/1	0.94	0.26	18,18,18,18	0
60	MG	CA	1604	1/1	0.94	0.21	1,1,1,1	0
60	MG	BA	3235	1/1	0.94	0.17	1,1,1,1	0
60	MG	DA	3033	1/1	0.94	0.20	4,4,4,4	0
60	MG	AA	1613	1/1	0.94	0.24	36,36,36,36	0
60	MG	DA	3071	1/1	0.94	0.27	19,19,19,19	0
60	MG	DA	3105	1/1	0.94	0.19	59,59,59,59	0
60	MG	BB	202	1/1	0.94	0.12	9,9,9,9	0
60	MG	BA	3145	1/1	0.94	0.29	31,31,31,31	0
60	MG	DA	3191	1/1	0.94	0.41	31,31,31,31	0
60	MG	BA	3139	1/1	0.94	0.25	1,1,1,1	0
60	MG	BA	3209	1/1	0.94	0.37	24,24,24,24	0
60	MG	DA	3076	1/1	0.94	0.12	25,25,25,25	0
60	MG	AA	1678	1/1	0.94	0.13	29,29,29,29	0
60	MG	BA	3136	1/1	0.94	0.28	42,42,42,42	0
60	MG	BA	3054	1/1	0.94	0.12	6,6,6,6	0
60	MG	BA	3305	1/1	0.94	0.26	32,32,32,32	0
60	MG	AA	1705	1/1	0.94	0.15	4,4,4,4	0
60	MG	AA	1687	1/1	0.94	0.18	20,20,20,20	0
60	MG	DA	3070	1/1	0.94	0.21	14,14,14,14	0
60	MG	BA	3002	1/1	0.94	0.31	17,17,17,17	0
60	MG	BA	3188	1/1	0.94	0.10	30,30,30,30	0
60	MG	BA	3098	1/1	0.94	0.44	1,1,1,1	0
60	MG	BA	3021	1/1	0.94	0.39	1,1,1,1	0
60	MG	BA	3273	1/1	0.94	0.09	1,1,1,1	0
60	MG	DA	3234	1/1	0.94	0.36	40,40,40,40	0
60	MG	DA	3238	1/1	0.94	0.69	42,42,42,42	0
60	MG	DA	3113	1/1	0.94	0.47	2,2,2,2	0
60	MG	BA	3245	1/1	0.94	0.11	25,25,25,25	0
60	MG	AA	1612	1/1	0.94	0.25	15,15,15,15	0
60	MG	AA	1689	1/1	0.94	0.16	2,2,2,2	0
60	MG	BA	3180	1/1	0.94	0.43	40,40,40,40	0
60	MG	DA	3038	1/1	0.94	0.57	8,8,8,8	0
60	MG	CA	1643	1/1	0.94	0.28	7,7,7,7	0
60	MG	BF	301	1/1	0.94	0.13	14,14,14,14	0
60	MG	DA	3037	1/1	0.94	0.20	24,24,24,24	0
60	MG	DA	3051	1/1	0.94	0.51	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1661	1/1	0.95	0.25	21,21,21,21	0
60	MG	AA	1690	1/1	0.95	0.43	23,23,23,23	0
60	MG	DA	3106	1/1	0.95	0.12	23,23,23,23	0
60	MG	BA	3330	1/1	0.95	0.20	12,12,12,12	0
60	MG	AA	1691	1/1	0.95	0.39	23,23,23,23	0
60	MG	DA	3151	1/1	0.95	0.34	26,26,26,26	0
60	MG	BA	3008	1/1	0.95	0.20	4,4,4,4	0
60	MG	BA	3081	1/1	0.95	0.13	19,19,19,19	0
60	MG	BA	3253	1/1	0.95	0.31	39,39,39,39	0
60	MG	BA	3037	1/1	0.95	0.39	33,33,33,33	0
60	MG	BA	3032	1/1	0.95	0.23	1,1,1,1	0
60	MG	DA	3067	1/1	0.95	0.19	23,23,23,23	0
60	MG	DA	3163	1/1	0.95	0.49	32,32,32,32	0
60	MG	CA	1650	1/1	0.95	0.46	1,1,1,1	0
60	MG	BA	3127	1/1	0.95	0.27	1,1,1,1	0
60	MG	CE	201	1/1	0.95	0.14	56,56,56,56	0
60	MG	BA	3232	1/1	0.95	0.29	1,1,1,1	0
60	MG	BA	3075	1/1	0.95	0.31	2,2,2,2	0
60	MG	CA	1662	1/1	0.95	0.13	38,38,38,38	0
60	MG	BA	3306	1/1	0.95	0.29	5,5,5,5	0
60	MG	BA	3153	1/1	0.95	0.51	16,16,16,16	0
60	MG	BA	3089	1/1	0.95	0.20	12,12,12,12	0
60	MG	BA	3115	1/1	0.95	0.14	1,1,1,1	0
60	MG	CA	1648	1/1	0.95	0.36	24,24,24,24	0
60	MG	BG	201	1/1	0.95	0.20	30,30,30,30	0
60	MG	BA	3080	1/1	0.95	0.45	15,15,15,15	0
60	MG	B5	101	1/1	0.95	0.11	16,16,16,16	0
60	MG	AA	1647	1/1	0.95	0.29	39,39,39,39	0
60	MG	BA	3216	1/1	0.95	0.17	25,25,25,25	0
60	MG	CA	1605	1/1	0.95	0.41	6,6,6,6	0
60	MG	CA	1687	1/1	0.95	0.25	17,17,17,17	0
60	MG	BA	3183	1/1	0.95	0.20	1,1,1,1	0
60	MG	BA	3315	1/1	0.95	0.35	29,29,29,29	0
60	MG	BA	3119	1/1	0.95	0.23	91,91,91,91	0
60	MG	CA	1625	1/1	0.95	0.25	3,3,3,3	0
60	MG	BA	3125	1/1	0.95	0.21	1,1,1,1	0
60	MG	DA	3010	1/1	0.95	0.46	1,1,1,1	0
60	MG	BA	3217	1/1	0.95	0.14	1,1,1,1	0
60	MG	BA	3102	1/1	0.95	0.17	1,1,1,1	0
60	MG	AA	1684	1/1	0.95	0.37	69,69,69,69	0
61	ZN	CD	301	1/1	0.95	0.26	49,49,49,49	0
60	MG	CA	1651	1/1	0.95	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1698	1/1	0.95	0.29	23,23,23,23	0
60	MG	DA	3100	1/1	0.95	0.22	18,18,18,18	0
60	MG	CA	1619	1/1	0.95	0.43	20,20,20,20	0
60	MG	BA	3296	1/1	0.95	0.28	26,26,26,26	0
60	MG	CA	1622	1/1	0.95	0.27	12,12,12,12	0
60	MG	BA	3182	1/1	0.95	0.24	1,1,1,1	0
60	MG	DA	3101	1/1	0.95	0.17	20,20,20,20	0
60	MG	AA	1619	1/1	0.95	0.20	10,10,10,10	0
60	MG	CA	1615	1/1	0.95	0.46	28,28,28,28	0
60	MG	BA	3041	1/1	0.96	0.29	1,1,1,1	0
60	MG	DA	3061	1/1	0.96	0.33	21,21,21,21	0
60	MG	BA	3167	1/1	0.96	0.26	22,22,22,22	0
60	MG	AA	1623	1/1	0.96	0.33	10,10,10,10	0
60	MG	BA	3169	1/1	0.96	0.30	16,16,16,16	0
60	MG	CA	1690	1/1	0.96	0.28	31,31,31,31	0
60	MG	AA	1654	1/1	0.96	0.21	68,68,68,68	0
60	MG	DD	301	1/1	0.96	0.08	21,21,21,21	0
60	MG	BA	3321	1/1	0.96	0.42	1,1,1,1	0
60	MG	BA	3244	1/1	0.96	0.21	34,34,34,34	0
60	MG	BA	3193	1/1	0.96	0.26	22,22,22,22	0
60	MG	DA	3180	1/1	0.96	0.56	5,5,5,5	0
61	ZN	AD	301	1/1	0.96	0.25	46,46,46,46	0
60	MG	CA	1630	1/1	0.96	0.14	57,57,57,57	0
60	MG	BA	3332	1/1	0.96	0.13	1,1,1,1	0
60	MG	CA	1635	1/1	0.96	0.29	20,20,20,20	0
60	MG	AA	1662	1/1	0.96	0.14	21,21,21,21	0
60	MG	BA	3166	1/1	0.96	0.28	8,8,8,8	0
60	MG	BA	3088	1/1	0.96	0.13	1,1,1,1	0
60	MG	BA	3062	1/1	0.96	0.23	1,1,1,1	0
60	MG	DA	3087	1/1	0.96	0.46	32,32,32,32	0
60	MG	CA	1699	1/1	0.96	0.08	30,30,30,30	0
60	MG	BA	3126	1/1	0.96	0.11	5,5,5,5	0
60	MG	BA	3320	1/1	0.96	0.10	23,23,23,23	0
60	MG	BA	3200	1/1	0.96	0.20	14,14,14,14	0
60	MG	BA	3221	1/1	0.96	0.47	35,35,35,35	0
60	MG	DA	3018	1/1	0.96	0.18	15,15,15,15	0
60	MG	BP	202	1/1	0.96	0.27	1,1,1,1	0
60	MG	BA	3033	1/1	0.96	0.42	1,1,1,1	0
60	MG	BA	3024	1/1	0.96	0.14	11,11,11,11	0
60	MG	BA	3157	1/1	0.96	0.25	10,10,10,10	0
60	MG	BA	3146	1/1	0.96	0.19	13,13,13,13	0
60	MG	BA	3117	1/1	0.96	0.28	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3067	1/1	0.96	0.10	1,1,1,1	0
60	MG	CA	1629	1/1	0.96	0.25	16,16,16,16	0
60	MG	BA	3324	1/1	0.96	0.15	1,1,1,1	0
60	MG	AA	1659	1/1	0.96	0.15	23,23,23,23	0
60	MG	BA	3242	1/1	0.96	0.48	49,49,49,49	0
60	MG	BA	3156	1/1	0.96	0.39	7,7,7,7	0
60	MG	BA	3150	1/1	0.96	0.42	9,9,9,9	0
60	MG	BA	3164	1/1	0.96	0.35	33,33,33,33	0
60	MG	DA	3004	1/1	0.96	0.29	7,7,7,7	0
60	MG	CA	1664	1/1	0.96	0.10	83,83,83,83	0
60	MG	AA	1603	1/1	0.96	0.17	32,32,32,32	0
60	MG	BA	3072	1/1	0.96	0.12	6,6,6,6	0
60	MG	BA	3068	1/1	0.96	0.07	11,11,11,11	0
60	MG	BA	3013	1/1	0.96	0.32	1,1,1,1	0
60	MG	AA	1663	1/1	0.96	0.28	14,14,14,14	0
60	MG	DA	3112	1/1	0.96	0.45	7,7,7,7	0
60	MG	AA	1658	1/1	0.96	0.15	1,1,1,1	0
60	MG	CA	1620	1/1	0.96	0.20	32,32,32,32	0
60	MG	AA	1710	1/1	0.96	0.61	29,29,29,29	0
60	MG	BA	3019	1/1	0.96	0.34	1,1,1,1	0
60	MG	CA	1681	1/1	0.96	0.47	44,44,44,44	0
60	MG	DA	3017	1/1	0.96	0.26	1,1,1,1	0
60	MG	BA	3208	1/1	0.96	0.27	1,1,1,1	0
60	MG	CA	1680	1/1	0.96	0.07	44,44,44,44	0
60	MG	BA	3267	1/1	0.96	0.15	6,6,6,6	0
60	MG	BA	3058	1/1	0.96	0.13	1,1,1,1	0
60	MG	BA	3129	1/1	0.96	0.21	1,1,1,1	0
60	MG	CA	1659	1/1	0.96	0.62	46,46,46,46	0
60	MG	BA	3093	1/1	0.96	0.30	1,1,1,1	0
60	MG	BA	3234	1/1	0.96	0.33	15,15,15,15	0
60	MG	DA	3008	1/1	0.96	0.46	13,13,13,13	0
60	MG	BB	204	1/1	0.96	0.14	21,21,21,21	0
60	MG	BA	3031	1/1	0.96	0.29	1,1,1,1	0
60	MG	CA	1617	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3308	1/1	0.96	0.33	30,30,30,30	0
60	MG	BA	3233	1/1	0.96	0.13	1,1,1,1	0
60	MG	CA	1666	1/1	0.96	0.20	9,9,9,9	0
60	MG	BP	201	1/1	0.96	0.17	11,11,11,11	0
60	MG	AX	109	1/1	0.96	0.12	16,16,16,16	0
60	MG	AA	1712	1/1	0.96	0.48	36,36,36,36	0
60	MG	DA	3044	1/1	0.96	0.19	1,1,1,1	0
60	MG	CA	1608	1/1	0.96	0.30	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3248	1/1	0.96	0.21	34,34,34,34	0
60	MG	AA	1639	1/1	0.96	0.11	29,29,29,29	0
60	MG	BA	3044	1/1	0.96	0.34	1,1,1,1	0
60	MG	BA	3063	1/1	0.96	0.20	1,1,1,1	0
60	MG	BE	303	1/1	0.96	0.32	58,58,58,58	0
60	MG	BA	3110	1/1	0.96	0.33	6,6,6,6	0
60	MG	BD	301	1/1	0.96	0.26	12,12,12,12	0
60	MG	AA	1636	1/1	0.96	0.41	28,28,28,28	0
60	MG	DA	3035	1/1	0.96	0.24	1,1,1,1	0
60	MG	AA	1667	1/1	0.96	0.17	15,15,15,15	0
60	MG	BA	3124	1/1	0.96	0.41	13,13,13,13	0
60	MG	BA	3057	1/1	0.96	0.11	3,3,3,3	0
60	MG	AA	1634	1/1	0.97	0.13	1,1,1,1	0
60	MG	AA	1666	1/1	0.97	0.09	9,9,9,9	0
60	MG	BA	3005	1/1	0.97	0.43	1,1,1,1	0
60	MG	BA	3323	1/1	0.97	0.14	2,2,2,2	0
60	MG	BA	3027	1/1	0.97	0.28	1,1,1,1	0
60	MG	DA	3230	1/1	0.97	0.05	17,17,17,17	0
60	MG	BA	3152	1/1	0.97	0.41	6,6,6,6	0
60	MG	AA	1649	1/1	0.97	0.25	25,25,25,25	0
60	MG	BA	3053	1/1	0.97	0.18	1,1,1,1	0
61	ZN	B9	101	1/1	0.97	0.07	44,44,44,44	0
60	MG	BA	3012	1/1	0.97	0.27	1,1,1,1	0
60	MG	BA	3237	1/1	0.97	0.19	1,1,1,1	0
60	MG	BA	3178	1/1	0.97	0.22	1,1,1,1	0
60	MG	BA	3143	1/1	0.97	0.23	32,32,32,32	0
60	MG	CA	1688	1/1	0.97	0.09	37,37,37,37	0
60	MG	BA	3052	1/1	0.97	0.33	1,1,1,1	0
60	MG	AA	1641	1/1	0.97	0.18	13,13,13,13	0
60	MG	AA	1676	1/1	0.97	0.31	11,11,11,11	0
60	MG	BA	3259	1/1	0.97	0.20	16,16,16,16	0
60	MG	BA	3123	1/1	0.97	0.14	6,6,6,6	0
60	MG	BA	3137	1/1	0.97	0.37	1,1,1,1	0
60	MG	BE	302	1/1	0.97	0.15	1,1,1,1	0
60	MG	BA	3043	1/1	0.97	0.40	1,1,1,1	0
60	MG	DA	3046	1/1	0.97	0.08	28,28,28,28	0
60	MG	AA	1669	1/1	0.97	0.18	35,35,35,35	0
60	MG	BA	3020	1/1	0.97	0.40	1,1,1,1	0
60	MG	BA	3231	1/1	0.97	0.19	2,2,2,2	0
60	MG	BA	3055	1/1	0.97	0.21	1,1,1,1	0
60	MG	BA	3176	1/1	0.97	0.37	1,1,1,1	0
60	MG	BA	3262	1/1	0.97	0.17	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3076	1/1	0.97	0.38	1,1,1,1	0
60	MG	CA	1661	1/1	0.97	0.21	9,9,9,9	0
60	MG	DA	3045	1/1	0.97	0.16	11,11,11,11	0
60	MG	BA	3134	1/1	0.97	0.36	12,12,12,12	0
60	MG	AX	107	1/1	0.97	0.12	8,8,8,8	0
60	MG	BA	3049	1/1	0.97	0.32	1,1,1,1	0
60	MG	BA	3069	1/1	0.97	0.18	1,1,1,1	0
60	MG	BA	3087	1/1	0.97	0.09	6,6,6,6	0
60	MG	BA	3100	1/1	0.97	0.11	10,10,10,10	0
60	MG	BA	3317	1/1	0.97	0.15	22,22,22,22	0
60	MG	BU	201	1/1	0.97	0.43	23,23,23,23	0
60	MG	BA	3029	1/1	0.97	0.26	36,36,36,36	0
60	MG	BA	3083	1/1	0.97	0.30	1,1,1,1	0
60	MG	BB	205	1/1	0.97	0.24	1,1,1,1	0
60	MG	BA	3206	1/1	0.97	0.33	6,6,6,6	0
60	MG	BA	3256	1/1	0.97	0.15	23,23,23,23	0
60	MG	DA	3132	1/1	0.97	0.26	6,6,6,6	0
60	MG	AA	1611	1/1	0.97	0.13	33,33,33,33	0
60	MG	BA	3288	1/1	0.97	0.24	29,29,29,29	0
60	MG	AA	1692	1/1	0.97	0.29	19,19,19,19	0
60	MG	BA	3090	1/1	0.97	0.05	13,13,13,13	0
60	MG	BA	3112	1/1	0.97	0.13	11,11,11,11	0
60	MG	DA	3121	1/1	0.97	0.59	34,34,34,34	0
60	MG	DA	3187	1/1	0.97	0.09	27,27,27,27	0
60	MG	AA	1656	1/1	0.97	0.25	10,10,10,10	0
60	MG	BE	301	1/1	0.97	0.14	1,1,1,1	0
60	MG	BA	3212	1/1	0.97	0.28	11,11,11,11	0
60	MG	BA	3071	1/1	0.97	0.34	1,1,1,1	0
60	MG	BA	3202	1/1	0.97	0.22	1,1,1,1	0
60	MG	AA	1618	1/1	0.97	0.40	22,22,22,22	0
60	MG	BA	3017	1/1	0.97	0.32	1,1,1,1	0
60	MG	BA	3046	1/1	0.98	0.24	10,10,10,10	0
60	MG	AA	1706	1/1	0.98	0.14	28,28,28,28	0
60	MG	AA	1650	1/1	0.98	0.15	15,15,15,15	0
60	MG	BA	3268	1/1	0.98	0.20	1,1,1,1	0
60	MG	BA	3038	1/1	0.98	0.25	1,1,1,1	0
60	MG	AA	1693	1/1	0.98	0.14	31,31,31,31	0
60	MG	BA	3073	1/1	0.98	0.30	1,1,1,1	0
60	MG	BA	3018	1/1	0.98	0.23	1,1,1,1	0
60	MG	DA	3099	1/1	0.98	0.24	14,14,14,14	0
60	MG	BA	3016	1/1	0.98	0.30	1,1,1,1	0
60	MG	DA	3055	1/1	0.98	0.23	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3326	1/1	0.98	0.13	21,21,21,21	0
60	MG	AA	1609	1/1	0.98	0.22	1,1,1,1	0
60	MG	BA	3151	1/1	0.98	0.17	22,22,22,22	0
60	MG	BA	3070	1/1	0.98	0.51	1,1,1,1	0
60	MG	BA	3278	1/1	0.98	0.10	15,15,15,15	0
60	MG	BA	3023	1/1	0.98	0.08	1,1,1,1	0
60	MG	BA	3011	1/1	0.98	0.16	1,1,1,1	0
60	MG	BA	3086	1/1	0.98	0.14	4,4,4,4	0
60	MG	BA	3030	1/1	0.98	0.38	7,7,7,7	0
60	MG	AA	1675	1/1	0.98	0.25	4,4,4,4	0
60	MG	AA	1714	1/1	0.98	0.18	6,6,6,6	0
60	MG	BA	3220	1/1	0.98	0.16	1,1,1,1	0
60	MG	BA	3116	1/1	0.98	0.11	26,26,26,26	0
60	MG	BA	3247	1/1	0.98	0.17	35,35,35,35	0
60	MG	BA	3132	1/1	0.98	0.31	1,1,1,1	0
60	MG	BA	3239	1/1	0.98	0.22	2,2,2,2	0
60	MG	BA	3040	1/1	0.98	0.20	1,1,1,1	0
60	MG	BA	3028	1/1	0.98	0.14	1,1,1,1	0
60	MG	BA	3327	1/1	0.98	0.31	17,17,17,17	0
60	MG	BA	3133	1/1	0.98	0.35	1,1,1,1	0
60	MG	BA	3322	1/1	0.98	0.30	10,10,10,10	0
60	MG	BA	3091	1/1	0.98	0.31	1,1,1,1	0
60	MG	CA	1663	1/1	0.98	0.12	31,31,31,31	0
60	MG	AA	1628	1/1	0.98	0.17	10,10,10,10	0
60	MG	BA	3009	1/1	0.98	0.35	1,1,1,1	0
60	MG	AA	1703	1/1	0.98	0.24	35,35,35,35	0
60	MG	BA	3039	1/1	0.98	0.22	1,1,1,1	0
60	MG	CA	1628	1/1	0.98	0.10	12,12,12,12	0
60	MG	AA	1696	1/1	0.98	0.46	20,20,20,20	0
60	MG	BA	3004	1/1	0.98	0.23	8,8,8,8	0
60	MG	AA	1668	1/1	0.98	0.13	24,24,24,24	0
60	MG	BA	3014	1/1	0.98	0.49	1,1,1,1	0
60	MG	BA	3199	1/1	0.99	0.19	1,1,1,1	0
60	MG	AA	1655	1/1	0.99	0.25	2,2,2,2	0
60	MG	BA	3252	1/1	0.99	0.06	4,4,4,4	0
60	MG	BA	3108	1/1	0.99	0.41	2,2,2,2	0
60	MG	BA	3147	1/1	0.99	0.12	8,8,8,8	0
60	MG	AA	1615	1/1	0.99	0.27	18,18,18,18	0
60	MG	BR	201	1/1	0.99	0.06	1,1,1,1	0
60	MG	BA	3065	1/1	0.99	0.16	2,2,2,2	0
60	MG	BA	3048	1/1	0.99	0.19	1,1,1,1	0
60	MG	BA	3135	1/1	0.99	0.13	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3099	1/1	0.99	0.19	8,8,8,8	0
60	MG	AA	1674	1/1	0.99	0.14	32,32,32,32	0
60	MG	BA	3257	1/1	0.99	0.06	22,22,22,22	0
60	MG	AA	1602	1/1	0.99	0.05	1,1,1,1	0
60	MG	AA	1606	1/1	0.99	0.29	1,1,1,1	0
60	MG	BA	3254	1/1	0.99	0.06	72,72,72,72	0
60	MG	BA	3045	1/1	0.99	0.24	2,2,2,2	0
60	MG	AA	1624	1/1	0.99	0.35	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.