



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 04:17 pm BST

PDB ID : 4V84
Title : Crystal structure of a complex containing domain 3 of CrPV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.40 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
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

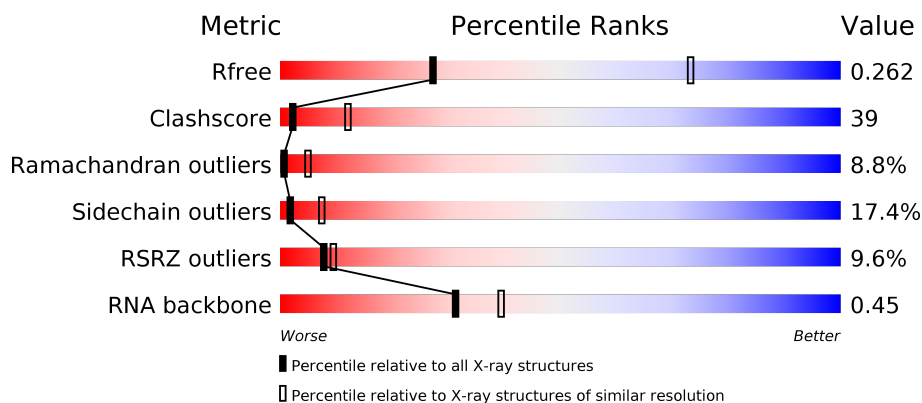
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	1506	<div> <div>4%</div> <div>20%</div> <div>63%</div> <div>16%</div> </div>
1	CA	1506	<div> <div>6%</div> <div>19%</div> <div>64%</div> <div>18%</div> </div>
2	AB	234	<div> <div>18%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
2	CB	234	<div> <div>19%</div> <div>32%</div> <div>56%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	
6	CF	101	
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	116	
13	CM	116	
14	AN	60	
14	CN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	43	
22	CV	43	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	

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Mol	Chain	Length	Quality of chain
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	
49	B1	30	
49	D1	30	
50	B2	52	
50	D2	52	
51	B3	44	
51	D3	44	
52	B4	48	
52	D4	48	

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Mol	Chain	Length	Quality of chain
53	B5	63	
53	D5	63	

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
54	MG	AA	1621	-	-	-	X
54	MG	AA	1640	-	-	-	X
54	MG	AA	1642	-	-	-	X
54	MG	AA	1645	-	-	-	X
54	MG	AA	1661	-	-	-	X
54	MG	AA	1673	-	-	-	X
54	MG	AA	1691	-	-	-	X
54	MG	AA	1698	-	-	-	X
54	MG	AA	1700	-	-	-	X
54	MG	AA	1702	-	-	-	X
54	MG	AA	1718	-	-	-	X
54	MG	AA	1723	-	-	-	X
54	MG	AA	1747	-	-	-	X
54	MG	AA	1757	-	-	-	X
54	MG	AV	6302	-	-	-	X
54	MG	AV	6304	-	-	-	X
54	MG	BA	3004	-	-	-	X
54	MG	BA	3006	-	-	-	X
54	MG	BA	3019	-	-	-	X
54	MG	BA	3027	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3072	-	-	-	X
54	MG	BA	3079	-	-	-	X
54	MG	BA	3084	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3114	-	-	-	X
54	MG	BA	3118	-	-	-	X
54	MG	BA	3149	-	-	-	X
54	MG	BA	3163	-	-	-	X
54	MG	BA	3164	-	-	-	X
54	MG	BA	3172	-	-	-	X
54	MG	BA	3178	-	-	-	X
54	MG	BA	3189	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3212	-	-	-	X
54	MG	BA	3218	-	-	-	X
54	MG	BA	3219	-	-	-	X
54	MG	BA	3225	-	-	-	X
54	MG	BA	3226	-	-	-	X
54	MG	BA	3267	-	-	-	X
54	MG	BA	3272	-	-	-	X
54	MG	BA	3275	-	-	-	X
54	MG	BA	3287	-	-	-	X
54	MG	BA	3305	-	-	-	X
54	MG	BA	3308	-	-	-	X
54	MG	BB	205	-	-	-	X
54	MG	CA	1616	-	-	-	X
54	MG	CA	1639	-	-	-	X
54	MG	CA	1658	-	-	-	X
54	MG	CA	1668	-	-	-	X
54	MG	CA	1685	-	-	-	X
54	MG	CA	1691	-	-	-	X
54	MG	CA	1697	-	-	-	X
54	MG	CA	1704	-	-	-	X
54	MG	D4	101	-	-	-	X
54	MG	DA	2940	-	-	-	X
54	MG	DA	2972	-	-	-	X
54	MG	DA	2987	-	-	-	X
54	MG	DA	2999	-	-	-	X
54	MG	DA	3030	-	-	-	X
54	MG	DA	3033	-	-	-	X
54	MG	DA	3043	-	-	-	X
54	MG	DA	3055	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3078	-	-	-	X
54	MG	DA	3080	-	-	-	X
54	MG	DA	3100	-	-	-	X
54	MG	DA	3101	-	-	-	X
54	MG	DA	3105	-	-	-	X
54	MG	DA	3115	-	-	-	X
54	MG	DA	3119	-	-	-	X
54	MG	DA	3165	-	-	-	X
54	MG	DA	3168	-	-	-	X
54	MG	DA	3174	-	-	-	X
54	MG	DA	3196	-	-	-	X
54	MG	DA	3199	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3209	-	-	-	X
54	MG	DA	3222	-	-	-	X
54	MG	DA	3226	-	-	-	X
54	MG	DA	3229	-	-	-	X
54	MG	DA	3235	-	-	-	X
54	MG	DA	3246	-	-	-	X
54	MG	DA	3258	-	-	-	X
54	MG	DA	3291	-	-	-	X
54	MG	DA	3298	-	-	-	X
54	MG	DA	3302	-	-	-	X
54	MG	DA	3312	-	-	-	X
54	MG	DA	3317	-	-	-	X
54	MG	DA	3324	-	-	-	X
54	MG	DA	3325	-	-	-	X
54	MG	DA	3332	-	-	-	X
54	MG	DB	215	-	-	-	X
54	MG	DG	201	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 282142 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	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	0
			1156	729	218	205	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	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	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
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	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
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	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			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	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	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
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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

- Molecule 22 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			
22	CV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59440	26455	11114	19112	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	conflict	GB 46197919
BA	2825	U	G	conflict	GB 46197919
DA	1142	U	C	conflict	GB 46197919
DA	2825	U	G	conflict	GB 46197919

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total	C	N	O	0	0	0
			771	486	154	131			
37	DO	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
38	DP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
39	DQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	deletion	UNP Q72L76
DQ	?	-	PHE	deletion	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	DR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O		0	0	0
			726	471	131	124				
42	DT	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total	C	N	O	0	0	0
			695	435	141	119			
46	DX	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
47	DY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
48	DZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	D1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
50	D2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	17	Total	Mg	0	0
			17	17		
54	DE	1	Total	Mg	0	0
			1	1		
54	BA	408	Total	Mg	0	0
			408	408		
54	CA	140	Total	Mg	0	0
			140	140		
54	DG	1	Total	Mg	0	0
			1	1		
54	CV	1	Total	Mg	0	0
			1	1		
54	AV	4	Total	Mg	0	0
			4	4		
54	D2	1	Total	Mg	0	0
			1	1		
54	DA	436	Total	Mg	0	0
			436	436		
54	B2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CP	1	Total 1	Mg 1	0	0
54	AA	163	Total 163	Mg 163	0	0
54	D4	1	Total 1	Mg 1	0	0
54	BK	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DB	17	Total 17	Mg 17	0	0

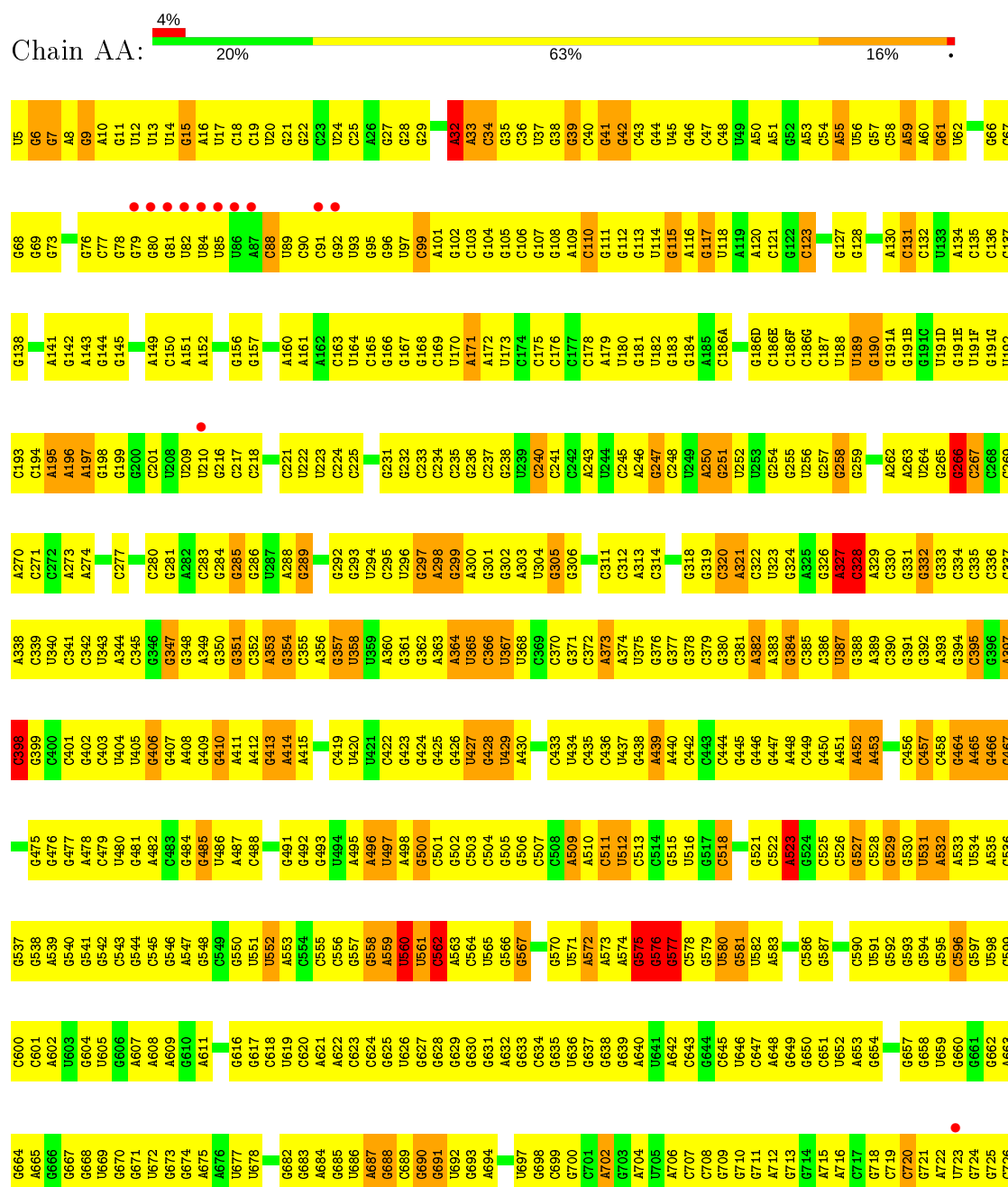
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CN	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0

3 Residue-property plots

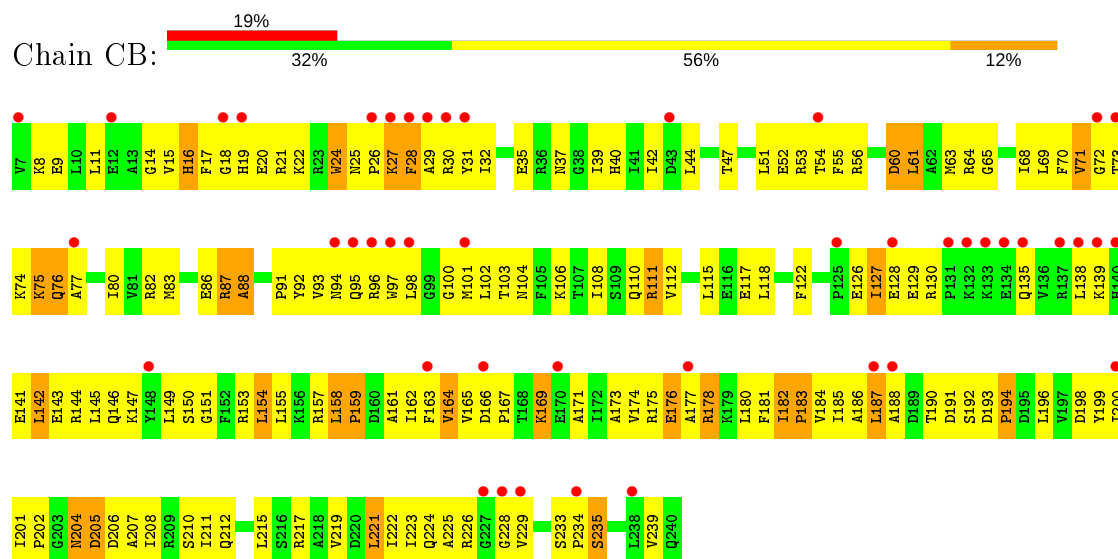
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: ribosomal RNA 16S

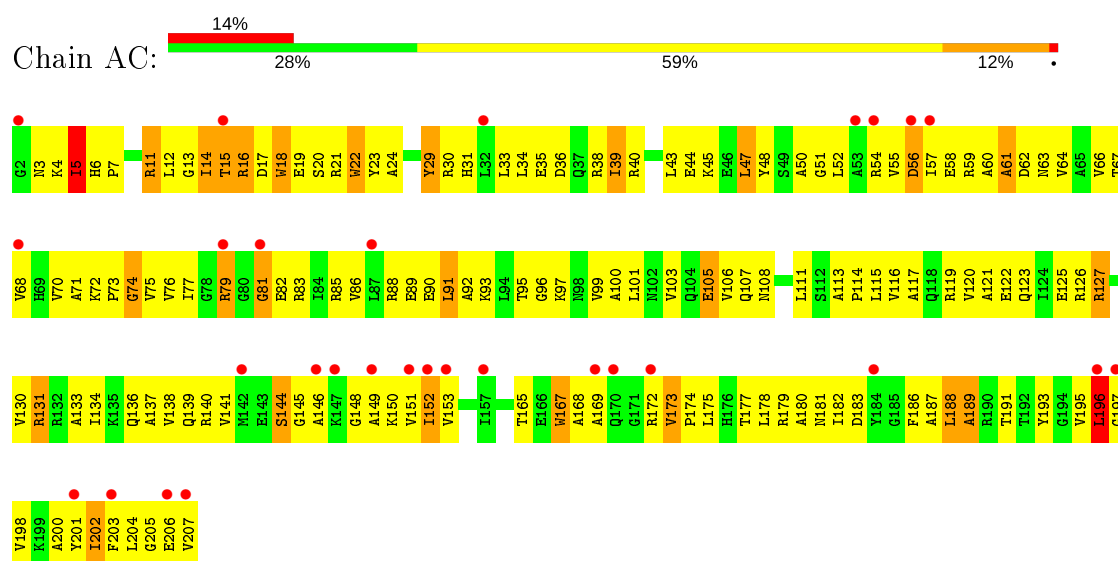


G922	G851	G778	G713	G649	C589	G529	C458	A393	G333	C269	U192	C135	U85	U5
A923	G852	C779	G714	G650	C590	G530	G464	G394	G334	C269	C193	C136	G66	G6
	G853	C780	A715	G651	C591	U531	G465	G395	C335	A270	C194	G137	C67	G7
G926	G854	A781	A716	U652	G592	A532	G466	G396	C336	C271	A195	G138	G68	A8
G927	G855	A782		G653	G593	A533	G467	A397	C337	C272	A196		G69	G9
G928	G856	C783	G719		G594	U534	A468	C398	A338	A273	A197	A141	G73	A10
G929	G857	C784	G720		G595	A535	G474	G399	C339	A274	G198	G142	C74	A11
C930	G858	G785	G721	G657	C596	C536	G475	C400	U340		G199	G143	C75	G12
C931	A859		A722	G658	G597	G537	G476	C401	C341	C277	G200	A144	C76	U13
C932	G860		A723	U659	U598	G538	G477	G402	U342	G278	G201	G145	C77	U14
C933	G861	U789	G724	G660	C599	A539	A478	C403	U343	A279	U208		C78	G15
G934	G862	G791	G725	G661	C600	G540	C479	U404	U344	C280	U209	A149	G79	A16
A935	U863	A792	G726	G662	C601	G541	U480	U405	C345	G281	U210	C150	G80	U17
C936	A864	U793	G727	A663	A602	G542	G481	G406	C346	A282	G216	A151	G81	C18
A865	A865	A794	A728	G664	U603	G543	G482	G407	G347	G283	C217	A152	C81	C19
A937			A729	A665	G604	G544	C483	A408	G348	C284	C218		U82	C20
C939	G868	G798	G730	G667	U605	G545	G484	C409	A349	G285	C221	G156	U85	G21
C940	U870	G800	G731	G668	U607	G546	G485	G410	G350	G286	U222	G157	U86	G22
G941	U871	U801	C732	U669	A608	A547	U486	A411	G351	U287	U223	G158	A87	C23
G942	A802	A802	A733	U670	A609	G549	A487	A412	C352	A288	U224	G159	C88	U24
G944	G803	G803	G734	G671	A610	U550	C488	G413	A353		C225	A161	U88	U25
G945	U804	U804	C735	U672	A611	U551	G490	A414	C354	G289		G162	C90	A26
G946	C875	C805	A737	G673	C612	U552	G491	A415	C355	G292	G231	C163	C91	G27
G947	G876	C806	C738	G674	C613	A553	G492	C419	A356	G293	G232	C164	G92	G28
C877	C807	A807	C739	A675	A614	G554	G493	U420	U358	U296	G233	C165	G95	U30
G948	G878		U740	U676	C615	C555	U494	U421	U359	G297	C234	G166	G96	G31
A949	C879	C810	G741	U677	G616	C556	A495	C422	A360	C297	C235	G167	U97	A32
U950	G880	C811	G742	U678	C617	G557	A496	G423	G361	A298	G236	C168	C98	A33
G951	G881		U743	U679	C618	G558	U497	G424	G362	C299	C237	C169	C99	A34
U952	C882	A814	C744	C680	U619	A559	A498	G425	A363	A300	G238	U170	C102	G35
G953	C883	A815		C681	C620	U560	G500	G426	A364	G301	U239	A171	C103	C36
G954	U894	A816	C748	C682	A621	U561	C501	U427	U365	G302	C240	A172	C104	U37
U955		C817	G749	G683	A622	C562	G502	G428	A366	A303	C241	U173	G105	U38
U956	U891	G818	U750	G684	C623	A563	C503	U429	U367	U304	C242	C174	C106	G39
A892	A892	A819	U751	G685	C624	C564	C504	A430	U368	G305	A243	C175	G107	C40
C958	C953	U820	G752	U686	G625	U565	G505	A431	G306	G306	U244	C176	G108	G41
U960		G821	A753	A887	U626	G566	G506	A432	C370	C307	C245	C177	A109	G42
U961	C896	C822	C754	G688	G627	G567	C507	C433	G371		C246	C178	C110	C43
C962	C897		G755	C689	G628	G568	C508	U434	C372	C311	A247	C179	G111	C44
G963	G898	C817	U756	G690	G629	C569	A509	C435	A373	C312	C248	U180	G112	U45
A964	C899	C826	U757	G691	G630	G570	A510	C436	A374	A313	U249	G181	G113	G46
A965	A900	U827	G758	U692	G631	U571	C511	U437	U375	C314	A250	U182	U114	C47
C966	A901	A828	A759	G693	A632	A572	U512	G438	G376	C314	G251	U183	G115	C48
	G902	G829	G760	G694	G633	A573	C513	A439	G377		U252	G183	A116	U49
A968		G830	G761	A695	C634	A574	C514	A440	G378	G317	U253	G186D	G116	
A969	A907	U831	C762	A696	G635	G575	G515		C379	G318	G254	C186E	U118	A50
C970	A908	C832	G763	U697	U636	G576	U516	C444	G380	G319	G255	C186F	A51	A51
G971	A909	U833	G764	G698	G637	G577	G517	G445	C381	C320	U256	C186G	G52	G52
C972	C910	C834	G765	C699	G638	C578	G518	G446	A382	A321	G257	C187	A120	A53
G973		U835	A766		G639	G579	C519	G447	A383	U323	G258	C187	C121	C54
A974	A913	G836	A767	A702	A640	U580	C520	A448	G384	G324	U189	U188	G122	A55
A975	A914	C837	A768		U641	U581	G521	A449	A385	A325	G260	G190	C123	U56
G976	A915	G838		A706	A642	U582	C522	C450	C386	G326	U261	G191A	G127	G57
A977	G916	U841	U772	C707	C643	A583	A523	A451	G387	A327	A262	G191B	G128	C58
A978	G917	C842	G773	C708	G644	G584	C524	A452	U387	C328	A263	G191C	A59	A59
C979	A918	U843	G774	G709	C645	G585	C525	A453	A389	A329	U264	U191D	G61	G61
C980	A919	C848	G775	G710	U646	C586	C526		C390	G330	G265	G191E	U62	U62
U981	U920	G849	G776	G711	C647	G587	G527	C456	G391	G331	G266	U191F	C132	C63
U982		U950	A777	A712	A648	G588	C528	C457	G392	G332	C267	G191G	C133	G64

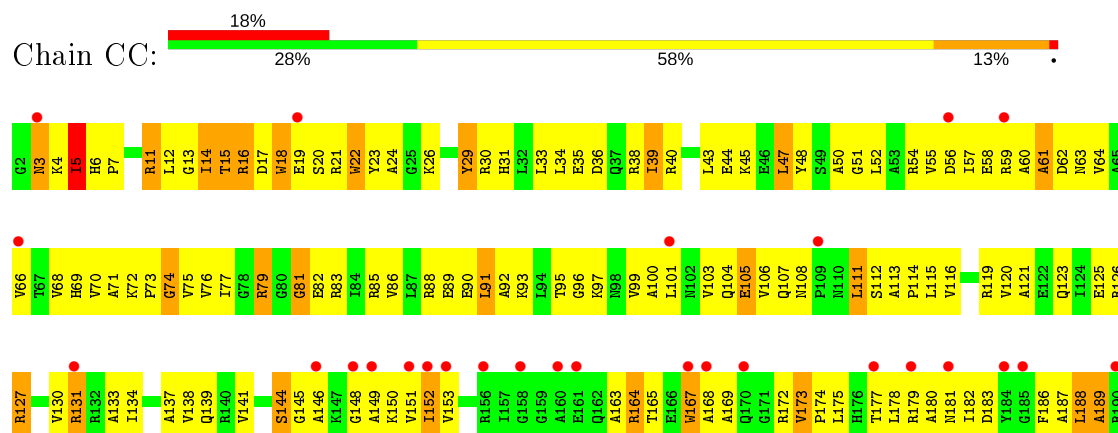
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

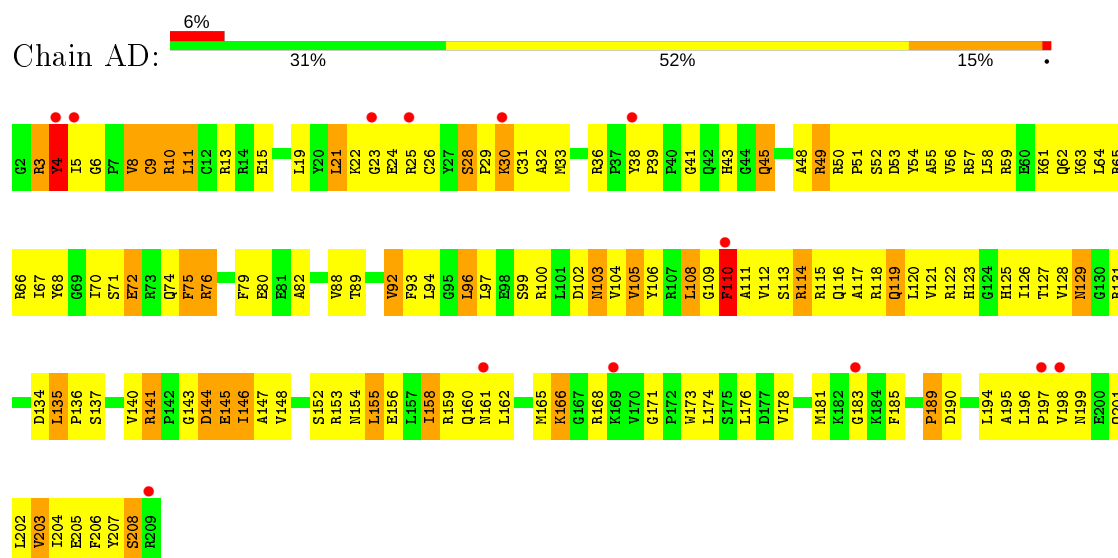


• Molecule 3: 30S ribosomal protein S3

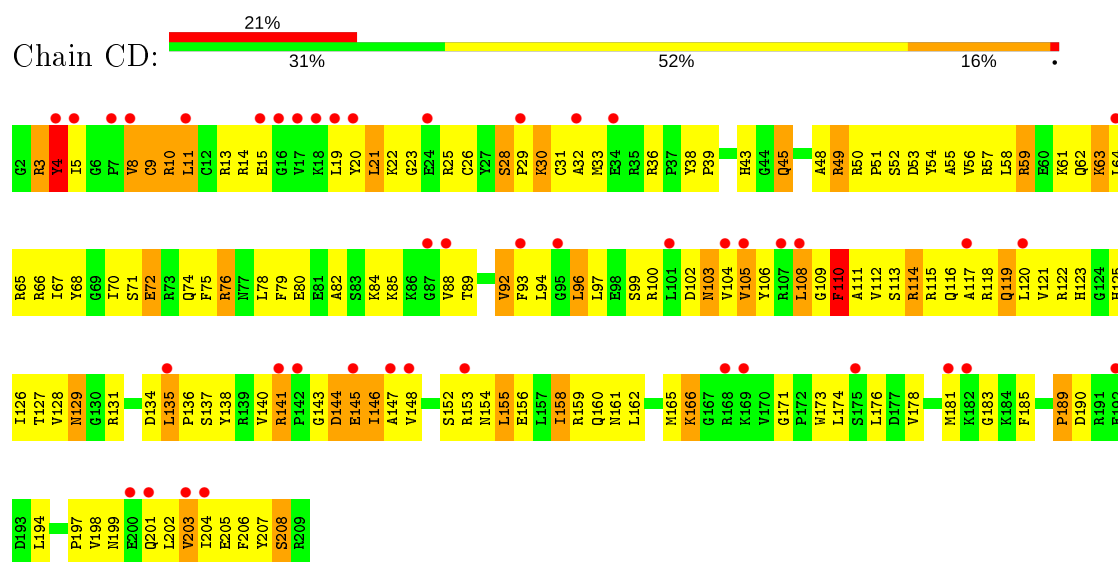




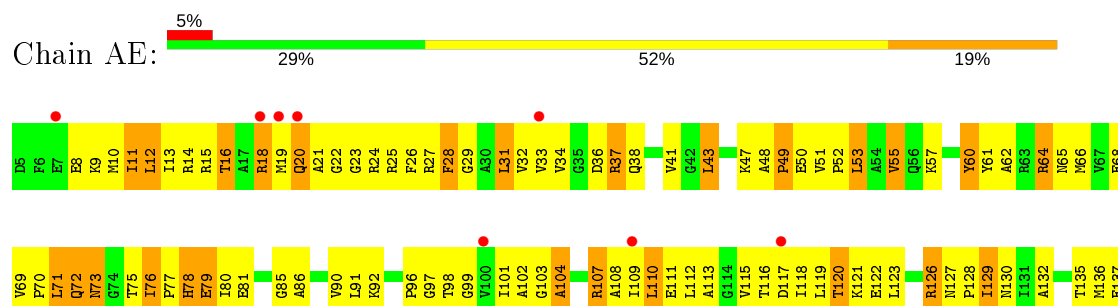
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

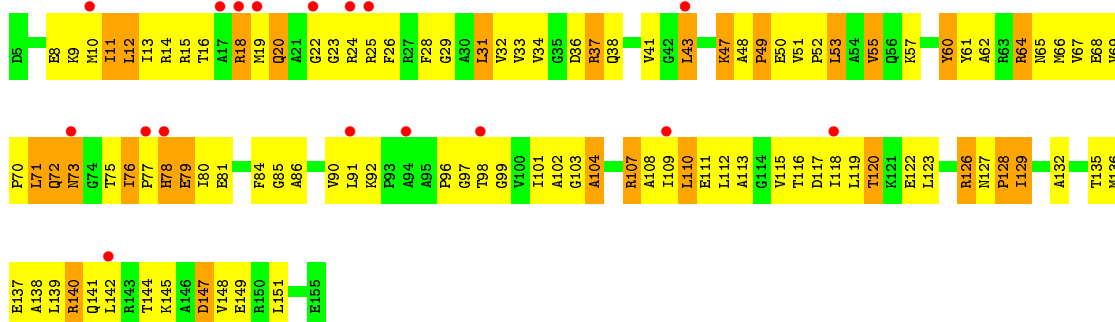


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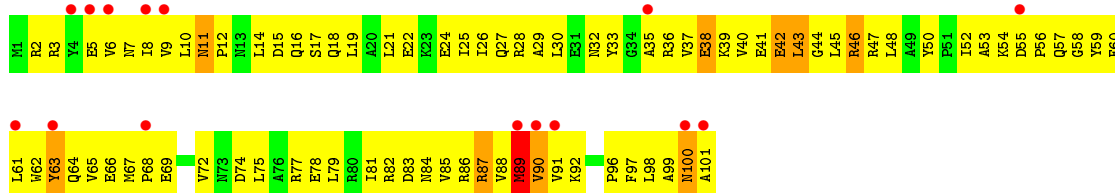




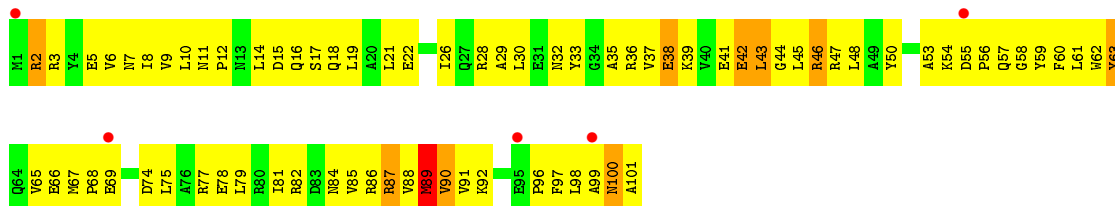
• Molecule 5: 30S ribosomal protein S5



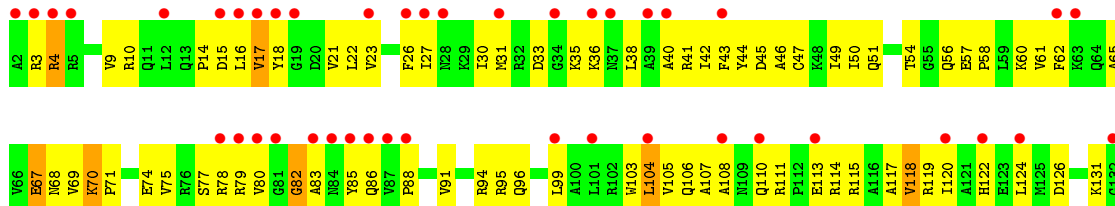
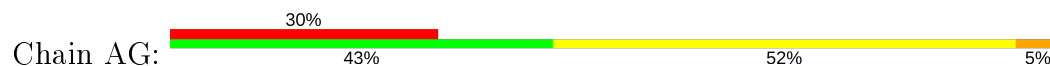
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

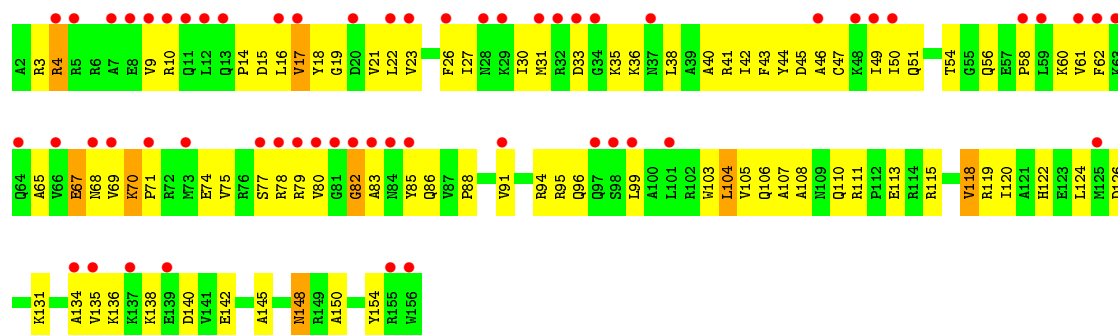
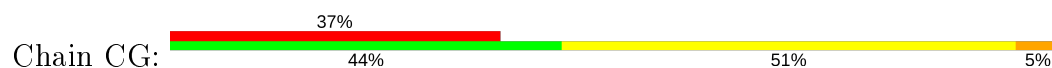


• Molecule 7: 30S ribosomal protein S7

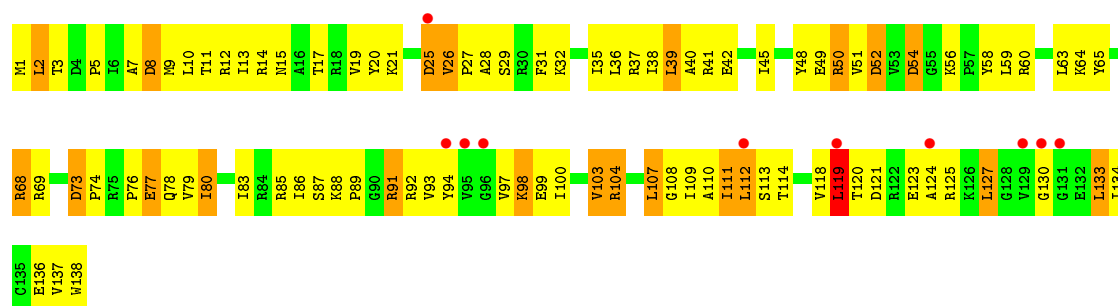




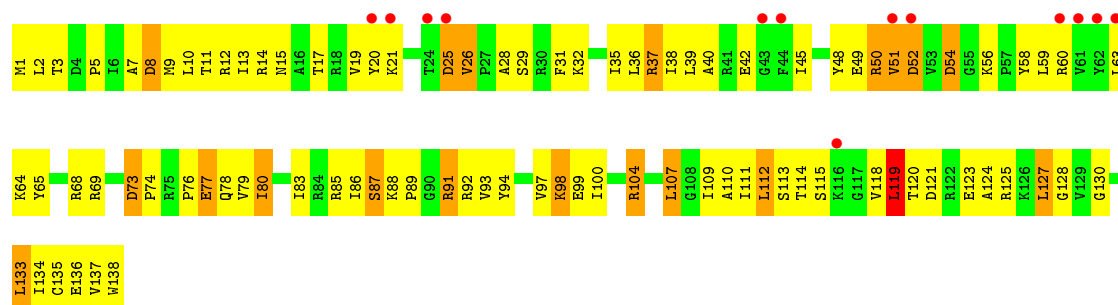
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

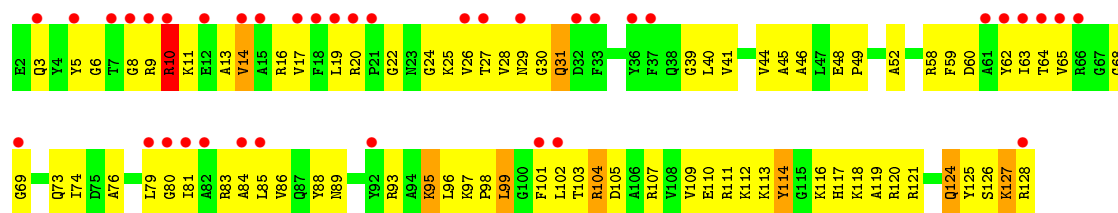


• Molecule 8: 30S ribosomal protein S8

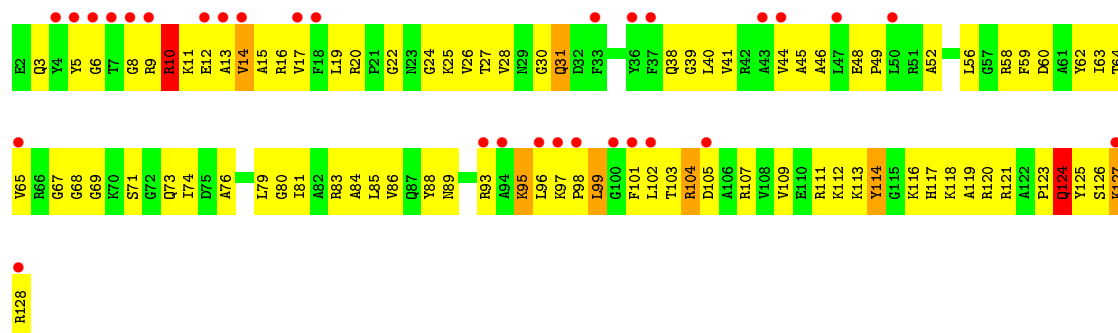


• Molecule 9: 30S ribosomal protein S9

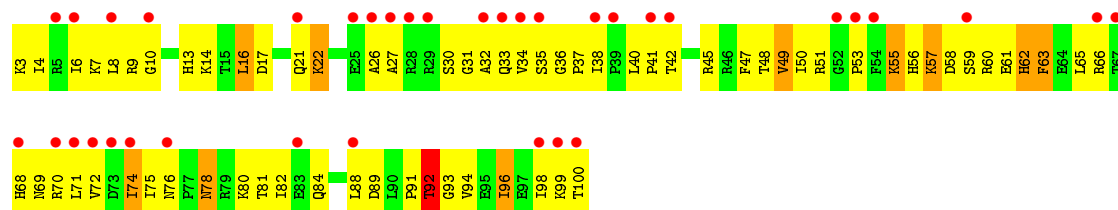




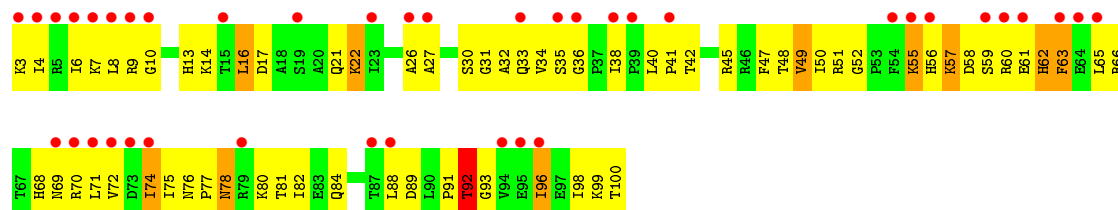
● Molecule 9: 30S ribosomal protein S9



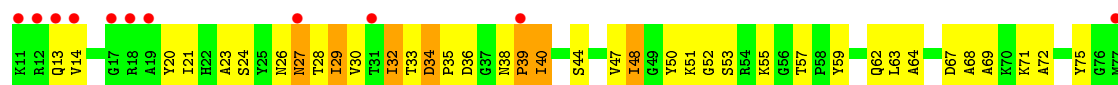
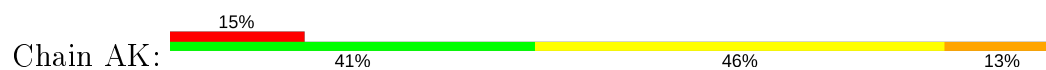
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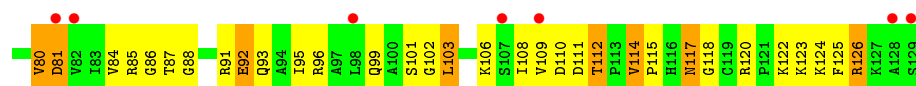


● Molecule 10: 30S ribosomal protein S10

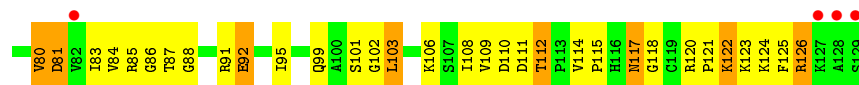
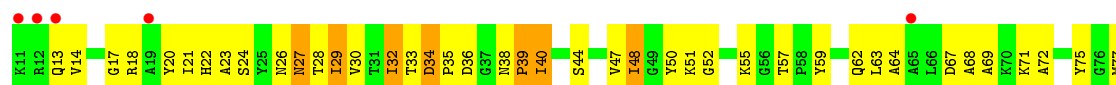


● Molecule 11: 30S ribosomal protein S11

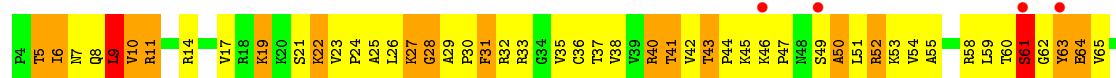




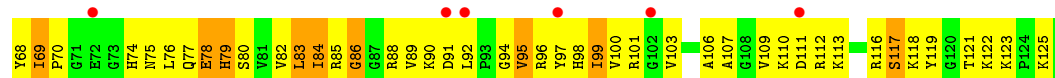
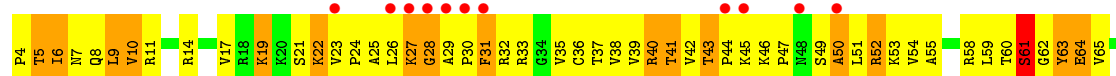
- Molecule 11: 30S ribosomal protein S11



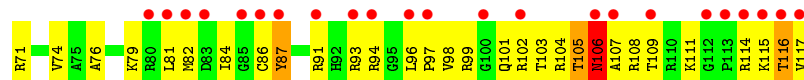
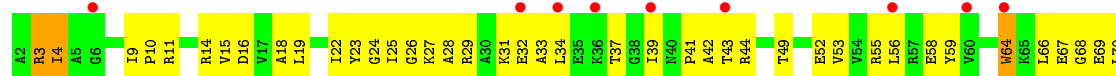
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

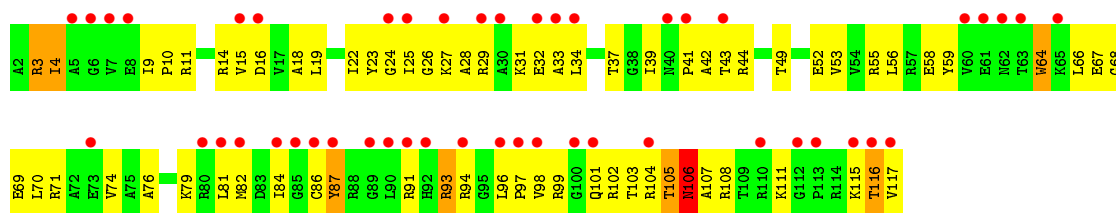


- Molecule 13: 30S ribosomal protein S13

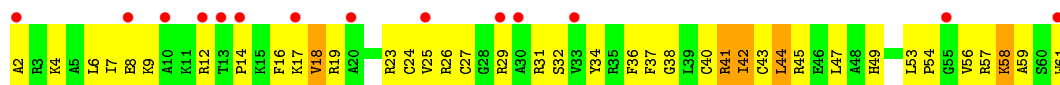


- Molecule 13: 30S ribosomal protein S13

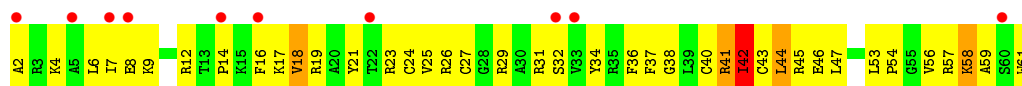




• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S15

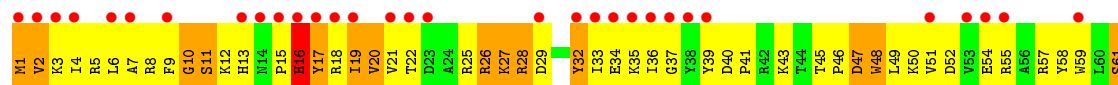
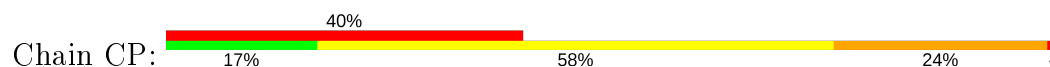


• Molecule 16: 30S ribosomal protein S16

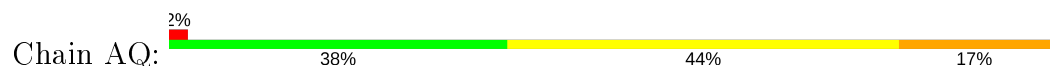




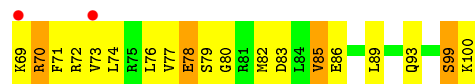
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

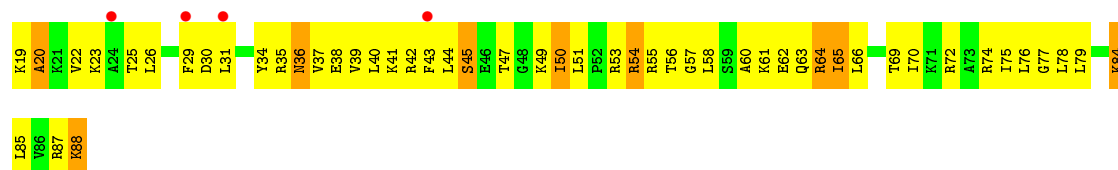


- Molecule 18: 30S ribosomal protein S18

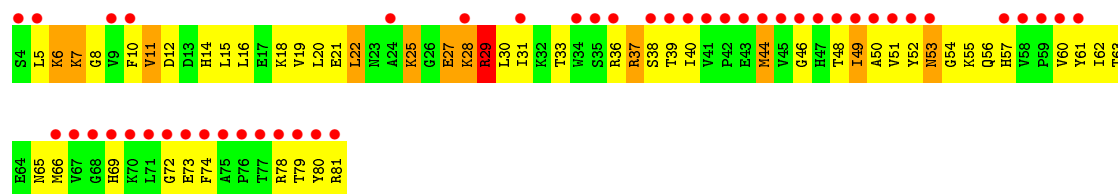


- Molecule 18: 30S ribosomal protein S18

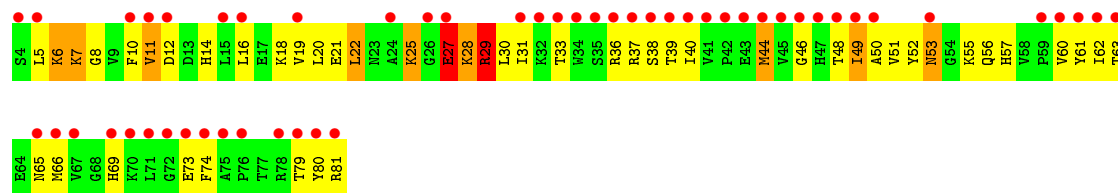




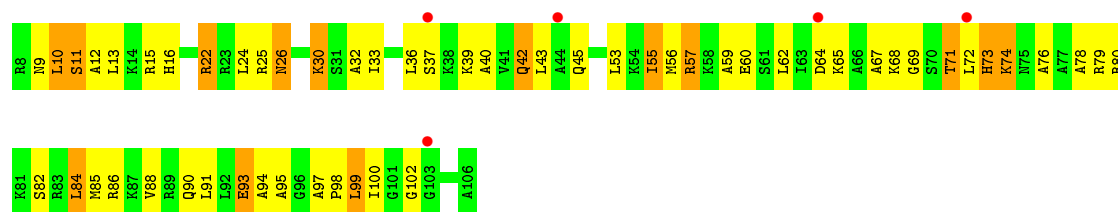
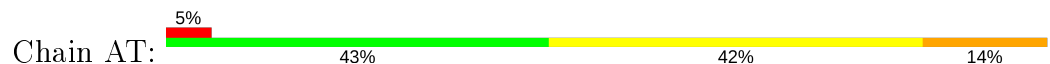
• Molecule 19: 30S ribosomal protein S19



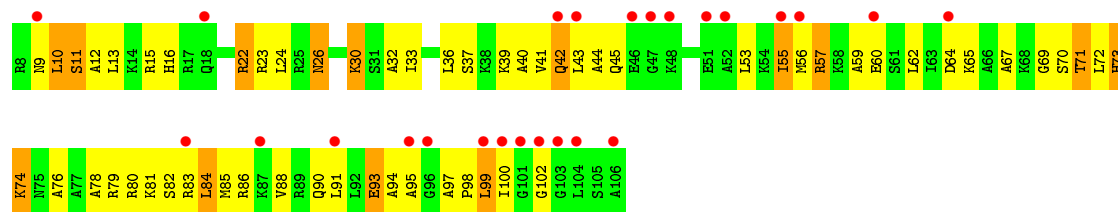
• Molecule 19: 30S ribosomal protein S19



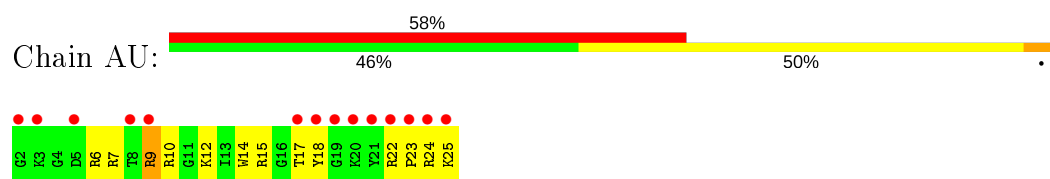
• Molecule 20: 30S ribosomal protein S20



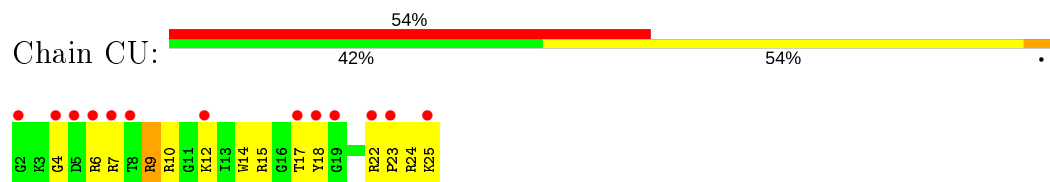
• Molecule 20: 30S ribosomal protein S20



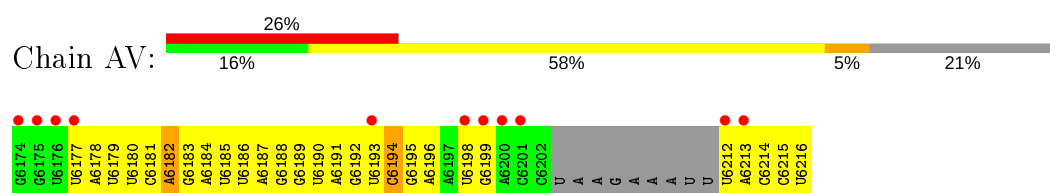
• Molecule 21: 30S ribosomal protein Thx



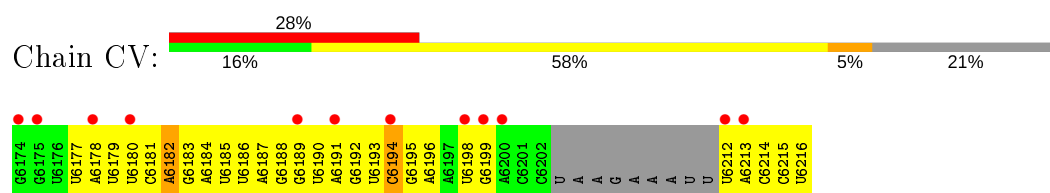
- Molecule 21: 30S ribosomal protein Thx



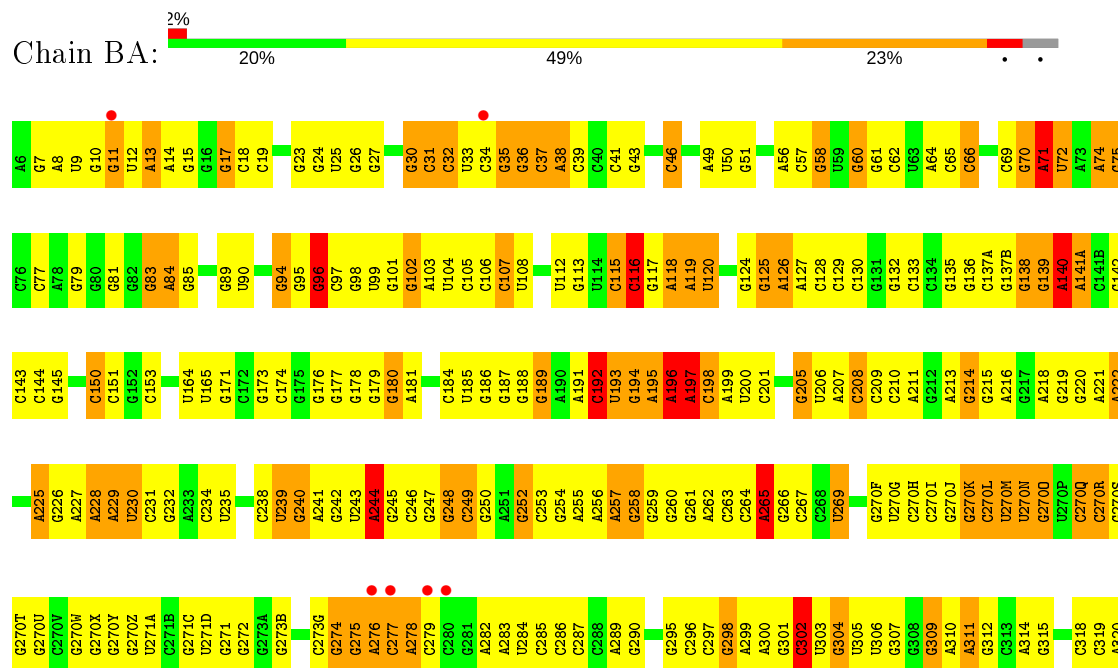
- Molecule 22: RNA (34-MER)



- Molecule 22: RNA (34-MER)

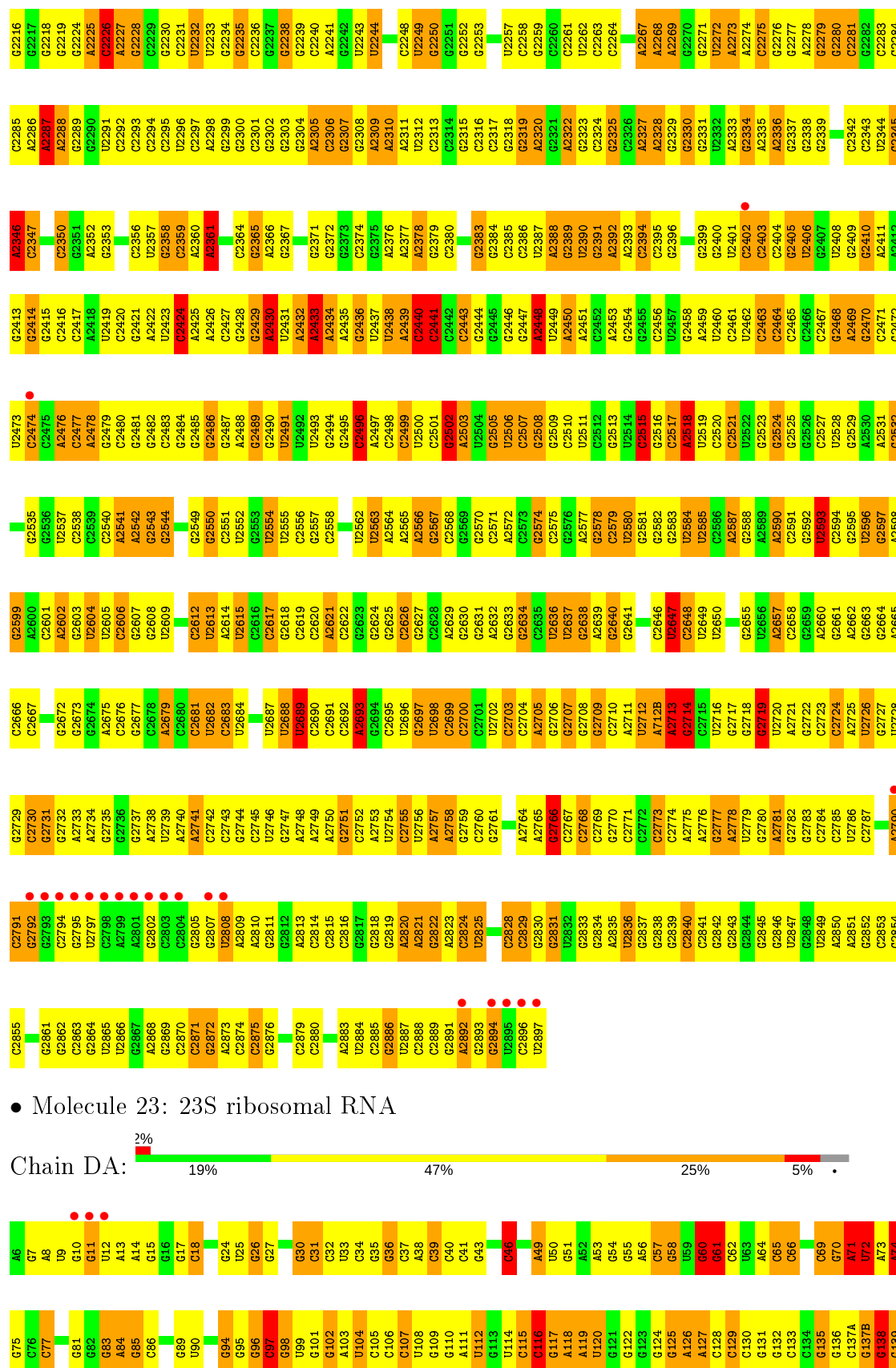


- Molecule 23: 23S ribosomal RNA





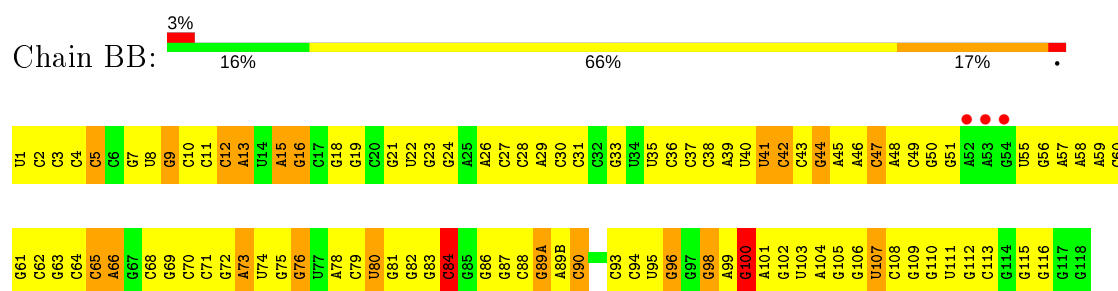




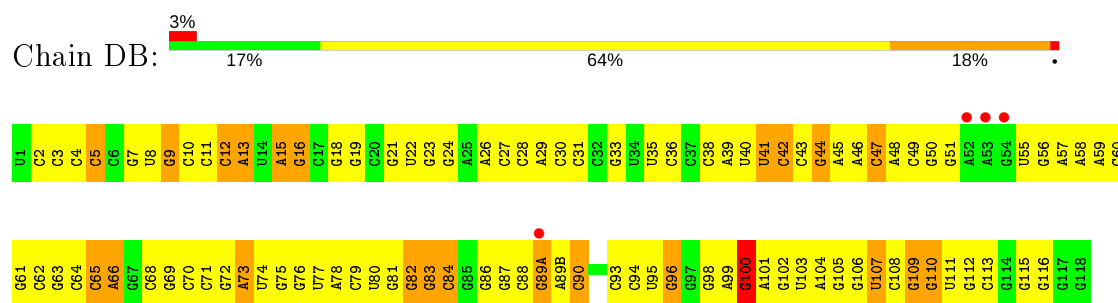
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U1002	G1002	A941	G869	U807	G745	A616	U554	G489	A416	G351	G281	A251	A190
A1003	G1003	G942	A870	G809	U747	G617	G556	G491	C417	G352	A282	G252	A191
G1004	U871	U943	U871	G748	G680	C618A	U557	A492		G353	U284	G253	C192
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A2051	U1991	C1926	U1851	A1786	U1706	G1642	C1515	C1451		A1393	C1333	G1270	U
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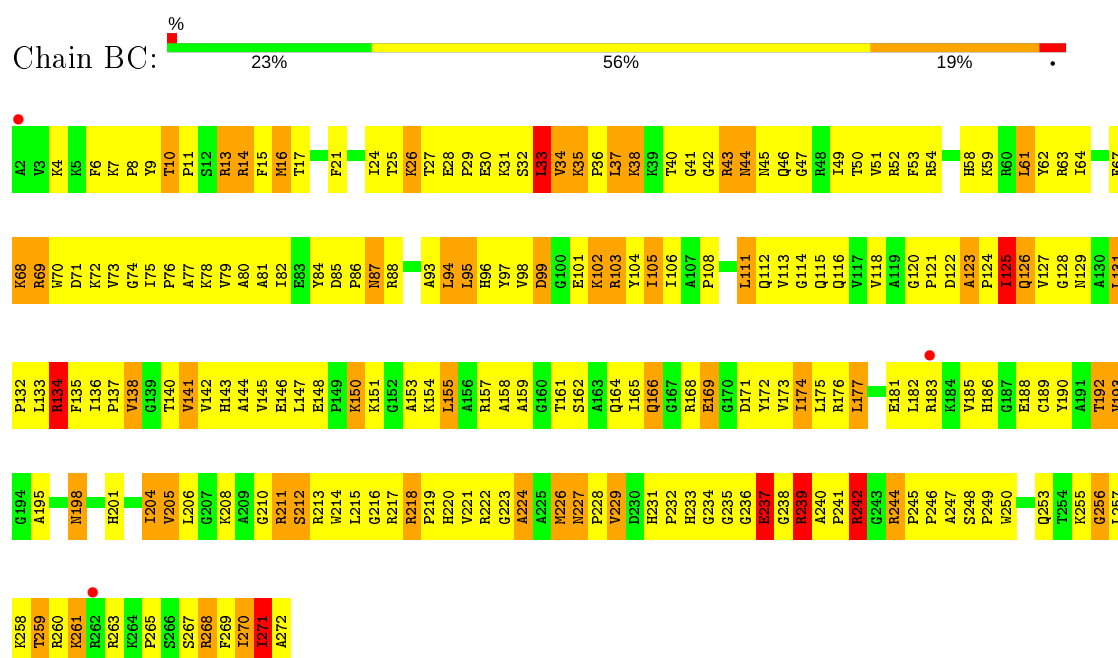




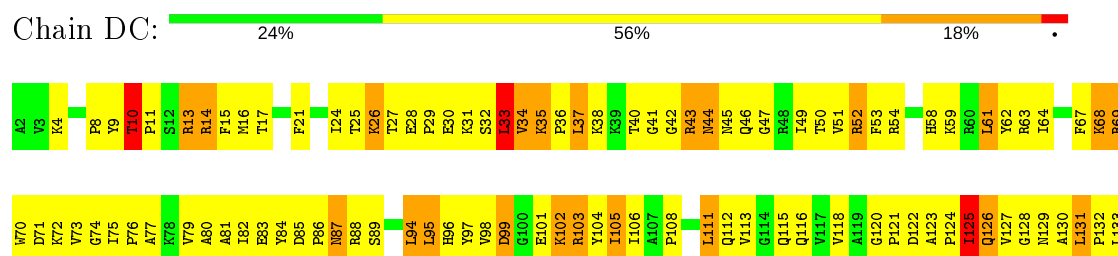
• Molecule 24: 5S ribosomal RNA

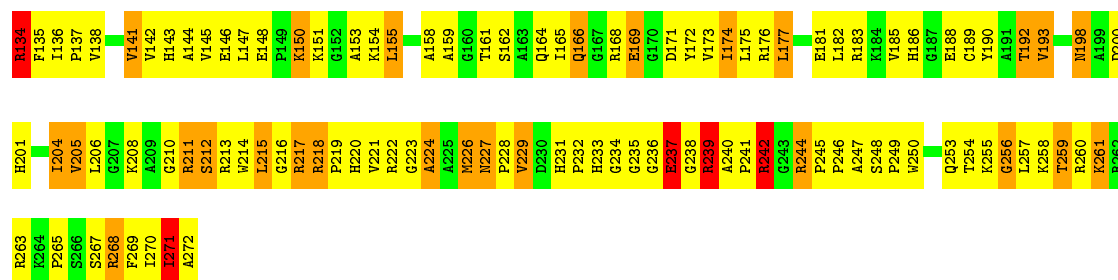


• Molecule 25: 50S ribosomal protein L2

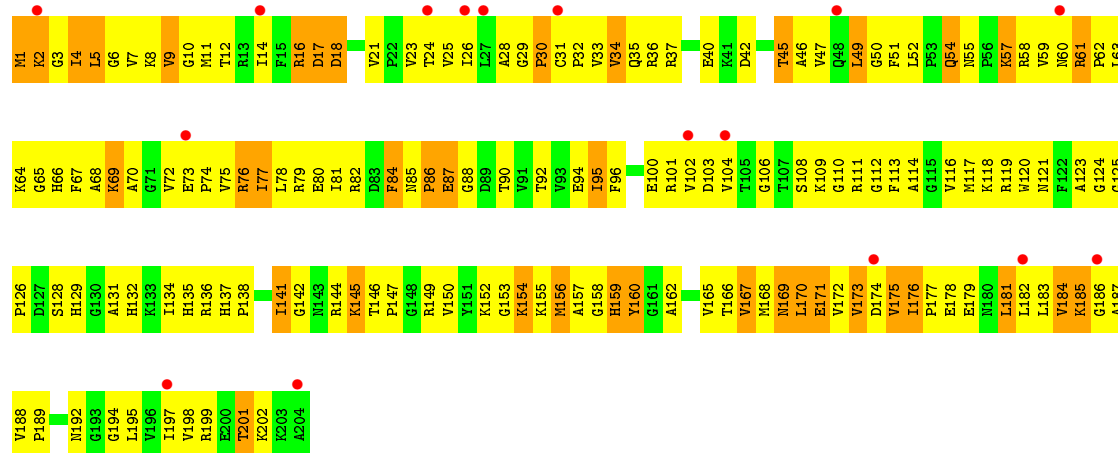


• Molecule 25: 50S ribosomal protein L2

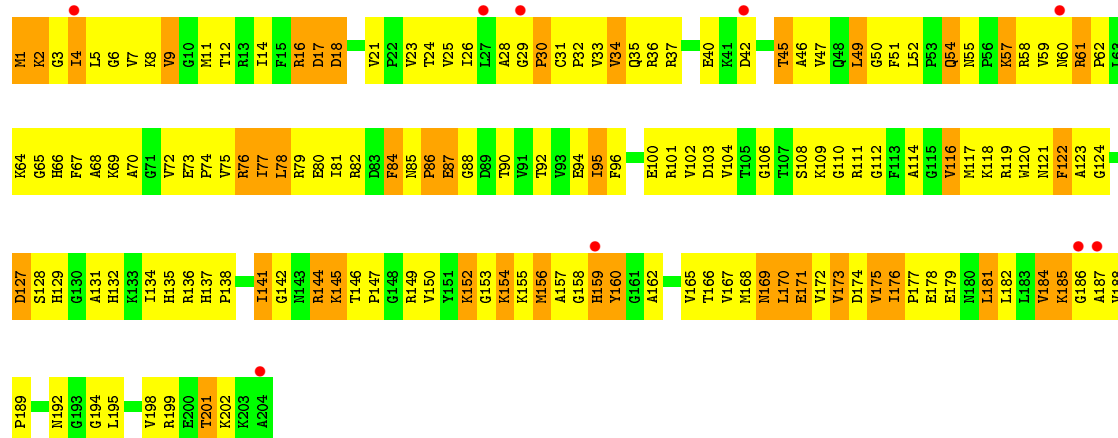




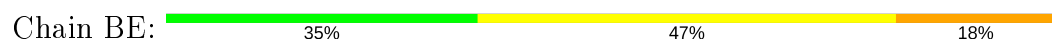
• Molecule 26: 50S ribosomal protein L3

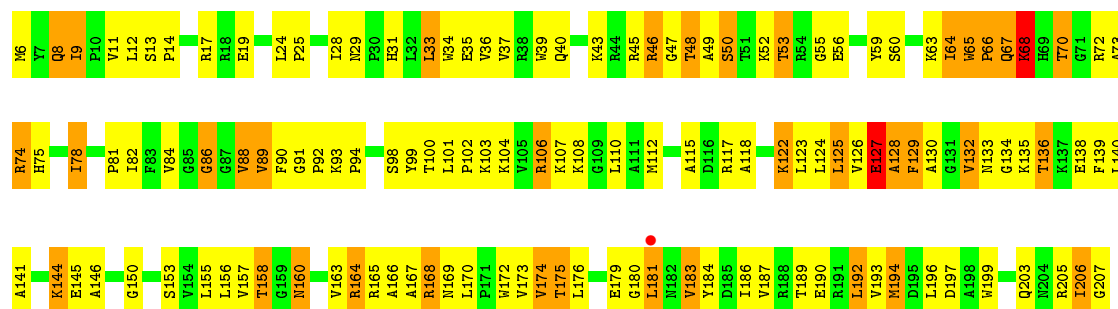


• Molecule 26: 50S ribosomal protein L3

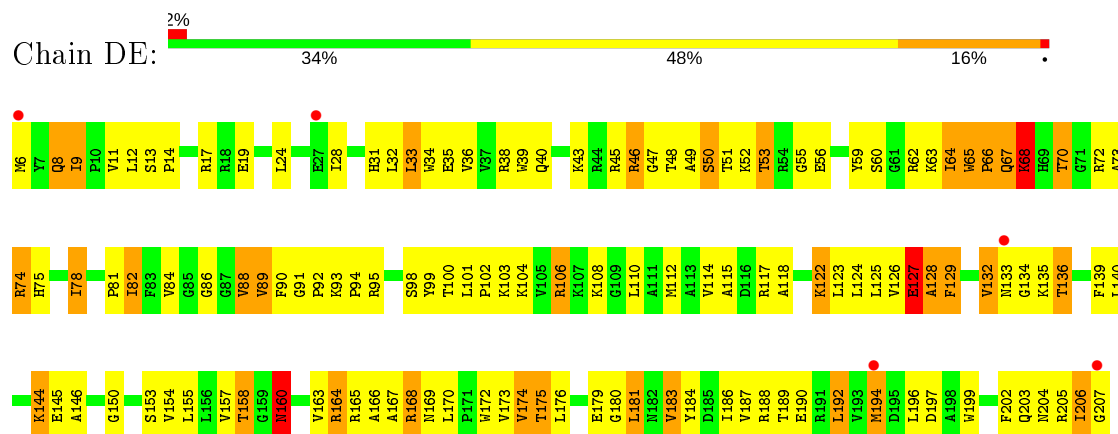


• Molecule 27: 50S ribosomal protein L4

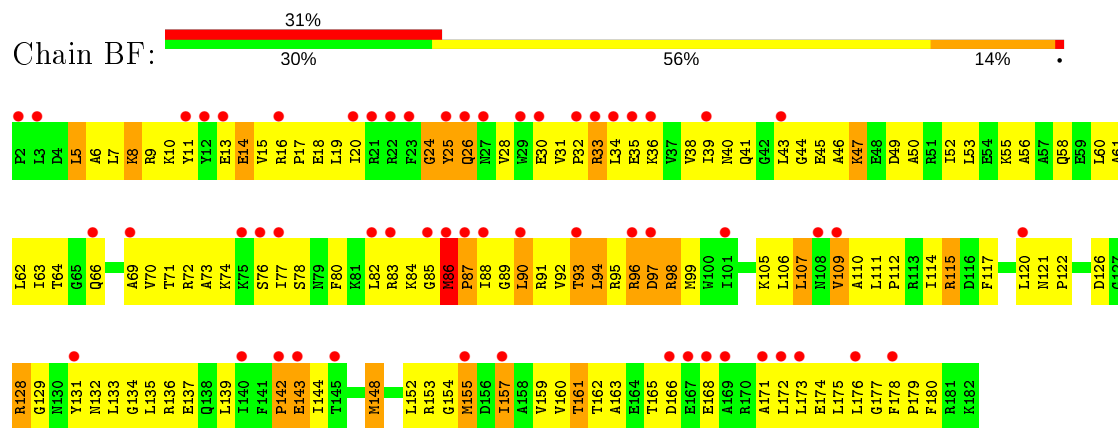




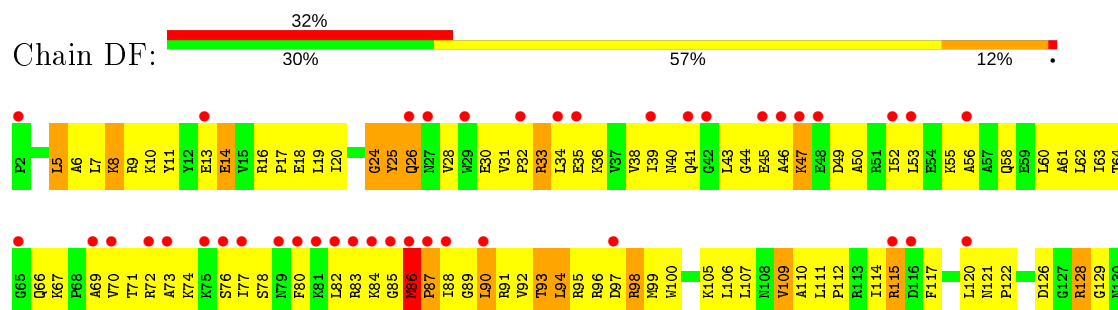
• Molecule 27: 50S ribosomal protein L4

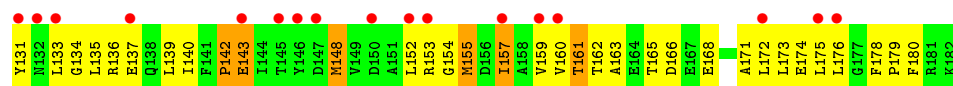


• Molecule 28: 50S ribosomal protein L5

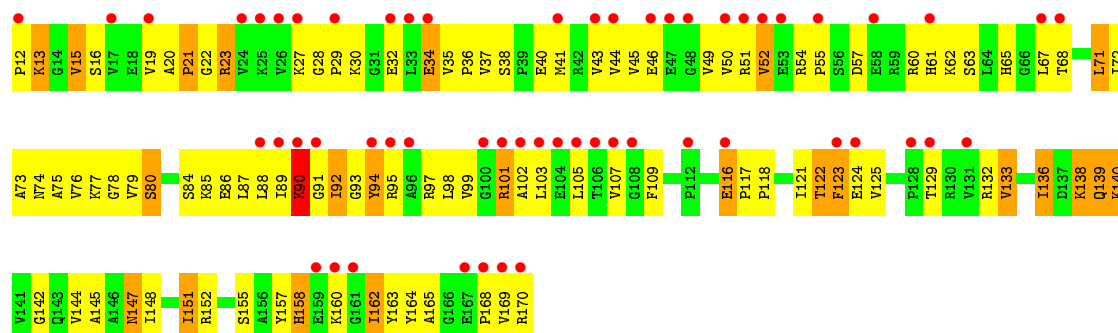


• Molecule 28: 50S ribosomal protein L5

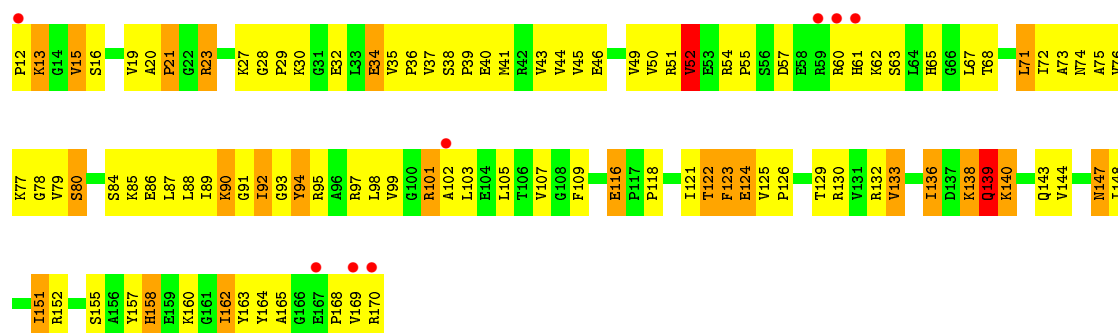




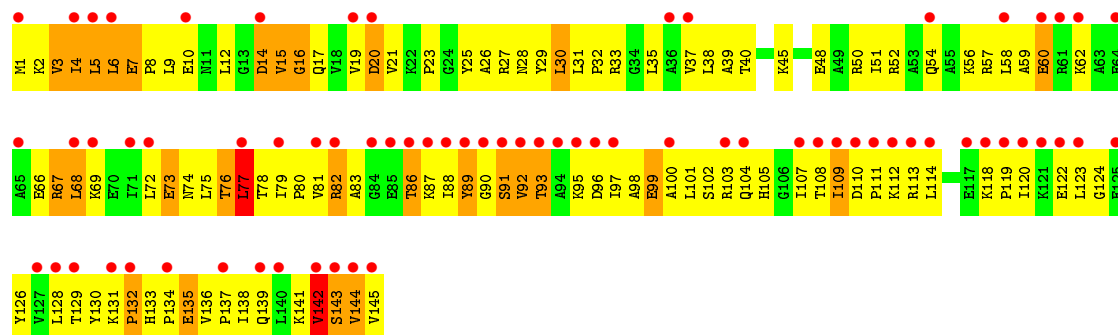
- Molecule 29: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L6

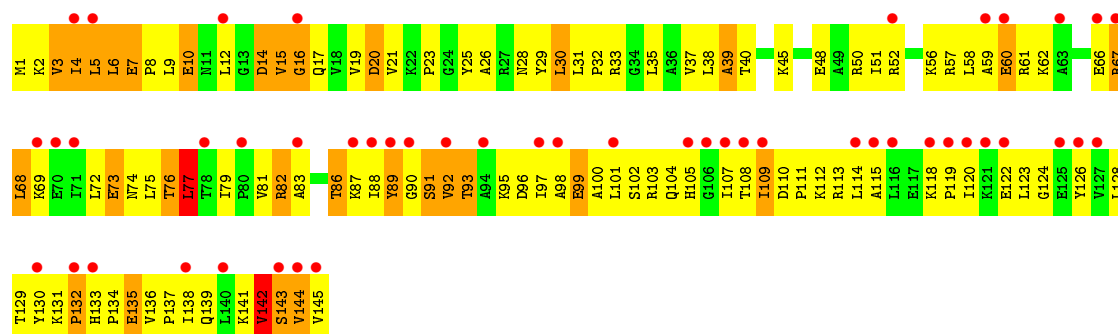


- Molecule 30: 50S ribosomal protein L9

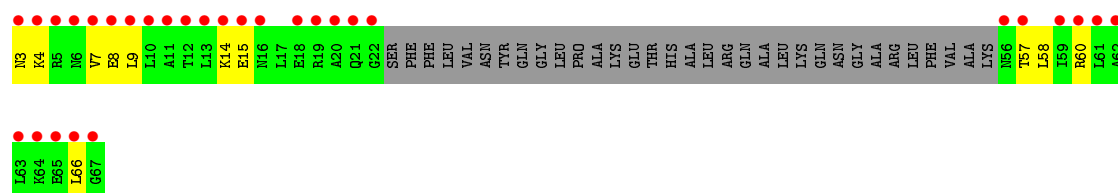


- Molecule 30: 50S ribosomal protein L9

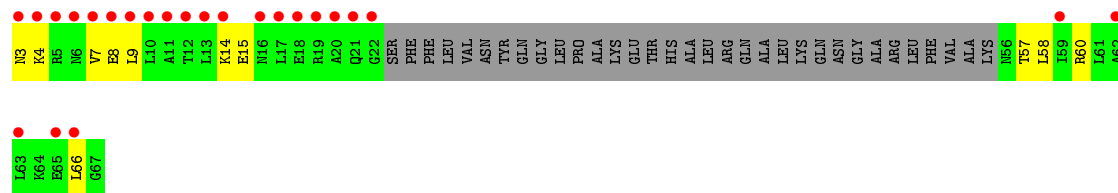
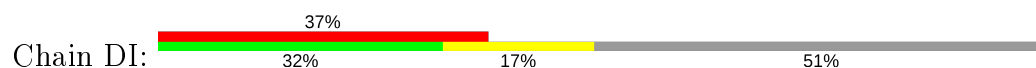




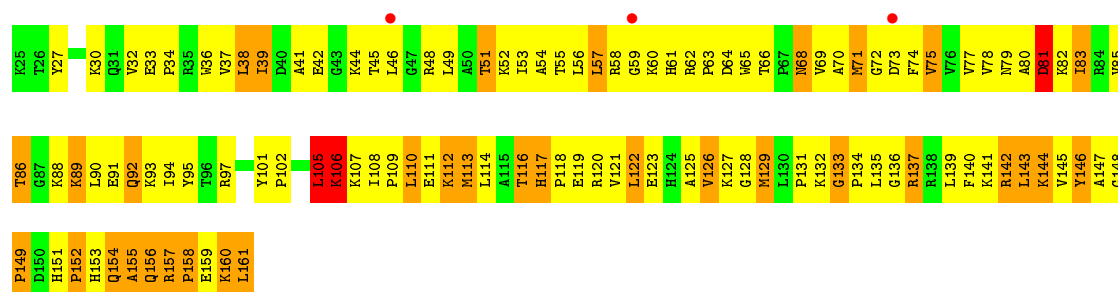
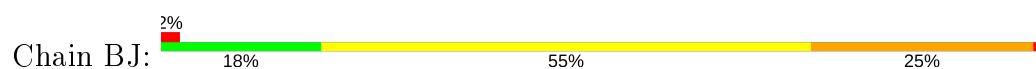
• Molecule 31: 50S ribosomal protein L10



• Molecule 31: 50S ribosomal protein L10

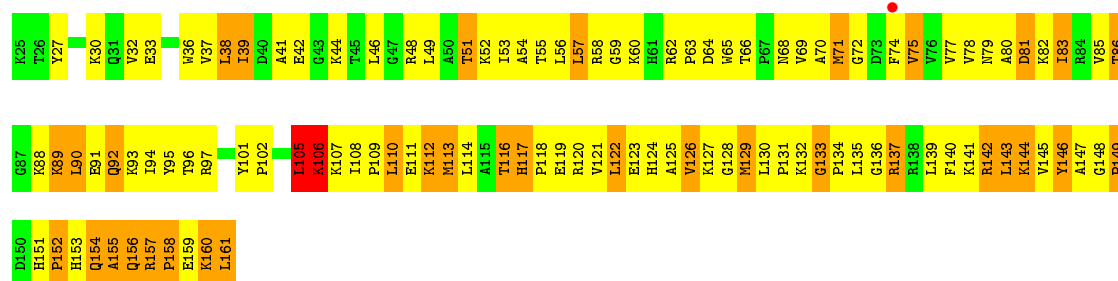


• Molecule 32: 50S ribosomal protein L13



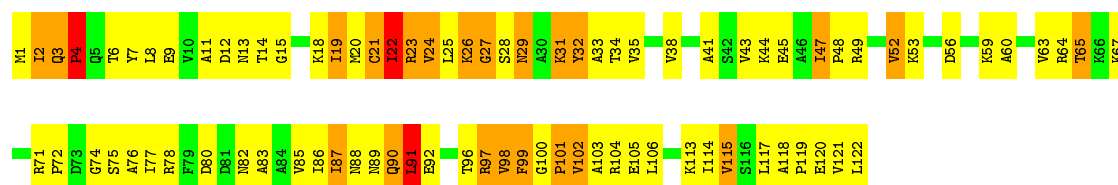
• Molecule 32: 50S ribosomal protein L13





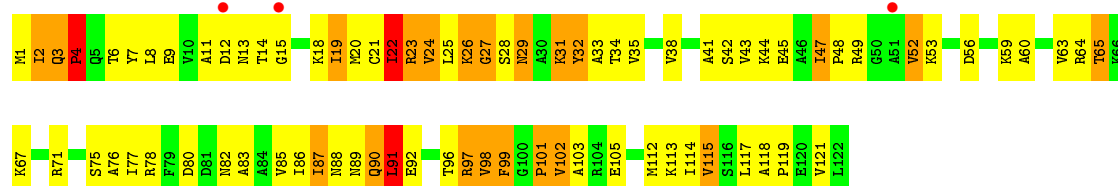
• Molecule 33: 50S ribosomal protein L14

Chain BK: 30% 49% 18%



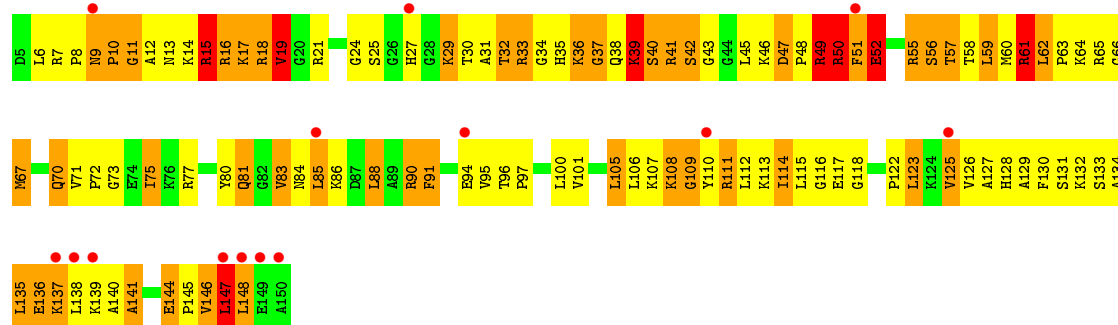
• Molecule 33: 50S ribosomal protein L14

Chain DK: 2% 34% 46% 17%



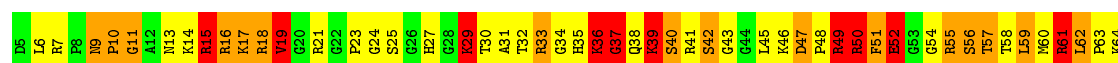
• Molecule 34: 50S ribosomal protein L15

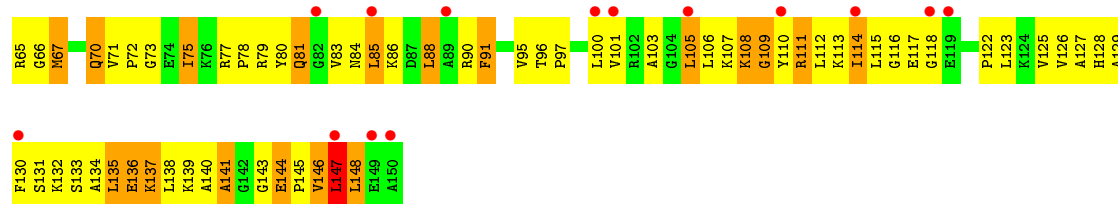
Chain BL: 10% 23% 42% 30% 5%



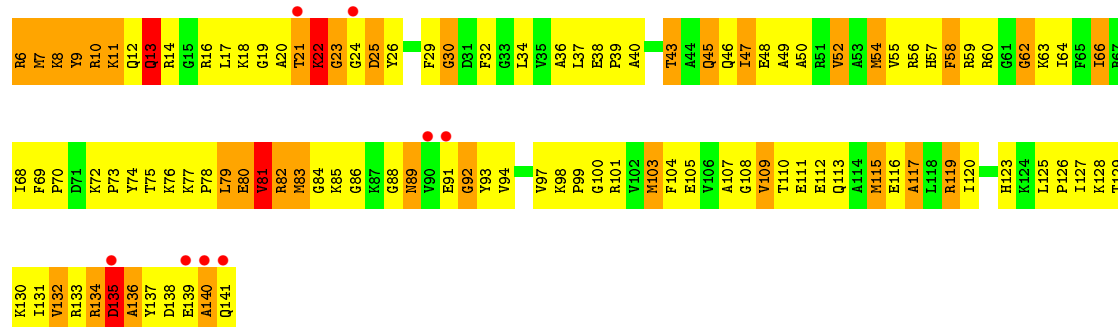
• Molecule 34: 50S ribosomal protein L15

Chain DL: 10% 21% 48% 24% 8%

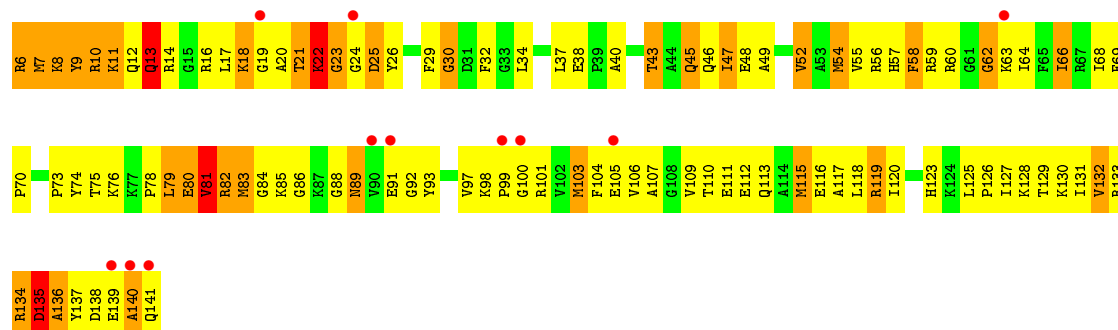




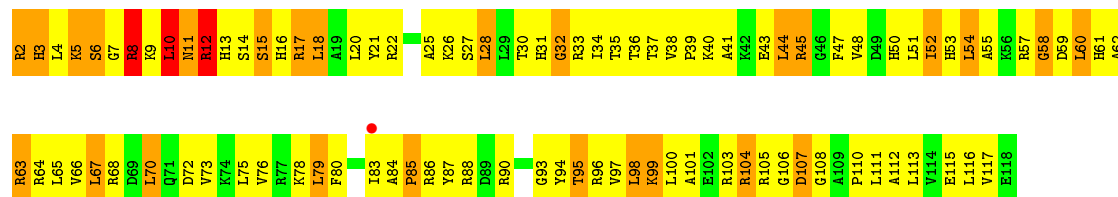
• Molecule 35: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L16

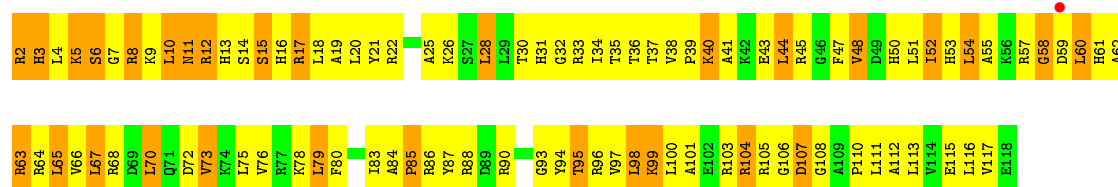


• Molecule 36: 50S ribosomal protein L17

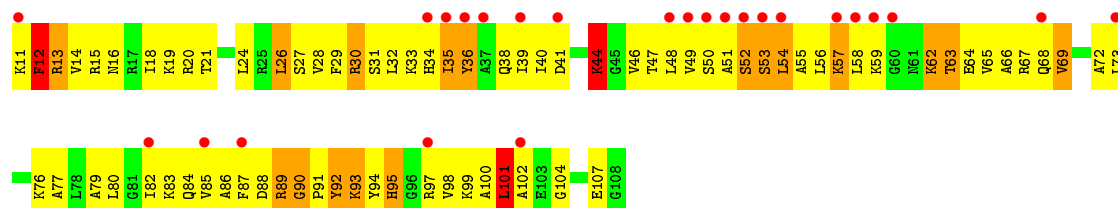


• Molecule 36: 50S ribosomal protein L17

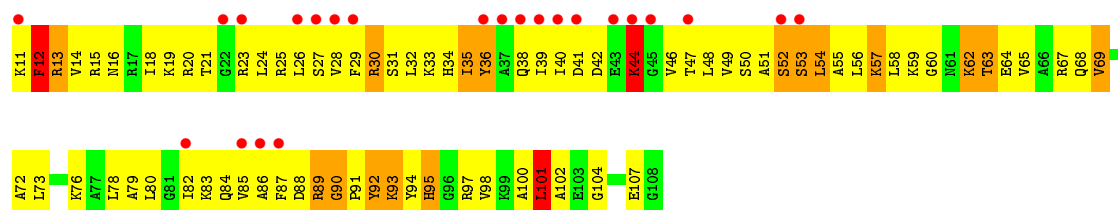




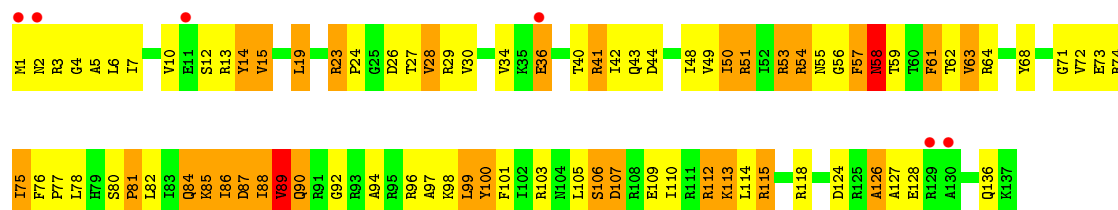
• Molecule 37: 50S ribosomal protein L18



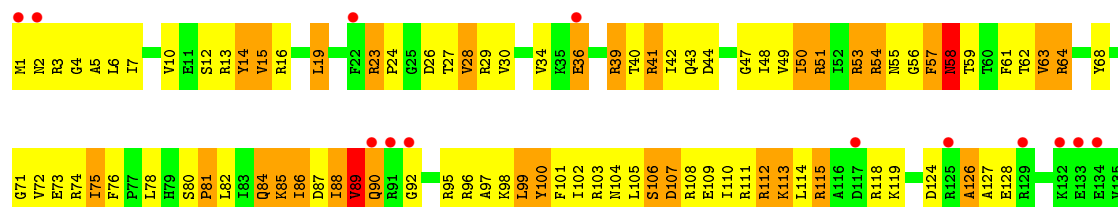
• Molecule 37: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L19



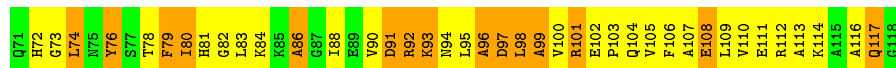
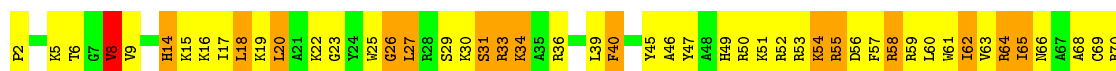
• Molecule 38: 50S ribosomal protein L19





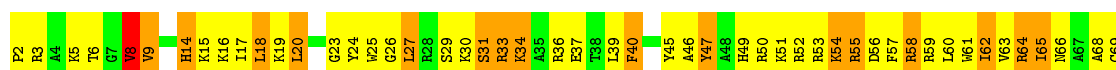
- Molecule 39: 50S ribosomal protein L20

Chain BQ: 23% 50% 26%



- Molecule 39: 50S ribosomal protein L20

Chain DQ: 23% 51% 25%



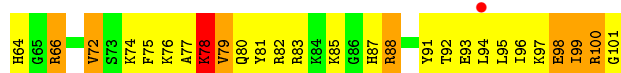
- Molecule 40: 50S ribosomal protein L21

Chain BR: 29% 48% 23%



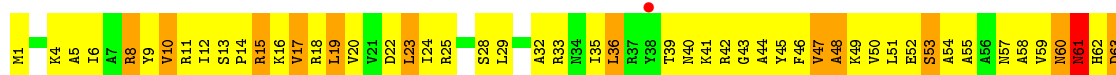
- Molecule 40: 50S ribosomal protein L21

Chain DR: 3% 24% 51% 24%



- Molecule 41: 50S ribosomal protein L22

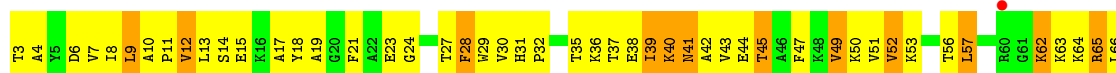
Chain BS: 2% 28% 55% 16%



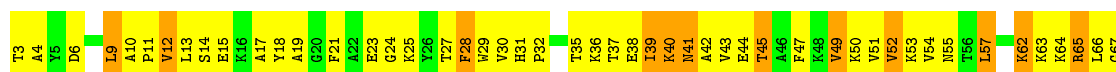
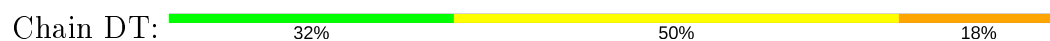
• Molecule 41: 50S ribosomal protein L22



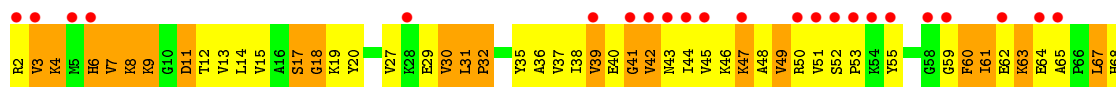
• Molecule 42: 50S ribosomal protein L23



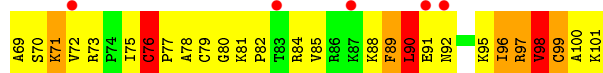
• Molecule 42: 50S ribosomal protein L23

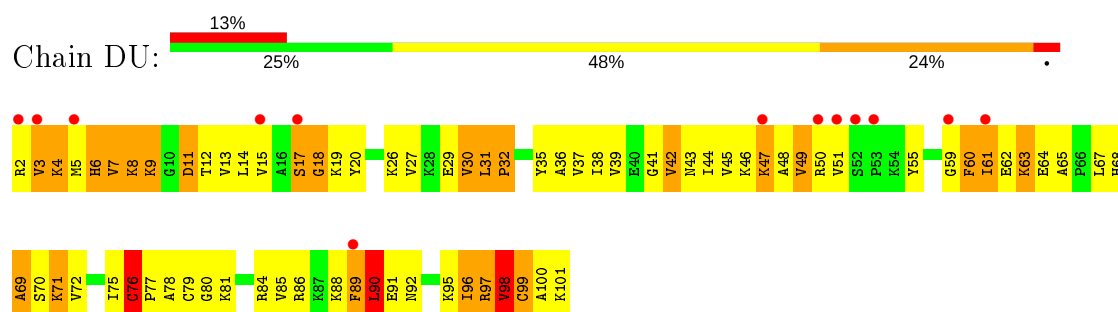


• Molecule 43: 50S ribosomal protein L24

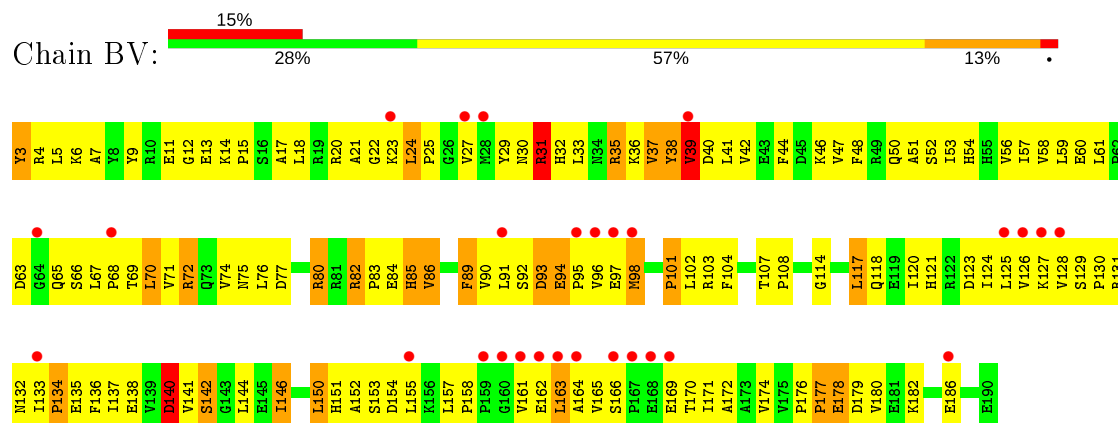


• Molecule 43: 50S ribosomal protein L24

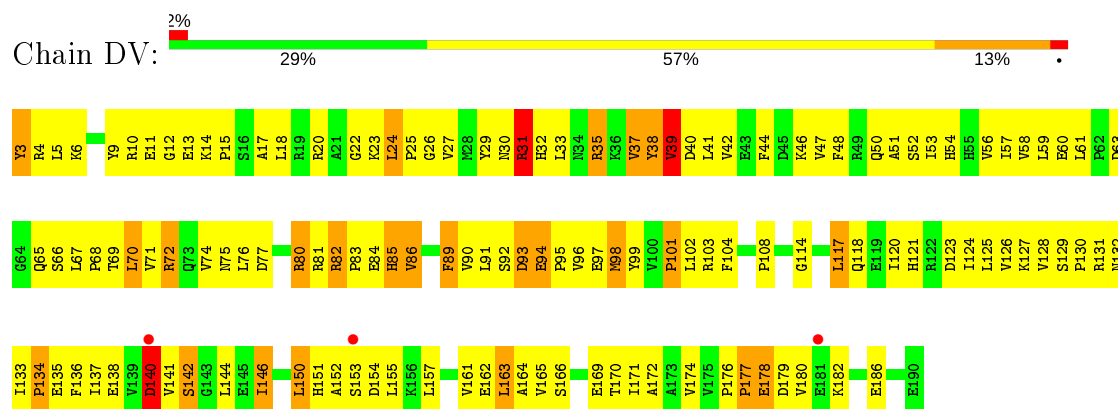




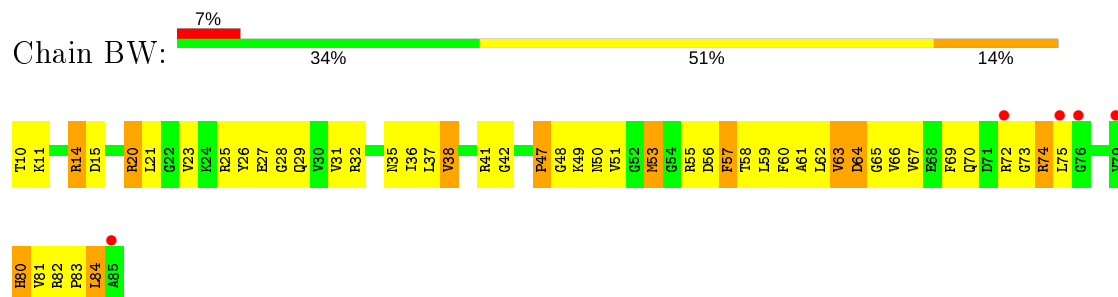
- Molecule 44: 50S ribosomal protein L25



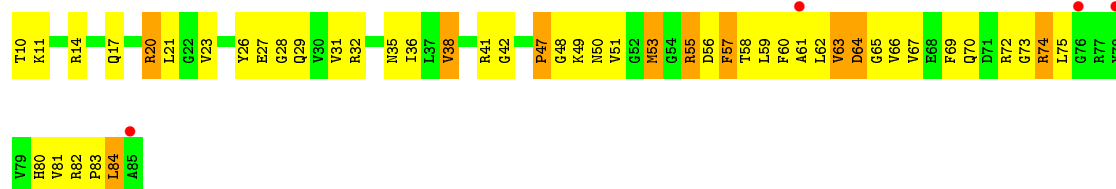
- Molecule 44: 50S ribosomal protein L25



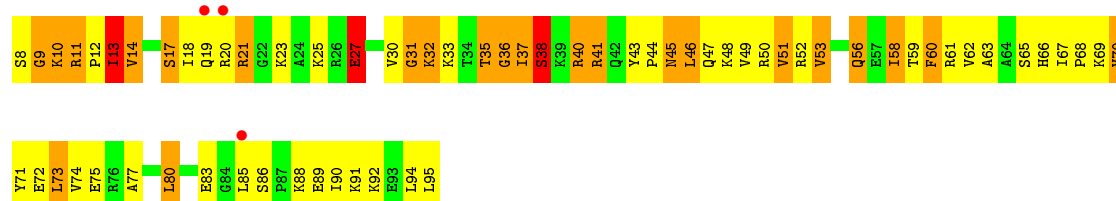
- Molecule 45: 50S ribosomal protein L27



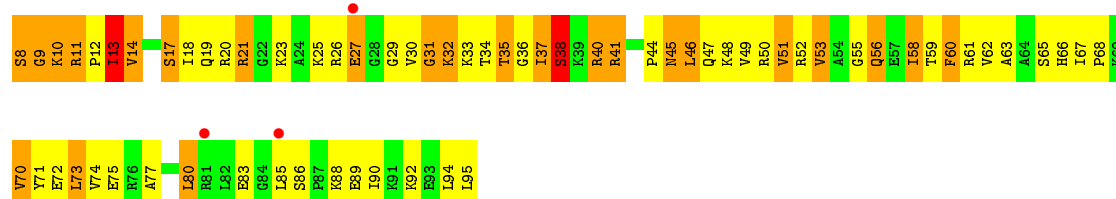
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29

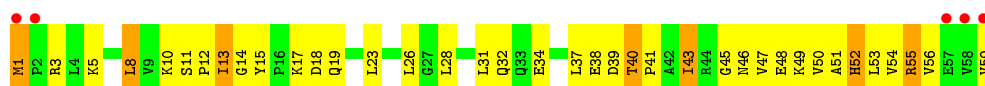


- Molecule 47: 50S ribosomal protein L29

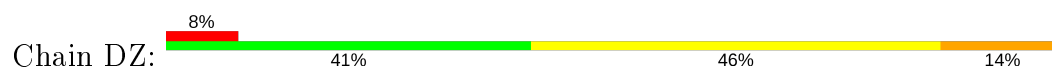


- Molecule 48: 50S ribosomal protein L30

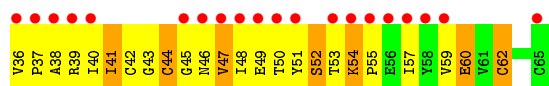




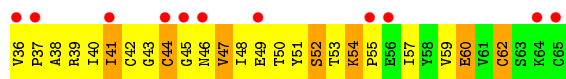
- Molecule 48: 50S ribosomal protein L30



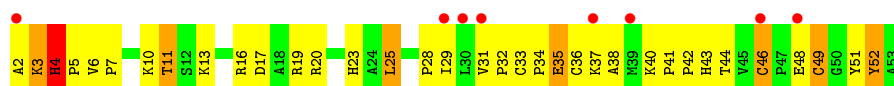
- Molecule 49: 50S ribosomal protein L31



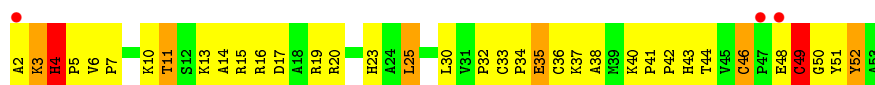
- Molecule 49: 50S ribosomal protein L31



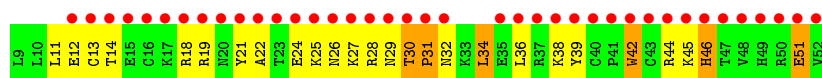
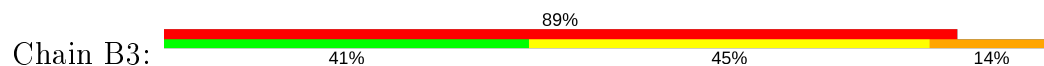
- Molecule 50: 50S ribosomal protein L32



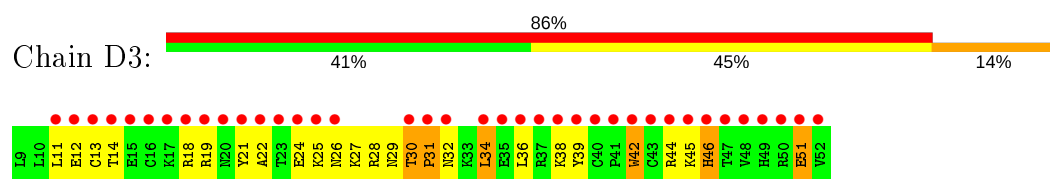
- Molecule 50: 50S ribosomal protein L32



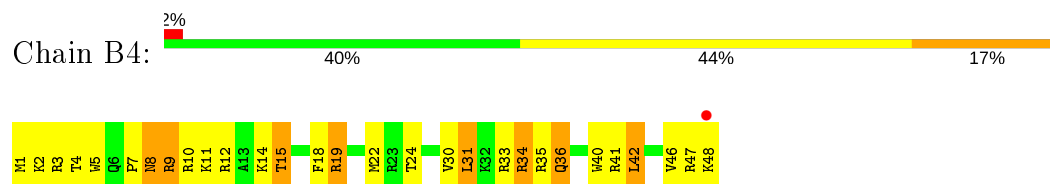
- Molecule 51: 50S ribosomal protein L33



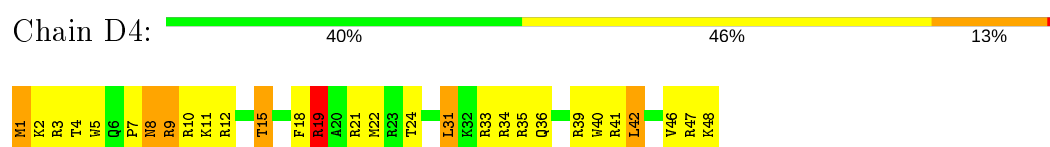
- Molecule 51: 50S ribosomal protein L33



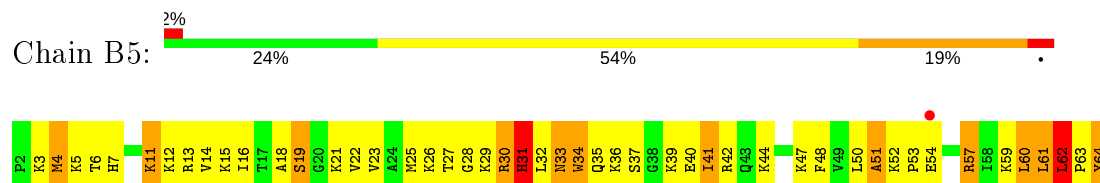
- Molecule 52: 50S ribosomal protein L34



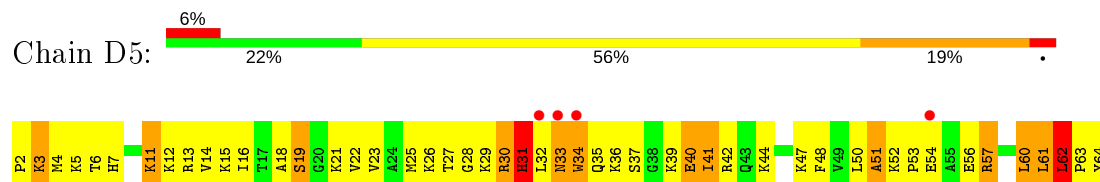
- Molecule 52: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.69Å 451.66Å 614.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 3.40 49.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.52-3.40) 97.6 (49.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, CNS	Depositor
R, R_{free}	0.228 , 0.266 0.224 , 0.262	Depositor DCC
R_{free} test set	7701 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	282142	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.63	4/36238 (0.0%)	1.02	99/56561 (0.2%)
1	CA	0.57	0/36238	0.96	75/56561 (0.1%)
2	AB	0.31	0/1936	0.51	0/2609
2	CB	0.28	0/1936	0.50	0/2609
3	AC	0.31	0/1637	0.47	0/2205
3	CC	0.29	0/1637	0.47	0/2205
4	AD	0.41	0/1733	0.59	0/2318
4	CD	0.34	0/1733	0.56	0/2318
5	AE	0.41	0/1172	0.61	0/1576
5	CE	0.36	0/1172	0.57	0/1576
6	AF	0.33	0/856	0.57	0/1154
6	CF	0.37	0/856	0.59	0/1154
7	AG	0.27	0/1276	0.46	0/1709
7	CG	0.27	0/1276	0.46	0/1709
8	AH	0.39	0/1136	0.61	0/1527
8	CH	0.33	0/1136	0.58	0/1527
9	AI	0.29	0/1029	0.45	0/1378
9	CI	0.27	0/1029	0.45	0/1378
10	AJ	0.28	0/808	0.48	0/1085
10	CJ	0.27	0/808	0.46	0/1085
11	AK	0.39	0/900	0.59	0/1213
11	CK	0.41	0/900	0.61	0/1213
12	AL	0.47	0/987	0.70	1/1320 (0.1%)
12	CL	0.44	0/987	0.68	0/1320
13	AM	0.25	0/939	0.44	0/1258
13	CM	0.24	0/939	0.44	0/1258
14	AN	0.31	0/501	0.50	0/664
14	CN	0.31	0/501	0.52	0/664
15	AO	0.39	0/745	0.57	0/992
15	CO	0.37	0/745	0.56	0/992
16	AP	0.42	0/717	0.62	0/963
16	CP	0.34	0/717	0.59	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.60	0/1117
17	CQ	0.37	0/837	0.56	0/1117
18	AR	0.38	0/579	0.61	0/768
18	CR	0.37	0/579	0.60	0/768
19	AS	0.25	0/643	0.43	0/865
19	CS	0.25	0/643	0.42	0/865
20	AT	0.38	0/764	0.57	0/1006
20	CT	0.33	0/764	0.54	0/1006
21	AU	0.23	0/213	0.43	0/277
21	CU	0.24	0/213	0.42	0/277
22	AV	0.43	0/802	0.68	0/1245
22	CV	0.43	0/802	0.69	0/1245
23	BA	1.07	153/66570 (0.2%)	1.48	1344/103918 (1.3%)
23	DA	1.19	253/66575 (0.4%)	1.59	1756/103930 (1.7%)
24	BB	0.58	0/2853	1.00	9/4451 (0.2%)
24	DB	0.59	0/2853	1.04	3/4451 (0.1%)
25	BC	0.71	1/2155 (0.0%)	0.90	3/2905 (0.1%)
25	DC	0.74	1/2155 (0.0%)	0.91	5/2905 (0.2%)
26	BD	0.58	0/1597	0.77	0/2153
26	DD	0.62	1/1597 (0.1%)	0.81	0/2153
27	BE	0.63	0/1622	0.77	0/2194
27	DE	0.67	0/1622	0.78	0/2194
28	BF	0.28	0/1500	0.49	0/2017
28	DF	0.28	0/1500	0.49	0/2017
29	BG	0.32	0/1246	0.58	0/1682
29	DG	0.44	0/1246	0.64	0/1682
30	BH	0.33	0/1148	0.56	0/1552
30	DH	0.38	0/1148	0.56	0/1552
31	BI	0.25	0/252	0.44	0/333
31	DI	0.27	0/252	0.46	0/333
32	BJ	0.56	0/1124	0.75	0/1515
32	DJ	0.59	0/1124	0.76	0/1515
33	BK	0.57	0/942	0.76	0/1268
33	DK	0.61	0/942	0.77	0/1268
34	BL	0.74	1/1131 (0.1%)	1.01	1/1504 (0.1%)
34	DL	0.75	2/1131 (0.2%)	1.03	5/1504 (0.3%)
35	BM	0.61	0/1099	0.83	2/1468 (0.1%)
35	DM	0.60	0/1099	0.83	1/1468 (0.1%)
36	BN	0.59	0/974	0.85	0/1302
36	DN	0.59	0/974	0.83	1/1302 (0.1%)
37	BO	0.36	0/779	0.58	0/1036
37	DO	0.39	0/779	0.61	0/1036
38	BP	0.50	0/1158	0.68	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.51	0/1158	0.69	0/1544
39	BQ	0.63	0/970	0.81	0/1290
39	DQ	0.67	0/970	0.81	0/1290
40	BR	0.58	0/790	0.73	1/1057 (0.1%)
40	DR	0.61	0/790	0.74	1/1057 (0.1%)
41	BS	0.63	0/902	0.78	0/1209
41	DS	0.66	0/902	0.76	0/1209
42	BT	0.64	0/740	0.79	0/993
42	DT	0.74	0/740	0.84	0/993
43	BU	0.53	0/789	0.76	0/1051
43	DU	0.56	0/789	0.76	0/1051
44	BV	0.36	0/1524	0.57	0/2068
44	DV	0.38	0/1524	0.57	0/2068
45	BW	0.50	0/613	0.71	0/816
45	DW	0.52	0/613	0.72	0/816
46	BX	0.73	0/702	0.98	2/932 (0.2%)
46	DX	0.82	0/702	1.04	2/932 (0.2%)
47	BY	0.55	0/523	0.87	1/690 (0.1%)
47	DY	0.72	0/523	0.98	3/690 (0.4%)
48	BZ	0.52	0/473	0.68	0/634
48	DZ	0.50	0/473	0.65	0/634
49	B1	0.23	0/229	0.40	0/309
49	D1	0.22	0/229	0.41	0/309
50	B2	0.61	0/419	0.80	0/567
50	D2	0.58	0/419	0.79	0/567
51	B3	0.28	0/388	0.46	0/518
51	D3	0.27	0/388	0.46	0/518
52	B4	0.72	0/427	0.89	0/561
52	D4	0.84	0/427	1.05	1/561 (0.2%)
53	B5	0.68	0/516	0.88	0/679
53	D5	0.69	0/516	0.88	1/679 (0.1%)
All	All	0.85	416/305211 (0.1%)	1.21	3317/456064 (0.7%)

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
25	DC	0	1
27	BE	0	1
27	DE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	BL	0	5
34	DL	0	5
35	BM	0	1
35	DM	0	1
36	BN	0	1
36	DN	0	1
39	BQ	0	2
39	DQ	0	2
All	All	0	21

The worst 5 of 416 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DA	774	A	N9-C4	-13.87	1.29	1.37
23	DA	1332	G	N9-C4	-11.99	1.28	1.38
23	DA	1602	U	C4-O4	11.31	1.32	1.23
23	BA	1332	G	N9-C4	-11.02	1.29	1.38
23	DA	2249	U	C4-O4	10.67	1.32	1.23

The worst 5 of 3317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DA	761	A	N1-C6-N6	30.82	137.09	118.60
23	BA	761	A	N1-C6-N6	25.08	133.65	118.60
23	DA	1332	G	N3-C4-N9	-24.42	111.35	126.00
23	DA	1332	G	N3-C4-C5	23.85	140.52	128.60
23	BA	1332	G	N3-C4-N9	-22.46	112.52	126.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BE	47	GLY	Peptide
34	BL	29	LYS	Peptide
34	BL	37	GLY	Peptide
34	BL	39	LYS	Peptide
34	BL	9	ASN	Peptide

5.2 Too-close contacts ⓘ

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	32372	0	16339	1680	0
1	CA	32372	0	16339	1784	0
2	AB	1901	0	1951	173	0
2	CB	1901	0	1951	180	0
3	AC	1613	0	1677	180	0
3	CC	1613	0	1677	186	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1764	182	1
5	AE	1156	0	1213	141	0
5	CE	1156	0	1213	141	0
6	AF	843	0	857	96	1
6	CF	843	0	857	93	0
7	AG	1257	0	1296	95	0
7	CG	1257	0	1296	92	0
8	AH	1116	0	1177	133	0
8	CH	1116	0	1177	140	0
9	AI	1011	0	1043	100	0
9	CI	1011	0	1043	112	0
10	AJ	795	0	840	93	0
10	CJ	795	0	840	92	0
11	AK	885	0	904	76	0
11	CK	885	0	904	72	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	139	0
13	AM	929	0	987	83	0
13	CM	929	0	987	83	0
14	AN	492	0	530	49	0
14	CN	492	0	532	61	0
15	AO	734	0	771	66	0
15	CO	734	0	771	60	0
16	AP	701	0	720	96	0
16	CP	701	0	720	90	0
17	AQ	824	0	893	66	0
17	CQ	824	0	893	77	0
18	AR	574	0	644	70	0
18	CR	574	0	644	70	0
19	AS	630	0	652	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	60	0
20	AT	762	0	859	64	0
20	CT	762	0	859	70	0
21	AU	209	0	221	16	0
21	CU	209	0	221	17	0
22	AV	719	0	366	58	0
22	CV	719	0	366	57	0
23	BA	59440	0	29964	2618	0
23	DA	59442	0	29965	2593	0
24	BB	2551	0	1295	147	0
24	DB	2551	0	1295	148	0
25	BC	2105	0	2182	353	0
25	DC	2105	0	2182	347	0
26	BD	1564	0	1629	224	0
26	DD	1564	0	1629	224	0
27	BE	1587	0	1632	147	0
27	DE	1587	0	1632	155	0
28	BF	1475	0	1537	155	0
28	DF	1475	0	1537	150	0
29	BG	1223	0	1282	114	0
29	DG	1223	0	1282	121	0
30	BH	1133	0	1220	131	0
30	DH	1133	0	1220	133	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	170	0
32	DJ	1097	0	1168	158	0
33	BK	932	0	994	97	0
33	DK	932	0	994	100	0
34	BL	1114	0	1187	270	0
34	DL	1114	0	1187	279	0
35	BM	1079	0	1127	170	0
35	DM	1079	0	1127	172	0
36	BN	960	0	1021	153	0
36	DN	960	0	1021	142	0
37	BO	771	0	832	95	0
37	DO	771	0	832	100	0
38	BP	1144	0	1211	129	0
38	DP	1144	0	1211	132	0
39	BQ	953	0	1013	150	0
39	DQ	953	0	1013	155	0
40	BR	779	0	852	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	779	0	852	128	0
41	BS	891	0	951	106	0
41	DS	891	0	951	110	0
42	BT	726	0	778	88	0
42	DT	726	0	778	92	0
43	BU	776	0	870	138	0
43	DU	776	0	870	139	0
44	BV	1492	0	1513	174	0
44	DV	1492	0	1513	171	0
45	BW	605	0	628	71	0
45	DW	605	0	628	63	0
46	BX	695	0	764	112	0
46	DX	695	0	764	106	0
47	BY	521	0	575	81	0
47	DY	521	0	575	81	0
48	BZ	468	0	523	46	0
48	DZ	468	0	523	46	0
49	B1	226	0	225	23	0
49	D1	226	0	225	24	0
50	B2	405	0	420	61	0
50	D2	405	0	420	64	0
51	B3	381	0	391	25	0
51	D3	381	0	391	26	0
52	B4	419	0	467	50	0
52	D4	419	0	467	48	0
53	B5	508	0	576	111	0
53	D5	508	0	576	110	0
54	AA	163	0	0	0	0
54	AD	1	0	0	0	0
54	AV	4	0	0	0	0
54	B2	1	0	0	0	0
54	BA	408	0	0	0	0
54	BB	17	0	0	0	0
54	BK	1	0	0	0	0
54	CA	140	0	0	0	0
54	CP	1	0	0	0	0
54	CV	1	0	0	0	0
54	D2	1	0	0	0	0
54	D4	1	0	0	0	0
54	DA	436	0	0	0	0
54	DB	17	0	0	0	0
54	DE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DG	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	282142	0	191729	18333	1

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 39.

The worst 5 of 18333 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)
34:DL:59:LEU:HA	34:DL:61:ARG:NE	1.55	1.20
34:DL:57:THR:HG23	34:DL:59:LEU:HD22	1.22	1.20
35:BM:81:VAL:O	35:BM:82:ARG:HG2	1.39	1.19
34:BL:57:THR:HG23	34:BL:59:LEU:HD22	1.21	1.19
52:D4:8:ASN:C	52:D4:8:ASN:HD22	1.42	1.18

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:15:ASP:OD1	4:CD:20:TYR:OH[4_555]	2.18	0.02

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	232/234 (99%)	172 (74%)	40 (17%)	20 (9%)	1 5
2	CB	232/234 (99%)	173 (75%)	38 (16%)	21 (9%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	136 (67%)	43 (21%)	25 (12%)	0	2
3	CC	204/206 (99%)	134 (66%)	45 (22%)	25 (12%)	0	2
4	AD	206/208 (99%)	152 (74%)	38 (18%)	16 (8%)	1	6
4	CD	206/208 (99%)	151 (73%)	40 (19%)	15 (7%)	1	7
5	AE	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1	5
5	CE	149/151 (99%)	104 (70%)	34 (23%)	11 (7%)	1	7
6	AF	99/101 (98%)	71 (72%)	17 (17%)	11 (11%)	0	3
6	CF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	0	4
7	AG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	4	22
7	CG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	4	22
8	AH	136/138 (99%)	97 (71%)	29 (21%)	10 (7%)	1	7
8	CH	136/138 (99%)	98 (72%)	28 (21%)	10 (7%)	1	7
9	AI	125/127 (98%)	91 (73%)	31 (25%)	3 (2%)	6	28
9	CI	125/127 (98%)	89 (71%)	32 (26%)	4 (3%)	4	22
10	AJ	96/98 (98%)	72 (75%)	20 (21%)	4 (4%)	3	18
10	CJ	96/98 (98%)	74 (77%)	18 (19%)	4 (4%)	3	18
11	AK	117/119 (98%)	83 (71%)	29 (25%)	5 (4%)	2	17
11	CK	117/119 (98%)	82 (70%)	30 (26%)	5 (4%)	2	17
12	AL	122/124 (98%)	78 (64%)	28 (23%)	16 (13%)	0	1
12	CL	122/124 (98%)	80 (66%)	27 (22%)	15 (12%)	0	2
13	AM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	21
13	CM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	21
14	AN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	13
14	CN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	13
15	AO	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1	5
15	CO	86/88 (98%)	61 (71%)	19 (22%)	6 (7%)	1	7
16	AP	81/83 (98%)	46 (57%)	24 (30%)	11 (14%)	0	1
16	CP	81/83 (98%)	46 (57%)	25 (31%)	10 (12%)	0	2
17	AQ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	7
17	CQ	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	1	10
18	AR	68/70 (97%)	40 (59%)	19 (28%)	9 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	68/70 (97%)	41 (60%)	18 (26%)	9 (13%)	0	1
19	AS	76/78 (97%)	51 (67%)	21 (28%)	4 (5%)	2	13
19	CS	76/78 (97%)	50 (66%)	21 (28%)	5 (7%)	1	8
20	AT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	7
20	CT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	7
21	AU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	16
21	CU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	16
25	BC	269/271 (99%)	213 (79%)	36 (13%)	20 (7%)	1	7
25	DC	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	7
26	BD	202/204 (99%)	154 (76%)	34 (17%)	14 (7%)	1	8
26	DD	202/204 (99%)	155 (77%)	32 (16%)	15 (7%)	1	7
27	BE	200/202 (99%)	152 (76%)	32 (16%)	16 (8%)	1	6
27	DE	200/202 (99%)	155 (78%)	30 (15%)	15 (8%)	1	7
28	BF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	8
28	DF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	8
29	BG	157/159 (99%)	112 (71%)	35 (22%)	10 (6%)	1	9
29	DG	157/159 (99%)	111 (71%)	36 (23%)	10 (6%)	1	9
30	BH	143/145 (99%)	95 (66%)	29 (20%)	19 (13%)	0	1
30	DH	143/145 (99%)	91 (64%)	31 (22%)	21 (15%)	0	1
31	BI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
31	DI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
32	BJ	135/137 (98%)	97 (72%)	26 (19%)	12 (9%)	1	5
32	DJ	135/137 (98%)	97 (72%)	24 (18%)	14 (10%)	0	3
33	BK	120/122 (98%)	100 (83%)	11 (9%)	9 (8%)	1	7
33	DK	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	8
34	BL	144/146 (99%)	87 (60%)	31 (22%)	26 (18%)	0	0
34	DL	144/146 (99%)	86 (60%)	35 (24%)	23 (16%)	0	0
35	BM	134/136 (98%)	86 (64%)	28 (21%)	20 (15%)	0	1
35	DM	134/136 (98%)	86 (64%)	30 (22%)	18 (13%)	0	1
36	BN	115/117 (98%)	91 (79%)	13 (11%)	11 (10%)	0	4
36	DN	115/117 (98%)	90 (78%)	15 (13%)	10 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	96/98 (98%)	57 (59%)	23 (24%)	16 (17%)	0	0
37	DO	96/98 (98%)	54 (56%)	25 (26%)	17 (18%)	0	0
38	BP	135/137 (98%)	101 (75%)	18 (13%)	16 (12%)	0	3
38	DP	135/137 (98%)	100 (74%)	19 (14%)	16 (12%)	0	3
39	BQ	114/116 (98%)	78 (68%)	22 (19%)	14 (12%)	0	2
39	DQ	114/116 (98%)	82 (72%)	20 (18%)	12 (10%)	0	3
40	BR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	4
40	DR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	4
41	BS	110/112 (98%)	88 (80%)	17 (16%)	5 (4%)	2	16
41	DS	110/112 (98%)	87 (79%)	17 (16%)	6 (6%)	2	12
42	BT	90/92 (98%)	69 (77%)	16 (18%)	5 (6%)	2	12
42	DT	90/92 (98%)	67 (74%)	18 (20%)	5 (6%)	2	12
43	BU	98/100 (98%)	55 (56%)	24 (24%)	19 (19%)	0	0
43	DU	98/100 (98%)	58 (59%)	21 (21%)	19 (19%)	0	0
44	BV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	4
44	DV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	4
45	BW	74/76 (97%)	61 (82%)	10 (14%)	3 (4%)	3	18
45	DW	74/76 (97%)	60 (81%)	10 (14%)	4 (5%)	2	13
46	BX	86/88 (98%)	57 (66%)	16 (19%)	13 (15%)	0	0
46	DX	86/88 (98%)	54 (63%)	19 (22%)	13 (15%)	0	0
47	BY	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	3
47	DY	60/62 (97%)	41 (68%)	12 (20%)	7 (12%)	0	3
48	BZ	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	8	32
48	DZ	57/59 (97%)	50 (88%)	6 (10%)	1 (2%)	8	32
49	B1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	0
49	D1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	0
50	B2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	6
50	D2	50/52 (96%)	39 (78%)	7 (14%)	4 (8%)	1	6
51	B3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	3
51	D3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	3
52	B4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	D4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	6	29
53	B5	61/63 (97%)	43 (70%)	12 (20%)	6 (10%)	0	4
53	D5	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	0	3
All	All	11192/11458 (98%)	8080 (72%)	2125 (19%)	987 (9%)	1	5

5 of 987 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	204	ASN
3	AC	189	ALA
3	AC	196	LEU
4	AD	28	SER
4	AD	30	LYS

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	202/202 (100%)	178 (88%)	24 (12%)	5	19
2	CB	202/202 (100%)	179 (89%)	23 (11%)	5	21
3	AC	160/160 (100%)	146 (91%)	14 (9%)	10	33
3	CC	160/160 (100%)	145 (91%)	15 (9%)	8	30
4	AD	180/180 (100%)	150 (83%)	30 (17%)	2	8
4	CD	180/180 (100%)	150 (83%)	30 (17%)	2	8
5	AE	116/116 (100%)	92 (79%)	24 (21%)	1	3
5	CE	116/116 (100%)	94 (81%)	22 (19%)	1	4
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	33
6	CF	90/90 (100%)	83 (92%)	7 (8%)	12	39
7	AG	126/126 (100%)	121 (96%)	5 (4%)	31	60
7	CG	126/126 (100%)	121 (96%)	5 (4%)	31	60
8	AH	119/119 (100%)	102 (86%)	17 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	104 (87%)	15 (13%)	4	17
9	AI	98/98 (100%)	88 (90%)	10 (10%)	7	26
9	CI	98/98 (100%)	88 (90%)	10 (10%)	7	26
10	AJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
10	CJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	8
11	CK	90/90 (100%)	76 (84%)	14 (16%)	2	11
12	AL	104/104 (100%)	83 (80%)	21 (20%)	1	3
12	CL	104/104 (100%)	83 (80%)	21 (20%)	1	3
13	AM	94/94 (100%)	87 (93%)	7 (7%)	13	42
13	CM	94/94 (100%)	87 (93%)	7 (7%)	13	42
14	AN	49/49 (100%)	45 (92%)	4 (8%)	11	37
14	CN	49/49 (100%)	45 (92%)	4 (8%)	11	37
15	AO	79/79 (100%)	69 (87%)	10 (13%)	4	16
15	CO	79/79 (100%)	69 (87%)	10 (13%)	4	16
16	AP	72/72 (100%)	57 (79%)	15 (21%)	1	3
16	CP	72/72 (100%)	56 (78%)	16 (22%)	1	2
17	AQ	94/94 (100%)	78 (83%)	16 (17%)	2	8
17	CQ	94/94 (100%)	79 (84%)	15 (16%)	2	10
18	AR	61/61 (100%)	58 (95%)	3 (5%)	25	55
18	CR	61/61 (100%)	58 (95%)	3 (5%)	25	55
19	AS	69/69 (100%)	60 (87%)	9 (13%)	4	16
19	CS	69/69 (100%)	60 (87%)	9 (13%)	4	16
20	AT	76/76 (100%)	65 (86%)	11 (14%)	3	12
20	CT	76/76 (100%)	65 (86%)	11 (14%)	3	12
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	CU	19/19 (100%)	19 (100%)	0	100	100
25	BC	213/213 (100%)	164 (77%)	49 (23%)	1	2
25	DC	213/213 (100%)	162 (76%)	51 (24%)	0	2
26	BD	165/165 (100%)	129 (78%)	36 (22%)	1	3
26	DD	165/165 (100%)	129 (78%)	36 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BE	161/161 (100%)	124 (77%)	37 (23%)	1	2
27	DE	161/161 (100%)	124 (77%)	37 (23%)	1	2
28	BF	155/155 (100%)	132 (85%)	23 (15%)	3	12
28	DF	155/155 (100%)	134 (86%)	21 (14%)	4	14
29	BG	132/132 (100%)	108 (82%)	24 (18%)	1	6
29	DG	132/132 (100%)	107 (81%)	25 (19%)	1	4
30	BH	122/122 (100%)	103 (84%)	19 (16%)	2	11
30	DH	122/122 (100%)	103 (84%)	19 (16%)	2	11
31	BI	27/53 (51%)	25 (93%)	2 (7%)	13	42
31	DI	27/53 (51%)	25 (93%)	2 (7%)	13	42
32	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	1
32	DJ	116/116 (100%)	85 (73%)	31 (27%)	0	1
33	BK	100/100 (100%)	78 (78%)	22 (22%)	1	3
33	DK	100/100 (100%)	78 (78%)	22 (22%)	1	3
34	BL	112/112 (100%)	75 (67%)	37 (33%)	0	1
34	DL	112/112 (100%)	76 (68%)	36 (32%)	0	1
35	BM	106/106 (100%)	82 (77%)	24 (23%)	1	2
35	DM	106/106 (100%)	81 (76%)	25 (24%)	1	2
36	BN	100/100 (100%)	75 (75%)	25 (25%)	0	2
36	DN	100/100 (100%)	76 (76%)	24 (24%)	0	2
37	BO	77/77 (100%)	63 (82%)	14 (18%)	1	6
37	DO	77/77 (100%)	63 (82%)	14 (18%)	1	6
38	BP	121/121 (100%)	96 (79%)	25 (21%)	1	3
38	DP	121/121 (100%)	94 (78%)	27 (22%)	1	2
39	BQ	92/92 (100%)	71 (77%)	21 (23%)	1	2
39	DQ	92/92 (100%)	71 (77%)	21 (23%)	1	2
40	BR	82/82 (100%)	63 (77%)	19 (23%)	1	2
40	DR	82/82 (100%)	61 (74%)	21 (26%)	0	2
41	BS	91/91 (100%)	65 (71%)	26 (29%)	0	1
41	DS	91/91 (100%)	65 (71%)	26 (29%)	0	1
42	BT	74/74 (100%)	60 (81%)	14 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	74/74 (100%)	60 (81%)	14 (19%)	1	4
43	BU	84/84 (100%)	66 (79%)	18 (21%)	1	3
43	DU	84/84 (100%)	67 (80%)	17 (20%)	1	3
44	BV	163/163 (100%)	142 (87%)	21 (13%)	4	16
44	DV	163/163 (100%)	141 (86%)	22 (14%)	4	14
45	BW	61/61 (100%)	52 (85%)	9 (15%)	3	12
45	DW	61/61 (100%)	53 (87%)	8 (13%)	4	15
46	BX	73/73 (100%)	50 (68%)	23 (32%)	0	1
46	DX	73/73 (100%)	50 (68%)	23 (32%)	0	1
47	BY	58/58 (100%)	46 (79%)	12 (21%)	1	3
47	DY	58/58 (100%)	46 (79%)	12 (21%)	1	3
48	BZ	51/51 (100%)	43 (84%)	8 (16%)	2	10
48	DZ	51/51 (100%)	43 (84%)	8 (16%)	2	10
49	B1	27/27 (100%)	26 (96%)	1 (4%)	34	62
49	D1	27/27 (100%)	26 (96%)	1 (4%)	34	62
50	B2	45/45 (100%)	40 (89%)	5 (11%)	6	22
50	D2	45/45 (100%)	39 (87%)	6 (13%)	4	15
51	B3	43/43 (100%)	38 (88%)	5 (12%)	5	20
51	D3	43/43 (100%)	38 (88%)	5 (12%)	5	20
52	B4	41/41 (100%)	29 (71%)	12 (29%)	0	1
52	D4	41/41 (100%)	28 (68%)	13 (32%)	0	1
53	B5	53/53 (100%)	42 (79%)	11 (21%)	1	3
53	D5	53/53 (100%)	43 (81%)	10 (19%)	1	4
All	All	9462/9514 (100%)	7811 (83%)	1651 (17%)	2	7

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BW	63	VAL
7	CG	67	GLU
42	DT	81	VAL
46	BX	73	LEU
2	CB	117	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
46	BX	45	ASN
7	CG	13	GLN
44	DV	121	HIS
47	BY	56	GLN
2	CB	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	293 (19%)	14 (0%)
1	CA	1505/1506 (99%)	294 (19%)	14 (0%)
22	AV	32/43 (74%)	3 (9%)	0
22	CV	32/43 (74%)	3 (9%)	0
23	BA	2755/2879 (95%)	584 (21%)	27 (0%)
23	DA	2757/2879 (95%)	589 (21%)	29 (1%)
24	BB	118/119 (99%)	26 (22%)	0
24	DB	118/119 (99%)	27 (22%)	0
All	All	8822/9094 (97%)	1819 (20%)	84 (0%)

5 of 1819 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2433	A
1	CA	793	U
23	DA	2272	U
23	BA	2542	A
1	CA	327	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1198 ligands modelled in this entry, 1198 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	1506/1506 (100%)	0.37	60 (3%) 38 37	51, 122, 245, 498	0
1	CA	1506/1506 (100%)	0.44	93 (6%) 20 21	51, 126, 251, 414	0
2	AB	234/234 (100%)	1.06	43 (18%) 1 1	113, 174, 244, 298	0
2	CB	234/234 (100%)	0.88	45 (19%) 1 1	111, 177, 259, 325	0
3	AC	206/206 (100%)	0.78	29 (14%) 2 3	106, 160, 225, 263	0
3	CC	206/206 (100%)	0.80	37 (17%) 1 1	105, 161, 226, 271	0
4	AD	208/208 (100%)	0.52	13 (6%) 20 21	90, 142, 199, 247	0
4	CD	208/208 (100%)	1.16	44 (21%) 0 1	94, 146, 220, 300	0
5	AE	151/151 (100%)	0.36	8 (5%) 26 27	73, 114, 172, 272	0
5	CE	151/151 (100%)	0.61	17 (11%) 5 6	73, 117, 188, 252	0
6	AF	101/101 (100%)	0.77	15 (14%) 2 2	83, 135, 192, 270	0
6	CF	101/101 (100%)	0.23	5 (4%) 28 29	79, 131, 184, 246	0
7	AG	155/155 (100%)	1.25	46 (29%) 0 0	118, 187, 237, 333	0
7	CG	155/155 (100%)	1.70	58 (37%) 0 0	119, 187, 237, 286	0
8	AH	138/138 (100%)	0.49	10 (7%) 15 17	77, 121, 166, 199	0
8	CH	138/138 (100%)	0.66	13 (9%) 8 10	81, 123, 167, 219	0
9	AI	127/127 (100%)	1.64	38 (29%) 0 0	119, 225, 289, 345	0
9	CI	127/127 (100%)	1.68	30 (23%) 0 0	121, 225, 286, 354	0
10	AJ	98/98 (100%)	1.86	36 (36%) 0 0	118, 198, 278, 356	0
10	CJ	98/98 (100%)	1.96	40 (40%) 0 0	122, 197, 264, 351	0
11	AK	119/119 (100%)	0.67	18 (15%) 2 2	71, 111, 171, 263	0
11	CK	119/119 (100%)	0.41	9 (7%) 13 15	74, 111, 178, 264	0
12	AL	124/124 (100%)	0.49	6 (4%) 30 31	67, 107, 165, 268	0
12	CL	124/124 (100%)	0.85	18 (14%) 2 3	70, 109, 178, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	116/116 (100%)	1.24	32 (27%) 0 0	134, 213, 299, 335	0
13	CM	116/116 (100%)	2.11	47 (40%) 0 0	135, 214, 309, 362	0
14	AN	60/60 (100%)	1.43	14 (23%) 0 0	114, 166, 217, 235	0
14	CN	60/60 (100%)	1.20	10 (16%) 1 2	116, 167, 227, 281	0
15	AO	88/88 (100%)	0.14	1 (1%) 80 79	66, 108, 159, 227	0
15	CO	88/88 (100%)	0.42	3 (3%) 45 44	67, 110, 166, 241	0
16	AP	83/83 (100%)	0.59	6 (7%) 15 17	84, 118, 174, 214	0
16	CP	83/83 (100%)	1.77	33 (39%) 0 0	87, 123, 177, 210	0
17	AQ	99/99 (100%)	0.27	2 (2%) 65 64	78, 112, 169, 216	0
17	CQ	99/99 (100%)	0.74	11 (11%) 5 6	79, 116, 166, 215	0
18	AR	70/70 (100%)	0.96	14 (20%) 1 1	84, 128, 183, 284	0
18	CR	70/70 (100%)	0.59	4 (5%) 23 24	82, 128, 192, 232	0
19	AS	78/78 (100%)	2.88	47 (60%) 0 0	152, 210, 275, 321	0
19	CS	78/78 (100%)	3.14	52 (66%) 0 0	151, 216, 291, 350	0
20	AT	99/99 (100%)	0.58	5 (5%) 28 28	86, 134, 203, 241	0
20	CT	99/99 (100%)	1.16	25 (25%) 0 0	92, 136, 212, 269	0
21	AU	24/24 (100%)	2.78	14 (58%) 0 0	160, 225, 264, 322	0
21	CU	24/24 (100%)	2.89	13 (54%) 0 0	163, 218, 265, 364	0
22	AV	34/43 (79%)	1.53	11 (32%) 0 0	89, 196, 324, 362	0
22	CV	34/43 (79%)	2.05	12 (35%) 0 0	92, 198, 333, 339	0
23	BA	2760/2879 (95%)	0.01	50 (1%) 68 67	27, 65, 180, 398	0
23	DA	2760/2879 (95%)	0.07	46 (1%) 70 68	25, 63, 178, 410	0
24	BB	119/119 (100%)	0.21	3 (2%) 57 55	77, 129, 182, 232	0
24	DB	119/119 (100%)	0.20	4 (3%) 45 44	78, 129, 184, 236	0
25	BC	271/271 (100%)	-0.09	3 (1%) 80 79	25, 58, 109, 175	0
25	DC	271/271 (100%)	-0.03	0 100 100	18, 57, 109, 177	0
26	BD	204/204 (100%)	0.42	16 (7%) 13 14	36, 73, 146, 341	0
26	DD	204/204 (100%)	0.42	9 (4%) 34 34	33, 71, 145, 347	0
27	BE	202/202 (100%)	-0.06	1 (0%) 91 90	31, 73, 155, 246	0
27	DE	202/202 (100%)	0.17	5 (2%) 57 55	25, 73, 155, 192	0
28	BF	181/181 (100%)	1.50	57 (31%) 0 0	102, 182, 254, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	181/181 (100%)	1.49	58 (32%) 0 0	104, 185, 268, 331	0
29	BG	159/159 (100%)	1.59	56 (35%) 0 0	85, 143, 221, 343	0
29	DG	159/159 (100%)	0.57	8 (5%) 28 29	79, 136, 186, 235	0
30	BH	145/145 (100%)	3.18	71 (48%) 0 0	67, 243, 391, 482	0
30	DH	145/145 (100%)	1.84	49 (33%) 0 0	64, 236, 379, 480	0
31	BI	32/65 (49%)	5.87	30 (93%) 0 0	171, 246, 347, 355	0
31	DI	32/65 (49%)	3.30	24 (75%) 0 0	168, 253, 310, 334	0
32	BJ	137/137 (100%)	0.13	3 (2%) 62 60	51, 81, 142, 201	0
32	DJ	137/137 (100%)	0.04	1 (0%) 87 87	52, 81, 146, 194	0
33	BK	122/122 (100%)	0.06	0 100 100	42, 70, 111, 150	0
33	DK	122/122 (100%)	0.20	3 (2%) 57 55	41, 69, 111, 162	0
34	BL	146/146 (100%)	0.61	14 (9%) 8 9	34, 97, 166, 309	0
34	DL	146/146 (100%)	0.52	14 (9%) 8 9	32, 97, 163, 293	0
35	BM	136/136 (100%)	0.32	8 (5%) 22 23	49, 89, 199, 370	0
35	DM	136/136 (100%)	0.54	11 (8%) 12 13	48, 88, 205, 406	0
36	BN	117/117 (100%)	0.31	1 (0%) 84 83	45, 73, 137, 249	0
36	DN	117/117 (100%)	0.21	1 (0%) 84 83	43, 73, 134, 235	0
37	BO	98/98 (100%)	1.25	25 (25%) 0 0	82, 137, 197, 223	0
37	DO	98/98 (100%)	1.00	23 (23%) 0 0	80, 136, 190, 215	0
38	BP	137/137 (100%)	0.13	6 (4%) 34 34	58, 93, 185, 250	0
38	DP	137/137 (100%)	0.42	15 (10%) 5 6	55, 92, 190, 273	0
39	BQ	116/116 (100%)	-0.06	0 100 100	35, 75, 124, 239	0
39	DQ	116/116 (100%)	-0.21	1 (0%) 84 83	26, 74, 126, 248	0
40	BR	101/101 (100%)	0.12	0 100 100	41, 105, 164, 264	0
40	DR	101/101 (100%)	0.56	3 (2%) 50 49	41, 110, 156, 259	0
41	BS	112/112 (100%)	0.08	2 (1%) 68 67	44, 59, 137, 254	0
41	DS	112/112 (100%)	0.11	5 (4%) 33 33	43, 59, 134, 255	0
42	BT	92/92 (100%)	0.00	1 (1%) 80 79	45, 77, 129, 170	0
42	DT	92/92 (100%)	0.16	0 100 100	36, 73, 127, 169	0
43	BU	100/100 (100%)	1.63	28 (28%) 0 0	62, 104, 257, 396	0
43	DU	100/100 (100%)	1.37	13 (13%) 3 4	61, 102, 251, 408	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	188/188 (100%)	0.75	28 (14%) 2 2	83, 138, 195, 245	0
44	DV	188/188 (100%)	0.29	3 (1%) 72 70	83, 139, 194, 230	0
45	BW	76/76 (100%)	0.46	5 (6%) 18 20	58, 84, 139, 261	0
45	DW	76/76 (100%)	0.59	4 (5%) 26 27	59, 84, 135, 256	0
46	BX	88/88 (100%)	0.40	3 (3%) 45 44	37, 74, 153, 322	0
46	DX	88/88 (100%)	0.46	3 (3%) 45 44	39, 70, 153, 326	0
47	BY	62/62 (100%)	0.29	5 (8%) 12 13	57, 98, 209, 292	0
47	DY	62/62 (100%)	0.80	7 (11%) 5 6	51, 96, 212, 328	0
48	BZ	59/59 (100%)	0.81	5 (8%) 10 12	43, 81, 156, 299	0
48	DZ	59/59 (100%)	1.03	5 (8%) 10 12	45, 85, 157, 305	0
49	B1	30/30 (100%)	2.71	20 (66%) 0 0	184, 253, 295, 311	0
49	D1	30/30 (100%)	2.01	11 (36%) 0 0	183, 261, 306, 358	0
50	B2	52/52 (100%)	0.47	8 (15%) 2 2	26, 71, 187, 233	0
50	D2	52/52 (100%)	0.01	3 (5%) 23 24	21, 72, 197, 229	0
51	B3	44/44 (100%)	7.97	39 (88%) 0 0	139, 249, 299, 320	0
51	D3	44/44 (100%)	9.15	38 (86%) 0 0	141, 245, 312, 333	0
52	B4	48/48 (100%)	0.06	1 (2%) 63 62	33, 43, 93, 194	0
52	D4	48/48 (100%)	-0.00	0 100 100	21, 41, 91, 200	0
53	B5	63/63 (100%)	0.14	1 (1%) 72 70	45, 68, 131, 215	0
53	D5	63/63 (100%)	0.26	4 (6%) 20 21	45, 70, 132, 216	0
All	All	20230/20552 (98%)	0.55	1948 (9%) 8 9	18, 104, 241, 498	0

The worst 5 of 1948 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	D3	47	THR	30.7
51	B3	41	PRO	25.8
43	DU	52	SER	24.8
51	B3	40	CYS	23.7
51	B3	13	CYS	23.7

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

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

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
54	MG	DA	3322	1/1	-0.12	0.38	95,95,95,95	0
54	MG	BA	3275	1/1	0.00	0.91	87,87,87,87	0
54	MG	DA	3284	1/1	0.05	0.33	134,134,134,134	0
54	MG	DG	201	1/1	0.07	0.44	101,101,101,101	0
54	MG	DA	3055	1/1	0.08	0.86	93,93,93,93	0
54	MG	AA	1729	1/1	0.28	0.13	75,75,75,75	0
54	MG	CA	1725	1/1	0.31	0.17	105,105,105,105	0
54	MG	AV	6304	1/1	0.32	0.44	118,118,118,118	0
54	MG	DA	3313	1/1	0.33	0.27	107,107,107,107	0
54	MG	BA	3176	1/1	0.38	0.33	99,99,99,99	0
54	MG	BA	2988	1/1	0.38	0.33	60,60,60,60	0
54	MG	CA	1704	1/1	0.41	0.52	108,108,108,108	0
54	MG	BA	3305	1/1	0.41	0.58	103,103,103,103	0
54	MG	CA	1648	1/1	0.41	0.34	64,64,64,64	0
54	MG	DA	3017	1/1	0.42	0.22	93,93,93,93	0
54	MG	AA	1754	1/1	0.42	0.22	110,110,110,110	0
54	MG	BA	3141	1/1	0.43	0.17	78,78,78,78	0
54	MG	DA	3033	1/1	0.45	0.47	101,101,101,101	0
54	MG	BA	3263	1/1	0.46	0.23	80,80,80,80	0
54	MG	BA	3164	1/1	0.46	0.63	88,88,88,88	0
54	MG	DA	3105	1/1	0.47	0.51	75,75,75,75	0
54	MG	BA	3073	1/1	0.47	0.28	89,89,89,89	0
54	MG	BA	3217	1/1	0.47	0.34	111,111,111,111	0
54	MG	DB	215	1/1	0.48	0.44	103,103,103,103	0
54	MG	DA	3278	1/1	0.49	0.34	75,75,75,75	0
54	MG	DA	3163	1/1	0.50	0.19	83,83,83,83	0
54	MG	CA	1697	1/1	0.50	0.47	74,74,74,74	0
54	MG	DA	3323	1/1	0.50	0.34	69,69,69,69	0
54	MG	DA	3110	1/1	0.51	0.31	86,86,86,86	0
54	MG	CA	1639	1/1	0.51	0.63	66,66,66,66	0
54	MG	BA	3271	1/1	0.52	0.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3236	1/1	0.52	0.30	119,119,119,119	0
54	MG	DA	3209	1/1	0.52	0.58	80,80,80,80	0
54	MG	CA	1688	1/1	0.53	0.35	99,99,99,99	0
54	MG	DA	3235	1/1	0.53	0.63	90,90,90,90	0
54	MG	AA	1757	1/1	0.54	0.53	89,89,89,89	0
54	MG	DA	3325	1/1	0.54	0.71	92,92,92,92	0
54	MG	CA	1740	1/1	0.54	0.23	117,117,117,117	0
54	MG	DA	2983	1/1	0.54	0.27	70,70,70,70	0
54	MG	BA	3163	1/1	0.55	0.49	72,72,72,72	0
54	MG	AA	1702	1/1	0.56	1.09	94,94,94,94	0
54	MG	AD	302	1/1	0.56	0.18	87,87,87,87	0
54	MG	DA	3115	1/1	0.56	0.49	65,65,65,65	0
54	MG	DA	3200	1/1	0.56	0.11	87,87,87,87	0
54	MG	DA	2999	1/1	0.57	0.43	76,76,76,76	0
54	MG	BA	3025	1/1	0.57	0.30	65,65,65,65	0
54	MG	DA	3078	1/1	0.58	0.60	79,79,79,79	0
54	MG	DA	3290	1/1	0.58	0.17	85,85,85,85	0
54	MG	DA	3324	1/1	0.58	0.51	78,78,78,78	0
54	MG	BA	3006	1/1	0.58	0.51	77,77,77,77	0
54	MG	DA	3226	1/1	0.59	0.49	80,80,80,80	0
54	MG	DA	3014	1/1	0.60	0.40	69,69,69,69	0
54	MG	DA	3302	1/1	0.60	0.56	77,77,77,77	0
54	MG	BA	3225	1/1	0.60	0.48	74,74,74,74	0
54	MG	BA	3117	1/1	0.60	0.11	77,77,77,77	0
54	MG	CA	1703	1/1	0.60	0.35	108,108,108,108	0
54	MG	CA	1696	1/1	0.60	0.18	133,133,133,133	0
54	MG	BA	3079	1/1	0.60	0.43	86,86,86,86	0
54	MG	DA	3243	1/1	0.60	0.35	72,72,72,72	0
54	MG	AA	1696	1/1	0.61	0.24	132,132,132,132	0
54	MG	BA	3213	1/1	0.61	0.25	101,101,101,101	0
54	MG	DA	3181	1/1	0.61	0.18	106,106,106,106	0
54	MG	DA	3043	1/1	0.61	0.69	70,70,70,70	0
54	MG	BA	3272	1/1	0.61	0.45	119,119,119,119	0
54	MG	AA	1623	1/1	0.62	0.39	93,93,93,93	0
54	MG	AA	1673	1/1	0.62	0.53	61,61,61,61	0
54	MG	DA	3238	1/1	0.62	0.29	58,58,58,58	0
54	MG	DA	3064	1/1	0.62	0.19	80,80,80,80	0
54	MG	BA	2986	1/1	0.63	0.23	67,67,67,67	0
54	MG	DA	3168	1/1	0.63	0.47	94,94,94,94	0
54	MG	AA	1745	1/1	0.64	0.27	97,97,97,97	0
54	MG	AA	1718	1/1	0.64	0.63	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1669	1/1	0.64	0.33	110,110,110,110	0
54	MG	DB	212	1/1	0.64	0.14	70,70,70,70	0
54	MG	AA	1698	1/1	0.64	0.47	88,88,88,88	0
54	MG	DA	3265	1/1	0.65	0.33	120,120,120,120	0
54	MG	AA	1680	1/1	0.65	0.14	90,90,90,90	0
54	MG	BA	3172	1/1	0.65	0.68	102,102,102,102	0
54	MG	CV	6301	1/1	0.65	0.22	98,98,98,98	0
54	MG	DA	3174	1/1	0.65	0.51	42,42,42,42	0
54	MG	DA	3119	1/1	0.65	0.65	88,88,88,88	0
54	MG	BA	3189	1/1	0.66	0.44	88,88,88,88	0
54	MG	CA	1705	1/1	0.66	0.24	54,54,54,54	0
54	MG	BA	3084	1/1	0.66	0.41	51,51,51,51	0
54	MG	DA	3249	1/1	0.67	0.36	56,56,56,56	0
54	MG	DA	3037	1/1	0.67	0.18	77,77,77,77	0
54	MG	BA	3060	1/1	0.67	0.69	74,74,74,74	0
54	MG	DA	3308	1/1	0.67	0.37	91,91,91,91	0
54	MG	AA	1618	1/1	0.67	0.09	91,91,91,91	0
54	MG	DA	3222	1/1	0.67	0.53	70,70,70,70	0
54	MG	DA	3030	1/1	0.67	0.41	71,71,71,71	0
54	MG	AA	1734	1/1	0.67	0.37	103,103,103,103	0
54	MG	AA	1646	1/1	0.68	0.26	99,99,99,99	0
54	MG	BA	3149	1/1	0.68	0.73	82,82,82,82	0
54	MG	AA	1642	1/1	0.68	0.51	97,97,97,97	0
54	MG	BA	3178	1/1	0.68	0.50	72,72,72,72	0
54	MG	BK	201	1/1	0.68	0.19	91,91,91,91	0
54	MG	CA	1724	1/1	0.68	0.32	74,74,74,74	0
54	MG	DA	2972	1/1	0.69	0.48	47,47,47,47	0
54	MG	BA	3219	1/1	0.69	0.80	66,66,66,66	0
54	MG	BA	3278	1/1	0.69	0.29	115,115,115,115	0
54	MG	BB	205	1/1	0.69	0.41	71,71,71,71	0
54	MG	CA	1717	1/1	0.69	0.28	84,84,84,84	0
54	MG	BA	3190	1/1	0.69	0.26	115,115,115,115	0
54	MG	DA	3087	1/1	0.70	0.30	67,67,67,67	0
54	MG	AA	1722	1/1	0.70	0.28	83,83,83,83	0
54	MG	DA	3246	1/1	0.70	0.60	67,67,67,67	0
54	MG	BA	3114	1/1	0.70	0.66	78,78,78,78	0
54	MG	DA	3143	1/1	0.70	0.25	77,77,77,77	0
54	MG	AA	1610	1/1	0.70	0.28	78,78,78,78	0
54	MG	DA	3100	1/1	0.70	0.45	59,59,59,59	0
54	MG	DA	3050	1/1	0.71	0.09	105,105,105,105	0
54	MG	DA	3327	1/1	0.71	0.33	68,68,68,68	0
54	MG	BA	3191	1/1	0.71	0.37	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3094	1/1	0.71	0.30	76,76,76,76	0
54	MG	BA	3027	1/1	0.71	0.51	62,62,62,62	0
54	MG	BA	3303	1/1	0.71	0.20	98,98,98,98	0
54	MG	DA	3271	1/1	0.71	0.18	97,97,97,97	0
54	MG	CA	1691	1/1	0.71	0.42	85,85,85,85	0
54	MG	AA	1709	1/1	0.71	0.38	83,83,83,83	0
54	MG	BA	3109	1/1	0.71	0.82	90,90,90,90	0
54	MG	BA	3259	1/1	0.71	0.38	75,75,75,75	0
54	MG	BA	3283	1/1	0.71	0.16	76,76,76,76	0
54	MG	BA	3004	1/1	0.71	1.28	74,74,74,74	0
54	MG	AA	1706	1/1	0.72	0.38	103,103,103,103	0
54	MG	BA	3075	1/1	0.72	0.21	67,67,67,67	0
54	MG	AA	1661	1/1	0.72	0.41	65,65,65,65	0
54	MG	CA	1668	1/1	0.72	1.09	116,116,116,116	0
54	MG	DA	3312	1/1	0.72	0.54	66,66,66,66	0
54	MG	BA	3013	1/1	0.72	0.10	90,90,90,90	0
54	MG	BA	3136	1/1	0.72	0.23	87,87,87,87	0
54	MG	BA	3036	1/1	0.72	0.24	92,92,92,92	0
54	MG	DA	3199	1/1	0.72	0.71	38,38,38,38	0
54	MG	CA	1685	1/1	0.72	0.60	106,106,106,106	0
54	MG	DA	3316	1/1	0.72	0.24	97,97,97,97	0
54	MG	DA	3251	1/1	0.72	0.37	63,63,63,63	0
54	MG	AA	1747	1/1	0.72	0.81	75,75,75,75	0
54	MG	DA	3024	1/1	0.72	0.39	36,36,36,36	0
54	MG	CA	1683	1/1	0.72	0.31	91,91,91,91	0
54	MG	DA	3080	1/1	0.72	0.41	69,69,69,69	0
54	MG	DA	3229	1/1	0.73	0.42	64,64,64,64	0
54	MG	AA	1700	1/1	0.73	0.56	98,98,98,98	0
54	MG	CA	1637	1/1	0.73	0.17	112,112,112,112	0
54	MG	BA	3103	1/1	0.73	0.30	88,88,88,88	0
54	MG	DA	3196	1/1	0.73	1.08	39,39,39,39	0
54	MG	AA	1713	1/1	0.73	0.30	93,93,93,93	0
54	MG	DB	216	1/1	0.73	0.36	88,88,88,88	0
54	MG	DA	3262	1/1	0.73	0.27	82,82,82,82	0
54	MG	CA	1636	1/1	0.73	0.33	93,93,93,93	0
54	MG	CA	1650	1/1	0.73	0.31	108,108,108,108	0
54	MG	DA	3291	1/1	0.74	0.48	78,78,78,78	0
54	MG	BA	3083	1/1	0.74	0.31	87,87,87,87	0
54	MG	DA	3318	1/1	0.74	0.35	101,101,101,101	0
54	MG	DA	3258	1/1	0.74	0.48	72,72,72,72	0
54	MG	BA	3115	1/1	0.74	0.32	91,91,91,91	0
54	MG	BA	3123	1/1	0.74	0.36	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3207	1/1	0.74	0.38	42,42,42,42	0
54	MG	AA	1762	1/1	0.74	0.10	155,155,155,155	0
54	MG	CA	1663	1/1	0.74	0.28	86,86,86,86	0
54	MG	DA	3185	1/1	0.74	0.32	108,108,108,108	0
54	MG	BA	3255	1/1	0.74	0.21	57,57,57,57	0
54	MG	DA	3332	1/1	0.74	0.45	60,60,60,60	0
54	MG	DA	2938	1/1	0.74	0.27	66,66,66,66	0
54	MG	CA	1698	1/1	0.75	0.30	117,117,117,117	0
54	MG	AA	1739	1/1	0.75	0.15	129,129,129,129	0
54	MG	DA	3244	1/1	0.75	0.27	87,87,87,87	0
54	MG	BA	3218	1/1	0.75	0.67	75,75,75,75	0
54	MG	CA	1614	1/1	0.75	0.33	89,89,89,89	0
54	MG	BA	3139	1/1	0.75	0.32	78,78,78,78	0
54	MG	BA	3308	1/1	0.75	0.47	94,94,94,94	0
54	MG	BA	3019	1/1	0.75	0.65	58,58,58,58	0
54	MG	BA	3110	1/1	0.75	0.14	86,86,86,86	0
54	MG	BA	3226	1/1	0.75	0.42	81,81,81,81	0
54	MG	AA	1641	1/1	0.75	0.35	85,85,85,85	0
54	MG	DA	3101	1/1	0.76	0.77	72,72,72,72	0
54	MG	AA	1693	1/1	0.76	0.32	74,74,74,74	0
54	MG	DA	3085	1/1	0.76	0.13	89,89,89,89	0
54	MG	AA	1626	1/1	0.76	0.15	62,62,62,62	0
54	MG	DA	2940	1/1	0.76	0.71	51,51,51,51	0
54	MG	AA	1645	1/1	0.76	0.59	79,79,79,79	0
54	MG	BA	3062	1/1	0.76	0.36	76,76,76,76	0
54	MG	BA	3281	1/1	0.76	0.33	84,84,84,84	0
54	MG	BA	3093	1/1	0.76	0.34	83,83,83,83	0
54	MG	DA	3300	1/1	0.76	0.21	68,68,68,68	0
54	MG	BA	3118	1/1	0.76	0.43	109,109,109,109	0
54	MG	AA	1763	1/1	0.76	0.13	96,96,96,96	0
54	MG	DA	3061	1/1	0.76	0.27	75,75,75,75	0
54	MG	BA	3306	1/1	0.77	0.38	74,74,74,74	0
54	MG	AA	1691	1/1	0.77	0.42	78,78,78,78	0
54	MG	BA	3299	1/1	0.77	0.28	80,80,80,80	0
54	MG	CA	1632	1/1	0.77	0.27	79,79,79,79	0
54	MG	DA	2987	1/1	0.77	0.44	70,70,70,70	0
54	MG	BA	3188	1/1	0.77	0.38	45,45,45,45	0
54	MG	DA	3134	1/1	0.77	0.16	71,71,71,71	0
54	MG	AA	1640	1/1	0.77	0.44	106,106,106,106	0
54	MG	CA	1616	1/1	0.77	0.47	75,75,75,75	0
54	MG	DA	3281	1/1	0.77	0.29	73,73,73,73	0
54	MG	DA	3057	1/1	0.77	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	209	1/1	0.77	0.12	75,75,75,75	0
54	MG	AA	1689	1/1	0.77	0.26	68,68,68,68	0
54	MG	BA	3240	1/1	0.77	0.10	114,114,114,114	0
54	MG	DB	206	1/1	0.78	0.29	99,99,99,99	0
54	MG	DA	3317	1/1	0.78	0.42	97,97,97,97	0
54	MG	BA	3072	1/1	0.78	0.43	67,67,67,67	0
54	MG	DA	3162	1/1	0.78	0.16	143,143,143,143	0
54	MG	AA	1695	1/1	0.78	0.38	83,83,83,83	0
54	MG	CA	1641	1/1	0.78	0.13	85,85,85,85	0
54	MG	DA	3263	1/1	0.78	0.36	63,63,63,63	0
54	MG	BA	3267	1/1	0.78	0.47	86,86,86,86	0
54	MG	BA	3287	1/1	0.78	0.44	74,74,74,74	0
54	MG	CP	101	1/1	0.78	0.17	96,96,96,96	0
54	MG	BA	3158	1/1	0.78	0.20	105,105,105,105	0
54	MG	DA	3186	1/1	0.78	0.13	90,90,90,90	0
54	MG	DA	3267	1/1	0.78	0.25	76,76,76,76	0
54	MG	AA	1621	1/1	0.78	0.61	74,74,74,74	0
54	MG	DA	3309	1/1	0.78	0.38	30,30,30,30	0
54	MG	BA	3253	1/1	0.78	0.36	76,76,76,76	0
54	MG	CA	1711	1/1	0.78	0.36	87,87,87,87	0
54	MG	AV	6302	1/1	0.78	0.48	121,121,121,121	0
54	MG	AA	1720	1/1	0.78	0.24	69,69,69,69	0
54	MG	BA	3095	1/1	0.78	0.13	83,83,83,83	0
54	MG	DA	3298	1/1	0.78	0.67	79,79,79,79	0
54	MG	DA	3049	1/1	0.78	0.21	56,56,56,56	0
54	MG	DA	3307	1/1	0.78	0.38	73,73,73,73	0
54	MG	BA	3157	1/1	0.78	0.29	68,68,68,68	0
54	MG	CA	1621	1/1	0.78	0.39	67,67,67,67	0
54	MG	DA	2993	1/1	0.78	0.08	69,69,69,69	0
54	MG	AA	1723	1/1	0.79	0.51	81,81,81,81	0
54	MG	DA	3116	1/1	0.79	0.25	115,115,115,115	0
54	MG	DA	3136	1/1	0.79	0.37	68,68,68,68	0
54	MG	CA	1610	1/1	0.79	0.28	77,77,77,77	0
54	MG	BA	3291	1/1	0.79	0.28	68,68,68,68	0
54	MG	DA	3072	1/1	0.79	0.60	73,73,73,73	0
54	MG	D4	101	1/1	0.79	0.55	55,55,55,55	0
54	MG	BA	3155	1/1	0.79	0.38	85,85,85,85	0
54	MG	DA	3296	1/1	0.79	0.15	104,104,104,104	0
54	MG	DA	3130	1/1	0.79	0.32	82,82,82,82	0
54	MG	BA	3061	1/1	0.79	0.21	91,91,91,91	0
54	MG	CA	1658	1/1	0.79	0.42	110,110,110,110	0
54	MG	DA	3311	1/1	0.79	0.15	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3212	1/1	0.79	0.40	69,69,69,69	0
54	MG	BA	3302	1/1	0.79	0.31	121,121,121,121	0
54	MG	DA	2959	1/1	0.79	0.39	56,56,56,56	0
54	MG	BA	3143	1/1	0.80	0.52	84,84,84,84	0
54	MG	DA	3111	1/1	0.80	0.39	67,67,67,67	0
54	MG	CA	1684	1/1	0.80	0.14	117,117,117,117	0
54	MG	DA	3169	1/1	0.80	0.12	112,112,112,112	0
54	MG	DA	3165	1/1	0.80	0.62	71,71,71,71	0
54	MG	BA	3078	1/1	0.80	0.10	83,83,83,83	0
54	MG	DA	3299	1/1	0.80	0.34	68,68,68,68	0
54	MG	AA	1719	1/1	0.80	0.28	78,78,78,78	0
54	MG	BB	206	1/1	0.80	0.23	70,70,70,70	0
54	MG	DA	3097	1/1	0.80	0.29	94,94,94,94	0
54	MG	BA	3037	1/1	0.80	0.14	93,93,93,93	0
54	MG	DA	2970	1/1	0.80	0.19	67,67,67,67	0
54	MG	DA	3142	1/1	0.80	0.18	109,109,109,109	0
54	MG	AA	1753	1/1	0.80	0.34	102,102,102,102	0
54	MG	BA	3229	1/1	0.80	0.28	62,62,62,62	0
54	MG	AA	1649	1/1	0.80	0.37	89,89,89,89	0
54	MG	BA	2969	1/1	0.80	0.15	37,37,37,37	0
54	MG	DA	3242	1/1	0.80	0.31	96,96,96,96	0
54	MG	BA	3033	1/1	0.80	0.19	67,67,67,67	0
54	MG	CA	1671	1/1	0.81	0.24	74,74,74,74	0
54	MG	BA	3026	1/1	0.81	0.40	82,82,82,82	0
54	MG	DA	2932	1/1	0.81	0.54	38,38,38,38	0
54	MG	DA	3202	1/1	0.81	0.67	44,44,44,44	0
54	MG	DA	3065	1/1	0.81	0.36	56,56,56,56	0
54	MG	DA	3098	1/1	0.81	0.37	71,71,71,71	0
54	MG	CA	1687	1/1	0.81	0.27	64,64,64,64	0
54	MG	DA	3141	1/1	0.81	0.14	95,95,95,95	0
54	MG	CA	1700	1/1	0.81	0.50	65,65,65,65	0
54	MG	BA	3204	1/1	0.81	0.35	74,74,74,74	0
54	MG	BA	3220	1/1	0.81	0.33	56,56,56,56	0
54	MG	AA	1701	1/1	0.81	0.36	83,83,83,83	0
54	MG	AA	1685	1/1	0.81	0.16	106,106,106,106	0
54	MG	DA	3149	1/1	0.81	0.45	74,74,74,74	0
54	MG	DA	3131	1/1	0.81	0.45	66,66,66,66	0
54	MG	DA	3127	1/1	0.81	0.37	90,90,90,90	0
54	MG	DA	3021	1/1	0.81	0.17	67,67,67,67	0
54	MG	CA	1701	1/1	0.81	0.34	112,112,112,112	0
54	MG	DA	3071	1/1	0.81	0.38	64,64,64,64	0
54	MG	DA	3074	1/1	0.81	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3159	1/1	0.81	0.42	78,78,78,78	0
54	MG	BA	3268	1/1	0.81	0.77	58,58,58,58	0
54	MG	AA	1612	1/1	0.81	0.25	64,64,64,64	0
54	MG	BA	3101	1/1	0.81	0.45	75,75,75,75	0
54	MG	BA	3038	1/1	0.81	0.17	65,65,65,65	0
54	MG	BA	3145	1/1	0.82	0.19	67,67,67,67	0
54	MG	BA	3262	1/1	0.82	0.39	60,60,60,60	0
54	MG	BA	3112	1/1	0.82	0.34	68,68,68,68	0
54	MG	BA	3175	1/1	0.82	0.35	85,85,85,85	0
54	MG	DA	3161	1/1	0.82	0.29	74,74,74,74	0
54	MG	DA	3295	1/1	0.82	0.27	63,63,63,63	0
54	MG	BB	217	1/1	0.82	0.15	78,78,78,78	0
54	MG	DA	3289	1/1	0.82	0.54	92,92,92,92	0
54	MG	DA	3029	1/1	0.82	0.23	70,70,70,70	0
54	MG	DA	3231	1/1	0.82	0.70	60,60,60,60	0
54	MG	CA	1736	1/1	0.82	1.14	115,115,115,115	0
54	MG	AA	1761	1/1	0.82	0.20	104,104,104,104	0
54	MG	BB	210	1/1	0.82	0.10	100,100,100,100	0
54	MG	DA	3092	1/1	0.82	0.09	98,98,98,98	0
54	MG	BA	3023	1/1	0.82	0.51	64,64,64,64	0
54	MG	CA	1727	1/1	0.82	0.26	75,75,75,75	0
54	MG	BA	3090	1/1	0.82	0.34	69,69,69,69	0
54	MG	DA	3334	1/1	0.82	0.25	72,72,72,72	0
54	MG	DA	3205	1/1	0.82	0.32	48,48,48,48	0
54	MG	BA	3119	1/1	0.82	0.28	64,64,64,64	0
54	MG	BA	3031	1/1	0.82	0.84	87,87,87,87	0
54	MG	BB	213	1/1	0.82	0.65	84,84,84,84	0
54	MG	BA	3208	1/1	0.82	0.24	48,48,48,48	0
54	MG	AA	1667	1/1	0.83	0.51	61,61,61,61	0
54	MG	AA	1737	1/1	0.83	0.25	86,86,86,86	0
54	MG	AA	1651	1/1	0.83	0.51	97,97,97,97	0
54	MG	DA	3113	1/1	0.83	0.09	71,71,71,71	0
54	MG	DA	3120	1/1	0.83	0.64	66,66,66,66	0
54	MG	BA	3138	1/1	0.83	0.14	100,100,100,100	0
54	MG	DA	3230	1/1	0.83	0.21	63,63,63,63	0
54	MG	DA	3268	1/1	0.83	0.43	81,81,81,81	0
54	MG	CA	1601	1/1	0.83	0.45	53,53,53,53	0
54	MG	DA	3175	1/1	0.83	0.18	81,81,81,81	0
54	MG	CA	1723	1/1	0.83	0.24	141,141,141,141	0
54	MG	BA	3295	1/1	0.83	0.60	70,70,70,70	0
54	MG	AA	1738	1/1	0.83	0.28	70,70,70,70	0
54	MG	AA	1664	1/1	0.83	0.62	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3059	1/1	0.83	0.21	67,67,67,67	0
54	MG	BA	3091	1/1	0.83	0.40	56,56,56,56	0
54	MG	DA	3297	1/1	0.83	0.38	49,49,49,49	0
54	MG	BA	2985	1/1	0.83	0.52	54,54,54,54	0
54	MG	DA	3212	1/1	0.83	0.49	78,78,78,78	0
54	MG	DA	3088	1/1	0.83	0.10	70,70,70,70	0
54	MG	DA	3010	1/1	0.84	0.65	51,51,51,51	0
54	MG	DA	3220	1/1	0.84	0.28	70,70,70,70	0
54	MG	DA	3178	1/1	0.84	0.27	83,83,83,83	0
54	MG	AA	1653	1/1	0.84	0.32	89,89,89,89	0
54	MG	BA	3009	1/1	0.84	0.51	87,87,87,87	0
54	MG	DA	3034	1/1	0.84	0.29	65,65,65,65	0
54	MG	BA	3146	1/1	0.84	0.29	83,83,83,83	0
54	MG	DA	3012	1/1	0.84	0.38	45,45,45,45	0
54	MG	AA	1755	1/1	0.84	0.32	103,103,103,103	0
54	MG	BA	3266	1/1	0.84	0.19	98,98,98,98	0
54	MG	AA	1682	1/1	0.84	0.40	85,85,85,85	0
54	MG	DA	3276	1/1	0.84	0.17	128,128,128,128	0
54	MG	CA	1708	1/1	0.84	0.14	143,143,143,143	0
54	MG	DA	3269	1/1	0.84	0.51	91,91,91,91	0
54	MG	BA	3069	1/1	0.84	0.13	109,109,109,109	0
54	MG	AA	1676	1/1	0.84	0.15	63,63,63,63	0
54	MG	DA	3103	1/1	0.84	0.41	79,79,79,79	0
54	MG	AA	1614	1/1	0.84	0.52	85,85,85,85	0
54	MG	BA	3165	1/1	0.84	0.26	71,71,71,71	0
54	MG	CA	1733	1/1	0.84	0.12	72,72,72,72	0
54	MG	AA	1681	1/1	0.84	0.16	99,99,99,99	0
54	MG	CA	1735	1/1	0.84	0.27	61,61,61,61	0
54	MG	CA	1672	1/1	0.84	0.30	62,62,62,62	0
54	MG	BA	3098	1/1	0.84	0.19	78,78,78,78	0
54	MG	DA	3047	1/1	0.84	0.34	66,66,66,66	0
54	MG	DA	3013	1/1	0.84	0.26	44,44,44,44	0
54	MG	CA	1706	1/1	0.84	0.53	101,101,101,101	0
54	MG	AA	1704	1/1	0.84	0.20	81,81,81,81	0
54	MG	DA	3177	1/1	0.84	0.32	62,62,62,62	0
54	MG	DA	3082	1/1	0.84	0.42	70,70,70,70	0
54	MG	BA	3066	1/1	0.84	0.46	56,56,56,56	0
54	MG	AA	1660	1/1	0.84	0.30	59,59,59,59	0
54	MG	AA	1712	1/1	0.84	0.50	75,75,75,75	0
54	MG	DB	203	1/1	0.84	0.19	82,82,82,82	0
54	MG	BA	3280	1/1	0.84	0.39	70,70,70,70	0
54	MG	DA	3166	1/1	0.84	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	216	1/1	0.84	0.18	79,79,79,79	0
54	MG	BA	2971	1/1	0.84	0.34	65,65,65,65	0
54	MG	CA	1608	1/1	0.84	0.11	61,61,61,61	0
54	MG	BA	2975	1/1	0.84	0.19	37,37,37,37	0
54	MG	DA	3128	1/1	0.85	0.21	114,114,114,114	0
54	MG	DA	3172	1/1	0.85	0.35	81,81,81,81	0
54	MG	AA	1674	1/1	0.85	0.50	79,79,79,79	0
54	MG	BA	3221	1/1	0.85	0.34	48,48,48,48	0
54	MG	CA	1699	1/1	0.85	0.72	71,71,71,71	0
54	MG	BA	3099	1/1	0.85	0.15	78,78,78,78	0
54	MG	BA	3005	1/1	0.85	0.53	69,69,69,69	0
54	MG	BA	3104	1/1	0.85	0.34	63,63,63,63	0
54	MG	CA	1674	1/1	0.85	0.15	74,74,74,74	0
54	MG	DA	3090	1/1	0.85	0.21	71,71,71,71	0
54	MG	BA	3100	1/1	0.85	0.07	77,77,77,77	0
54	MG	BA	3258	1/1	0.85	0.21	104,104,104,104	0
54	MG	BA	3051	1/1	0.85	0.34	66,66,66,66	0
54	MG	DA	2995	1/1	0.85	0.56	48,48,48,48	0
54	MG	DA	3023	1/1	0.85	0.24	49,49,49,49	0
54	MG	AV	6301	1/1	0.85	0.10	72,72,72,72	0
54	MG	DA	3201	1/1	0.85	0.45	72,72,72,72	0
54	MG	BA	3282	1/1	0.85	0.37	62,62,62,62	0
54	MG	BA	3034	1/1	0.85	0.87	102,102,102,102	0
54	MG	BA	3054	1/1	0.85	0.18	46,46,46,46	0
54	MG	DA	3004	1/1	0.85	0.33	67,67,67,67	0
54	MG	AA	1679	1/1	0.85	0.58	78,78,78,78	0
54	MG	DA	3003	1/1	0.85	0.36	41,41,41,41	0
54	MG	AA	1677	1/1	0.85	0.44	64,64,64,64	0
54	MG	DA	3256	1/1	0.85	0.21	82,82,82,82	0
54	MG	DA	3228	1/1	0.85	0.45	51,51,51,51	0
54	MG	BA	3068	1/1	0.85	0.34	59,59,59,59	0
54	MG	DA	3274	1/1	0.85	0.39	62,62,62,62	0
54	MG	DA	3259	1/1	0.85	0.53	108,108,108,108	0
54	MG	DA	3223	1/1	0.85	0.61	45,45,45,45	0
54	MG	BA	3248	1/1	0.85	0.16	77,77,77,77	0
54	MG	BA	3301	1/1	0.85	0.65	66,66,66,66	0
54	MG	AA	1678	1/1	0.85	0.25	115,115,115,115	0
54	MG	AA	1644	1/1	0.85	0.27	53,53,53,53	0
54	MG	BB	211	1/1	0.86	0.49	112,112,112,112	0
54	MG	DA	3279	1/1	0.86	0.09	88,88,88,88	0
54	MG	BA	3201	1/1	0.86	0.20	80,80,80,80	0
54	MG	CA	1738	1/1	0.86	0.51	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3116	1/1	0.86	0.39	85,85,85,85	0
54	MG	AA	1717	1/1	0.86	0.35	81,81,81,81	0
54	MG	BA	3140	1/1	0.86	0.43	76,76,76,76	0
54	MG	BA	3012	1/1	0.86	0.16	91,91,91,91	0
54	MG	BA	3197	1/1	0.86	0.37	57,57,57,57	0
54	MG	AA	1658	1/1	0.86	0.09	94,94,94,94	0
54	MG	DA	3189	1/1	0.86	0.25	37,37,37,37	0
54	MG	BA	3030	1/1	0.86	0.15	57,57,57,57	0
54	MG	AA	1639	1/1	0.86	0.35	79,79,79,79	0
54	MG	BA	3242	1/1	0.86	0.35	44,44,44,44	0
54	MG	BA	3284	1/1	0.86	0.89	85,85,85,85	0
54	MG	AV	6303	1/1	0.86	0.13	67,67,67,67	0
54	MG	BA	3125	1/1	0.86	0.26	87,87,87,87	0
54	MG	DA	3068	1/1	0.86	0.41	72,72,72,72	0
54	MG	AA	1675	1/1	0.86	0.15	77,77,77,77	0
54	MG	AA	1643	1/1	0.86	0.33	70,70,70,70	0
54	MG	CA	1620	1/1	0.86	0.11	79,79,79,79	0
54	MG	DA	3187	1/1	0.86	0.22	90,90,90,90	0
54	MG	CA	1612	1/1	0.86	0.93	58,58,58,58	0
54	MG	DA	3027	1/1	0.86	0.49	53,53,53,53	0
54	MG	AA	1697	1/1	0.86	0.36	80,80,80,80	0
54	MG	CA	1694	1/1	0.86	0.32	59,59,59,59	0
54	MG	AA	1731	1/1	0.86	0.27	76,76,76,76	0
54	MG	BA	2948	1/1	0.86	0.72	39,39,39,39	0
54	MG	B2	101	1/1	0.86	0.54	64,64,64,64	0
54	MG	BA	3169	1/1	0.87	0.52	75,75,75,75	0
54	MG	CA	1628	1/1	0.87	0.20	100,100,100,100	0
54	MG	DA	3121	1/1	0.87	0.21	69,69,69,69	0
54	MG	BA	3050	1/1	0.87	0.17	41,41,41,41	0
54	MG	CA	1618	1/1	0.87	0.72	63,63,63,63	0
54	MG	BA	3171	1/1	0.87	0.19	68,68,68,68	0
54	MG	CA	1645	1/1	0.87	0.64	72,72,72,72	0
54	MG	AA	1625	1/1	0.87	1.01	88,88,88,88	0
54	MG	AA	1655	1/1	0.87	0.72	72,72,72,72	0
54	MG	BA	3113	1/1	0.87	0.29	71,71,71,71	0
54	MG	CA	1646	1/1	0.87	0.15	78,78,78,78	0
54	MG	BA	2968	1/1	0.87	0.47	51,51,51,51	0
54	MG	DA	3091	1/1	0.87	0.49	125,125,125,125	0
54	MG	DA	3077	1/1	0.87	0.61	67,67,67,67	0
54	MG	BA	3265	1/1	0.87	0.33	80,80,80,80	0
54	MG	CA	1662	1/1	0.87	0.76	86,86,86,86	0
54	MG	AA	1699	1/1	0.87	0.26	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3109	1/1	0.87	0.31	54,54,54,54	0
54	MG	AA	1758	1/1	0.87	0.14	73,73,73,73	0
54	MG	DB	214	1/1	0.87	0.20	90,90,90,90	0
54	MG	BA	3000	1/1	0.87	0.16	65,65,65,65	0
54	MG	BA	3039	1/1	0.87	0.19	94,94,94,94	0
54	MG	BA	2963	1/1	0.87	0.19	54,54,54,54	0
54	MG	AA	1752	1/1	0.87	0.93	81,81,81,81	0
54	MG	CA	1634	1/1	0.87	0.26	60,60,60,60	0
54	MG	BA	2996	1/1	0.87	0.29	54,54,54,54	0
54	MG	BA	3111	1/1	0.87	0.54	46,46,46,46	0
54	MG	BA	3173	1/1	0.87	0.51	80,80,80,80	0
54	MG	DA	2994	1/1	0.87	0.13	67,67,67,67	0
54	MG	BA	3168	1/1	0.87	0.20	76,76,76,76	0
54	MG	BA	3041	1/1	0.87	0.22	67,67,67,67	0
54	MG	BA	3288	1/1	0.87	0.62	62,62,62,62	0
54	MG	DA	3006	1/1	0.87	0.12	74,74,74,74	0
54	MG	DA	3272	1/1	0.87	0.43	41,41,41,41	0
54	MG	DA	3320	1/1	0.87	0.41	58,58,58,58	0
54	MG	AA	1740	1/1	0.87	0.34	80,80,80,80	0
54	MG	DA	3260	1/1	0.87	0.50	102,102,102,102	0
54	MG	CA	1607	1/1	0.87	0.27	52,52,52,52	0
54	MG	BA	3048	1/1	0.87	0.34	67,67,67,67	0
54	MG	DA	3152	1/1	0.87	0.21	77,77,77,77	0
54	MG	DA	3288	1/1	0.87	0.43	78,78,78,78	0
54	MG	BA	2931	1/1	0.87	0.47	32,32,32,32	0
54	MG	D2	101	1/1	0.87	0.27	66,66,66,66	0
54	MG	DB	208	1/1	0.87	0.31	96,96,96,96	0
54	MG	AA	1707	1/1	0.87	0.29	100,100,100,100	0
54	MG	DA	3294	1/1	0.87	0.28	61,61,61,61	0
54	MG	BA	3200	1/1	0.88	0.33	64,64,64,64	0
54	MG	BA	3150	1/1	0.88	0.38	79,79,79,79	0
54	MG	BA	3127	1/1	0.88	0.76	56,56,56,56	0
54	MG	AA	1650	1/1	0.88	0.29	103,103,103,103	0
54	MG	BA	3300	1/1	0.88	0.45	83,83,83,83	0
54	MG	DA	3287	1/1	0.88	0.51	69,69,69,69	0
54	MG	DA	3330	1/1	0.88	0.38	69,69,69,69	0
54	MG	DA	3145	1/1	0.88	0.42	70,70,70,70	0
54	MG	BA	2991	1/1	0.88	0.16	36,36,36,36	0
54	MG	DA	3041	1/1	0.88	0.17	51,51,51,51	0
54	MG	DB	207	1/1	0.88	0.28	72,72,72,72	0
54	MG	DA	3070	1/1	0.88	0.27	70,70,70,70	0
54	MG	DA	3173	1/1	0.88	0.18	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3241	1/1	0.88	0.26	60,60,60,60	0
54	MG	DA	3282	1/1	0.88	0.14	96,96,96,96	0
54	MG	AA	1605	1/1	0.88	0.57	42,42,42,42	0
54	MG	BA	3022	1/1	0.88	0.14	77,77,77,77	0
54	MG	DA	3286	1/1	0.88	0.34	98,98,98,98	0
54	MG	BA	3252	1/1	0.88	0.12	92,92,92,92	0
54	MG	AA	1629	1/1	0.88	0.36	72,72,72,72	0
54	MG	DA	3069	1/1	0.88	0.17	81,81,81,81	0
54	MG	BA	3133	1/1	0.88	0.26	67,67,67,67	0
54	MG	AA	1684	1/1	0.88	0.37	95,95,95,95	0
54	MG	BA	2966	1/1	0.88	0.09	75,75,75,75	0
54	MG	DA	3032	1/1	0.88	0.10	49,49,49,49	0
54	MG	CA	1728	1/1	0.88	0.55	82,82,82,82	0
54	MG	CA	1633	1/1	0.88	0.48	102,102,102,102	0
54	MG	BA	3148	1/1	0.88	0.35	68,68,68,68	0
54	MG	AA	1665	1/1	0.88	0.26	82,82,82,82	0
54	MG	CA	1731	1/1	0.88	0.13	90,90,90,90	0
54	MG	AA	1663	1/1	0.88	0.13	70,70,70,70	0
54	MG	BA	3243	1/1	0.88	0.17	82,82,82,82	0
54	MG	BB	208	1/1	0.88	0.47	109,109,109,109	0
54	MG	AA	1690	1/1	0.88	0.09	117,117,117,117	0
54	MG	CA	1715	1/1	0.88	0.36	74,74,74,74	0
54	MG	DA	2977	1/1	0.88	0.18	47,47,47,47	0
54	MG	DA	3154	1/1	0.88	0.33	94,94,94,94	0
54	MG	DA	3285	1/1	0.88	0.34	113,113,113,113	0
54	MG	BA	3289	1/1	0.88	0.25	65,65,65,65	0
54	MG	DA	3170	1/1	0.88	0.20	80,80,80,80	0
54	MG	CA	1611	1/1	0.88	0.19	76,76,76,76	0
54	MG	BA	2976	1/1	0.88	0.47	70,70,70,70	0
54	MG	DA	3158	1/1	0.88	0.18	59,59,59,59	0
54	MG	DA	3089	1/1	0.88	0.26	76,76,76,76	0
54	MG	DA	3009	1/1	0.88	0.48	49,49,49,49	0
54	MG	DE	301	1/1	0.88	0.24	44,44,44,44	0
54	MG	BA	3108	1/1	0.88	0.42	99,99,99,99	0
54	MG	DA	2945	1/1	0.88	0.61	41,41,41,41	0
54	MG	CA	1681	1/1	0.88	0.42	81,81,81,81	0
54	MG	BA	3049	1/1	0.88	0.14	86,86,86,86	0
54	MG	DA	3184	1/1	0.88	0.28	117,117,117,117	0
54	MG	BA	3094	1/1	0.89	0.68	70,70,70,70	0
54	MG	BA	3056	1/1	0.89	0.48	62,62,62,62	0
54	MG	DA	3007	1/1	0.89	0.19	43,43,43,43	0
54	MG	DA	3036	1/1	0.89	0.34	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	2979	1/1	0.89	0.22	69,69,69,69	0
54	MG	DA	3303	1/1	0.89	0.15	66,66,66,66	0
54	MG	DA	3305	1/1	0.89	0.12	110,110,110,110	0
54	MG	DA	3277	1/1	0.89	0.31	52,52,52,52	0
54	MG	DA	3038	1/1	0.89	0.26	71,71,71,71	0
54	MG	DA	2992	1/1	0.89	0.18	46,46,46,46	0
54	MG	DA	3310	1/1	0.89	0.27	52,52,52,52	0
54	MG	DA	3241	1/1	0.89	0.51	54,54,54,54	0
54	MG	BB	209	1/1	0.89	0.24	83,83,83,83	0
54	MG	DA	3221	1/1	0.89	0.18	68,68,68,68	0
54	MG	AA	1694	1/1	0.89	0.23	129,129,129,129	0
54	MG	BA	3097	1/1	0.89	0.29	53,53,53,53	0
54	MG	AA	1714	1/1	0.89	0.35	58,58,58,58	0
54	MG	DA	3137	1/1	0.89	0.18	68,68,68,68	0
54	MG	AA	1748	1/1	0.89	0.15	96,96,96,96	0
54	MG	BA	3017	1/1	0.89	0.22	69,69,69,69	0
54	MG	BA	3160	1/1	0.89	0.55	106,106,106,106	0
54	MG	DA	3264	1/1	0.89	0.24	61,61,61,61	0
54	MG	AA	1657	1/1	0.89	0.31	101,101,101,101	0
54	MG	BA	3080	1/1	0.89	0.14	73,73,73,73	0
54	MG	CA	1720	1/1	0.89	0.35	63,63,63,63	0
54	MG	DA	3138	1/1	0.89	0.12	70,70,70,70	0
54	MG	BA	3256	1/1	0.89	0.39	79,79,79,79	0
54	MG	AA	1637	1/1	0.89	0.45	61,61,61,61	0
54	MG	DA	3066	1/1	0.89	0.47	85,85,85,85	0
54	MG	DA	3329	1/1	0.89	0.71	69,69,69,69	0
54	MG	BA	3124	1/1	0.89	0.30	89,89,89,89	0
54	MG	BA	3129	1/1	0.89	0.14	75,75,75,75	0
54	MG	DA	2916	1/1	0.89	0.27	22,22,22,22	0
54	MG	BB	212	1/1	0.89	0.14	89,89,89,89	0
54	MG	BA	3074	1/1	0.89	0.34	61,61,61,61	0
54	MG	DA	3306	1/1	0.89	0.31	51,51,51,51	0
54	MG	DA	3008	1/1	0.90	0.47	59,59,59,59	0
54	MG	BB	214	1/1	0.90	0.20	101,101,101,101	0
54	MG	BA	3016	1/1	0.90	0.31	60,60,60,60	0
54	MG	BA	3166	1/1	0.90	0.39	74,74,74,74	0
54	MG	BA	3144	1/1	0.90	0.34	75,75,75,75	0
54	MG	DA	3155	1/1	0.90	0.07	124,124,124,124	0
54	MG	BA	3035	1/1	0.90	0.38	44,44,44,44	0
54	MG	DA	3224	1/1	0.90	0.17	72,72,72,72	0
54	MG	DA	3159	1/1	0.90	1.09	87,87,87,87	0
54	MG	BA	3126	1/1	0.90	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	2981	1/1	0.90	0.31	55,55,55,55	0
54	MG	DA	3180	1/1	0.90	0.26	77,77,77,77	0
54	MG	DA	3095	1/1	0.90	0.17	67,67,67,67	0
54	MG	DA	2936	1/1	0.90	0.36	27,27,27,27	0
54	MG	DA	3126	1/1	0.90	0.08	77,77,77,77	0
54	MG	BA	3001	1/1	0.90	0.31	59,59,59,59	0
54	MG	DA	3257	1/1	0.90	0.16	94,94,94,94	0
54	MG	CA	1638	1/1	0.90	0.19	65,65,65,65	0
54	MG	BA	2970	1/1	0.90	0.58	45,45,45,45	0
54	MG	AA	1751	1/1	0.90	0.18	72,72,72,72	0
54	MG	AA	1631	1/1	0.90	0.31	70,70,70,70	0
54	MG	DA	2975	1/1	0.90	0.07	58,58,58,58	0
54	MG	DA	2988	1/1	0.90	0.51	41,41,41,41	0
54	MG	BA	3045	1/1	0.90	0.20	80,80,80,80	0
54	MG	BA	2958	1/1	0.90	0.32	42,42,42,42	0
54	MG	DA	3301	1/1	0.90	0.29	80,80,80,80	0
54	MG	DA	3079	1/1	0.90	0.33	38,38,38,38	0
54	MG	AA	1647	1/1	0.90	0.24	85,85,85,85	0
54	MG	BA	2992	1/1	0.90	0.50	70,70,70,70	0
54	MG	AA	1735	1/1	0.90	0.20	104,104,104,104	0
54	MG	DA	3018	1/1	0.90	0.13	73,73,73,73	0
54	MG	BA	3131	1/1	0.90	0.26	67,67,67,67	0
54	MG	CA	1624	1/1	0.90	0.13	66,66,66,66	0
54	MG	DA	3035	1/1	0.90	0.42	77,77,77,77	0
54	MG	DA	3076	1/1	0.90	0.16	63,63,63,63	0
54	MG	BA	3285	1/1	0.90	0.23	87,87,87,87	0
54	MG	DA	3099	1/1	0.90	0.18	81,81,81,81	0
54	MG	DA	2991	1/1	0.90	0.24	31,31,31,31	0
54	MG	DA	3132	1/1	0.90	0.07	70,70,70,70	0
54	MG	BB	201	1/1	0.90	0.35	56,56,56,56	0
54	MG	BA	2962	1/1	0.90	0.17	17,17,17,17	0
54	MG	BB	207	1/1	0.90	0.11	105,105,105,105	0
54	MG	BA	3085	1/1	0.90	0.28	68,68,68,68	0
54	MG	AA	1687	1/1	0.90	0.08	73,73,73,73	0
54	MG	BA	3177	1/1	0.90	0.23	93,93,93,93	0
54	MG	AA	1749	1/1	0.90	0.24	90,90,90,90	0
54	MG	AA	1654	1/1	0.90	0.30	76,76,76,76	0
54	MG	DA	3108	1/1	0.90	0.19	50,50,50,50	0
54	MG	AA	1692	1/1	0.90	0.33	84,84,84,84	0
54	MG	AA	1721	1/1	0.90	0.55	66,66,66,66	0
54	MG	BA	2995	1/1	0.90	0.21	47,47,47,47	0
54	MG	BA	3223	1/1	0.90	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3014	1/1	0.90	0.20	47,47,47,47	0
54	MG	DA	3216	1/1	0.90	0.62	46,46,46,46	0
54	MG	DA	2982	1/1	0.90	0.20	33,33,33,33	0
54	MG	BA	3105	1/1	0.90	0.21	60,60,60,60	0
54	MG	CA	1739	1/1	0.90	0.11	99,99,99,99	0
54	MG	CA	1692	1/1	0.90	0.80	78,78,78,78	0
54	MG	BA	2961	1/1	0.90	0.38	43,43,43,43	0
54	MG	BA	3297	1/1	0.91	0.52	67,67,67,67	0
54	MG	DA	3005	1/1	0.91	0.32	33,33,33,33	0
54	MG	DA	3148	1/1	0.91	0.23	99,99,99,99	0
54	MG	CA	1647	1/1	0.91	0.28	77,77,77,77	0
54	MG	AA	1716	1/1	0.91	0.16	120,120,120,120	0
54	MG	BA	3147	1/1	0.91	0.32	72,72,72,72	0
54	MG	DA	3112	1/1	0.91	0.20	60,60,60,60	0
54	MG	DA	3046	1/1	0.91	0.09	76,76,76,76	0
54	MG	AA	1602	1/1	0.91	0.58	49,49,49,49	0
54	MG	AA	1634	1/1	0.91	0.19	70,70,70,70	0
54	MG	BB	203	1/1	0.91	0.14	83,83,83,83	0
54	MG	DA	2920	1/1	0.91	0.44	30,30,30,30	0
54	MG	AA	1688	1/1	0.91	0.14	68,68,68,68	0
54	MG	DA	2927	1/1	0.91	0.24	22,22,22,22	0
54	MG	CA	1631	1/1	0.91	0.13	68,68,68,68	0
54	MG	DA	3083	1/1	0.91	0.24	67,67,67,67	0
54	MG	DA	3146	1/1	0.91	0.13	95,95,95,95	0
54	MG	DA	3060	1/1	0.91	0.21	87,87,87,87	0
54	MG	BA	3238	1/1	0.91	0.14	91,91,91,91	0
54	MG	DA	3133	1/1	0.91	0.13	89,89,89,89	0
54	MG	BA	2964	1/1	0.91	0.47	30,30,30,30	0
54	MG	BA	2980	1/1	0.91	0.26	40,40,40,40	0
54	MG	DA	3157	1/1	0.91	0.14	71,71,71,71	0
54	MG	AA	1630	1/1	0.91	0.37	70,70,70,70	0
54	MG	CA	1710	1/1	0.91	0.18	119,119,119,119	0
54	MG	DA	3086	1/1	0.91	0.69	92,92,92,92	0
54	MG	DA	3210	1/1	0.91	0.10	59,59,59,59	0
54	MG	DA	3093	1/1	0.91	0.39	69,69,69,69	0
54	MG	CA	1676	1/1	0.91	0.36	82,82,82,82	0
54	MG	DA	3011	1/1	0.91	0.14	99,99,99,99	0
54	MG	BA	3032	1/1	0.91	0.26	59,59,59,59	0
54	MG	DA	3245	1/1	0.91	0.55	54,54,54,54	0
54	MG	CA	1689	1/1	0.91	0.29	83,83,83,83	0
54	MG	BA	3135	1/1	0.91	0.23	77,77,77,77	0
54	MG	AA	1732	1/1	0.91	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3152	1/1	0.91	0.22	75,75,75,75	0
54	MG	BA	3261	1/1	0.91	0.30	53,53,53,53	0
54	MG	DA	2915	1/1	0.91	0.47	14,14,14,14	0
54	MG	CA	1702	1/1	0.91	0.70	68,68,68,68	0
54	MG	DA	3218	1/1	0.91	0.49	48,48,48,48	0
54	MG	CA	1657	1/1	0.91	0.39	78,78,78,78	0
54	MG	BA	3007	1/1	0.91	0.19	55,55,55,55	0
54	MG	BA	3067	1/1	0.91	0.08	86,86,86,86	0
54	MG	DA	3319	1/1	0.91	0.64	83,83,83,83	0
54	MG	DA	2960	1/1	0.91	0.29	42,42,42,42	0
54	MG	DA	3250	1/1	0.92	0.38	74,74,74,74	0
54	MG	BA	2993	1/1	0.92	0.24	58,58,58,58	0
54	MG	CA	1625	1/1	0.92	0.10	94,94,94,94	0
54	MG	BA	3018	1/1	0.92	0.31	68,68,68,68	0
54	MG	BA	3250	1/1	0.92	0.13	95,95,95,95	0
54	MG	AA	1746	1/1	0.92	0.27	100,100,100,100	0
54	MG	DA	3040	1/1	0.92	0.36	41,41,41,41	0
54	MG	DA	3129	1/1	0.92	0.43	63,63,63,63	0
54	MG	BA	3029	1/1	0.92	0.59	63,63,63,63	0
54	MG	DA	3253	1/1	0.92	0.17	92,92,92,92	0
54	MG	BA	3065	1/1	0.92	0.20	61,61,61,61	0
54	MG	CA	1677	1/1	0.92	0.28	85,85,85,85	0
54	MG	BA	3207	1/1	0.92	0.36	94,94,94,94	0
54	MG	BA	3257	1/1	0.92	0.32	64,64,64,64	0
54	MG	CA	1679	1/1	0.92	0.12	93,93,93,93	0
54	MG	DA	3315	1/1	0.92	0.16	52,52,52,52	0
54	MG	BA	2955	1/1	0.92	0.18	50,50,50,50	0
54	MG	DA	2998	1/1	0.92	0.38	68,68,68,68	0
54	MG	BA	3222	1/1	0.92	1.17	91,91,91,91	0
54	MG	AA	1632	1/1	0.92	0.11	68,68,68,68	0
54	MG	DA	3147	1/1	0.92	0.14	78,78,78,78	0
54	MG	BA	3230	1/1	0.92	0.51	44,44,44,44	0
54	MG	BA	3082	1/1	0.92	0.18	61,61,61,61	0
54	MG	BA	3122	1/1	0.92	0.30	101,101,101,101	0
54	MG	DA	3240	1/1	0.92	0.38	60,60,60,60	0
54	MG	BA	3239	1/1	0.92	0.57	82,82,82,82	0
54	MG	CA	1656	1/1	0.92	0.14	79,79,79,79	0
54	MG	CA	1709	1/1	0.92	0.39	81,81,81,81	0
54	MG	DA	2950	1/1	0.92	0.21	29,29,29,29	0
54	MG	DA	2939	1/1	0.92	0.17	40,40,40,40	0
54	MG	AA	1725	1/1	0.92	0.20	72,72,72,72	0
54	MG	BA	3199	1/1	0.92	0.63	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3248	1/1	0.92	0.29	75,75,75,75	0
54	MG	BA	3298	1/1	0.92	0.10	74,74,74,74	0
54	MG	AA	1760	1/1	0.92	0.16	84,84,84,84	0
54	MG	CA	1623	1/1	0.92	0.48	99,99,99,99	0
54	MG	DA	3124	1/1	0.92	0.09	90,90,90,90	0
54	MG	AA	1609	1/1	0.92	0.62	70,70,70,70	0
54	MG	DA	3254	1/1	0.92	0.53	79,79,79,79	0
54	MG	DA	3336	1/1	0.92	0.07	89,89,89,89	0
54	MG	BA	3270	1/1	0.92	0.31	61,61,61,61	0
54	MG	DA	3125	1/1	0.92	0.28	81,81,81,81	0
54	MG	CA	1713	1/1	0.92	0.17	80,80,80,80	0
54	MG	DA	2913	1/1	0.92	0.41	17,17,17,17	0
54	MG	BA	3294	1/1	0.92	0.17	64,64,64,64	0
54	MG	CA	1609	1/1	0.92	0.23	93,93,93,93	0
54	MG	CA	1680	1/1	0.92	0.32	58,58,58,58	0
54	MG	BA	3047	1/1	0.92	0.39	65,65,65,65	0
54	MG	DA	2974	1/1	0.92	0.08	46,46,46,46	0
54	MG	BA	3187	1/1	0.92	0.46	40,40,40,40	0
54	MG	DB	205	1/1	0.92	0.10	79,79,79,79	0
54	MG	BA	2987	1/1	0.92	0.28	59,59,59,59	0
54	MG	AA	1756	1/1	0.92	0.20	106,106,106,106	0
54	MG	CA	1726	1/1	0.92	0.34	87,87,87,87	0
54	MG	DA	3335	1/1	0.92	0.29	90,90,90,90	0
54	MG	BA	2944	1/1	0.92	0.16	17,17,17,17	0
54	MG	BA	3128	1/1	0.92	0.48	59,59,59,59	0
54	MG	BA	2997	1/1	0.92	0.38	57,57,57,57	0
54	MG	DA	3026	1/1	0.92	0.08	48,48,48,48	0
54	MG	DA	2948	1/1	0.92	0.33	52,52,52,52	0
54	MG	BA	3088	1/1	0.92	0.55	73,73,73,73	0
54	MG	DA	3280	1/1	0.92	0.30	84,84,84,84	0
54	MG	DA	2935	1/1	0.93	0.61	30,30,30,30	0
54	MG	BA	3043	1/1	0.93	0.30	70,70,70,70	0
54	MG	DA	3273	1/1	0.93	0.29	85,85,85,85	0
54	MG	DA	3179	1/1	0.93	0.19	68,68,68,68	0
54	MG	AA	1662	1/1	0.93	0.23	53,53,53,53	0
54	MG	DA	2925	1/1	0.93	0.45	24,24,24,24	0
54	MG	DA	3275	1/1	0.93	0.17	78,78,78,78	0
54	MG	BA	2914	1/1	0.93	0.43	31,31,31,31	0
54	MG	AA	1683	1/1	0.93	0.16	102,102,102,102	0
54	MG	BA	3276	1/1	0.93	0.21	65,65,65,65	0
54	MG	AA	1652	1/1	0.93	0.20	89,89,89,89	0
54	MG	DA	3028	1/1	0.93	0.15	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2978	1/1	0.93	0.35	59,59,59,59	0
54	MG	DA	3247	1/1	0.93	0.21	40,40,40,40	0
54	MG	DA	3107	1/1	0.93	0.27	67,67,67,67	0
54	MG	BA	3228	1/1	0.93	0.12	66,66,66,66	0
54	MG	CA	1622	1/1	0.93	0.23	79,79,79,79	0
54	MG	BA	3055	1/1	0.93	0.17	60,60,60,60	0
54	MG	AA	1733	1/1	0.93	0.22	91,91,91,91	0
54	MG	BA	3142	1/1	0.93	0.09	89,89,89,89	0
54	MG	DA	2953	1/1	0.93	0.45	58,58,58,58	0
54	MG	BA	3092	1/1	0.93	0.17	63,63,63,63	0
54	MG	DA	3118	1/1	0.93	0.25	62,62,62,62	0
54	MG	DA	2952	1/1	0.93	0.30	50,50,50,50	0
54	MG	BA	3202	1/1	0.93	0.60	63,63,63,63	0
54	MG	DA	3002	1/1	0.93	0.43	59,59,59,59	0
54	MG	AA	1726	1/1	0.93	0.08	108,108,108,108	0
54	MG	BA	2982	1/1	0.93	0.31	41,41,41,41	0
54	MG	DA	3153	1/1	0.93	0.28	85,85,85,85	0
54	MG	AA	1742	1/1	0.93	0.42	87,87,87,87	0
54	MG	DA	2965	1/1	0.93	0.39	57,57,57,57	0
54	MG	BA	3071	1/1	0.93	0.17	72,72,72,72	0
54	MG	DA	3025	1/1	0.93	0.16	69,69,69,69	0
54	MG	DA	3171	1/1	0.93	0.27	61,61,61,61	0
54	MG	CA	1732	1/1	0.93	0.23	73,73,73,73	0
54	MG	BA	3269	1/1	0.93	0.24	63,63,63,63	0
54	MG	DA	2941	1/1	0.93	0.23	37,37,37,37	0
54	MG	BA	3063	1/1	0.93	0.23	56,56,56,56	0
54	MG	DA	3314	1/1	0.93	0.54	102,102,102,102	0
54	MG	AA	1727	1/1	0.93	0.13	100,100,100,100	0
54	MG	DA	3052	1/1	0.93	0.16	107,107,107,107	0
54	MG	DA	2978	1/1	0.93	0.28	44,44,44,44	0
54	MG	DA	2942	1/1	0.93	0.29	39,39,39,39	0
54	MG	BA	3290	1/1	0.93	0.27	42,42,42,42	0
54	MG	CA	1693	1/1	0.93	0.34	65,65,65,65	0
54	MG	BA	3002	1/1	0.93	0.38	45,45,45,45	0
54	MG	BA	3205	1/1	0.93	0.23	38,38,38,38	0
54	MG	CA	1718	1/1	0.93	0.15	78,78,78,78	0
54	MG	BA	3193	1/1	0.93	0.38	53,53,53,53	0
54	MG	DA	3084	1/1	0.93	0.11	146,146,146,146	0
54	MG	AA	1711	1/1	0.93	0.56	53,53,53,53	0
54	MG	BA	3292	1/1	0.93	0.19	72,72,72,72	0
54	MG	BA	3307	1/1	0.93	0.14	68,68,68,68	0
54	MG	BA	3194	1/1	0.93	0.53	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3121	1/1	0.93	0.26	77,77,77,77	0
54	MG	BA	3003	1/1	0.93	0.28	48,48,48,48	0
54	MG	CA	1654	1/1	0.93	0.13	111,111,111,111	0
54	MG	CA	1666	1/1	0.93	0.08	116,116,116,116	0
54	MG	DA	3139	1/1	0.93	0.28	60,60,60,60	0
54	MG	DA	3261	1/1	0.93	0.27	73,73,73,73	0
54	MG	CA	1737	1/1	0.93	0.20	70,70,70,70	0
54	MG	BA	3249	1/1	0.93	0.23	37,37,37,37	0
54	MG	BA	3081	1/1	0.93	0.14	65,65,65,65	0
54	MG	DA	2986	1/1	0.93	0.22	55,55,55,55	0
54	MG	BA	2921	1/1	0.94	0.39	21,21,21,21	0
54	MG	CA	1714	1/1	0.94	0.30	74,74,74,74	0
54	MG	DA	3117	1/1	0.94	0.20	87,87,87,87	0
54	MG	AA	1608	1/1	0.94	0.36	47,47,47,47	0
54	MG	DA	2964	1/1	0.94	0.20	34,34,34,34	0
54	MG	BA	3235	1/1	0.94	0.13	62,62,62,62	0
54	MG	AA	1703	1/1	0.94	0.15	83,83,83,83	0
54	MG	BA	3040	1/1	0.94	0.26	58,58,58,58	0
54	MG	DA	3022	1/1	0.94	0.32	60,60,60,60	0
54	MG	DA	2989	1/1	0.94	0.34	45,45,45,45	0
54	MG	DA	3192	1/1	0.94	0.29	30,30,30,30	0
54	MG	BA	2905	1/1	0.94	0.54	12,12,12,12	0
54	MG	DA	3266	1/1	0.94	0.34	83,83,83,83	0
54	MG	BA	3042	1/1	0.94	0.15	90,90,90,90	0
54	MG	DA	2946	1/1	0.94	0.55	24,24,24,24	0
54	MG	DA	3234	1/1	0.94	0.10	130,130,130,130	0
54	MG	CA	1604	1/1	0.94	0.23	59,59,59,59	0
54	MG	DA	2934	1/1	0.94	0.44	25,25,25,25	0
54	MG	DA	2967	1/1	0.94	0.35	54,54,54,54	0
54	MG	AA	1750	1/1	0.94	0.46	109,109,109,109	0
54	MG	BA	2979	1/1	0.94	0.25	40,40,40,40	0
54	MG	BA	3244	1/1	0.94	0.78	47,47,47,47	0
54	MG	CA	1642	1/1	0.94	0.17	71,71,71,71	0
54	MG	BA	3058	1/1	0.94	0.11	114,114,114,114	0
54	MG	DA	3019	1/1	0.94	0.36	51,51,51,51	0
54	MG	AA	1728	1/1	0.94	0.88	105,105,105,105	0
54	MG	CA	1651	1/1	0.94	0.09	99,99,99,99	0
54	MG	DB	204	1/1	0.94	0.07	75,75,75,75	0
54	MG	BA	3192	1/1	0.94	0.58	52,52,52,52	0
54	MG	BA	3059	1/1	0.94	0.22	60,60,60,60	0
54	MG	DA	2963	1/1	0.94	0.39	53,53,53,53	0
54	MG	CA	1682	1/1	0.94	0.21	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2935	1/1	0.94	0.56	34,34,34,34	0
54	MG	BA	2915	1/1	0.94	0.17	4,4,4,4	0
54	MG	BA	3028	1/1	0.94	0.45	62,62,62,62	0
54	MG	BA	3057	1/1	0.94	0.42	63,63,63,63	0
54	MG	BA	3209	1/1	0.94	0.27	69,69,69,69	0
54	MG	DA	3333	1/1	0.94	0.15	126,126,126,126	0
54	MG	CA	1627	1/1	0.94	0.18	67,67,67,67	0
54	MG	DA	3215	1/1	0.94	0.45	39,39,39,39	0
54	MG	DA	3283	1/1	0.94	0.27	53,53,53,53	0
54	MG	BA	2973	1/1	0.94	0.15	61,61,61,61	0
54	MG	BA	3206	1/1	0.94	0.10	60,60,60,60	0
54	MG	BA	2912	1/1	0.94	0.66	36,36,36,36	0
54	MG	BA	3107	1/1	0.94	0.26	87,87,87,87	0
54	MG	DA	3031	1/1	0.94	0.07	62,62,62,62	0
54	MG	BA	3106	1/1	0.94	0.21	70,70,70,70	0
54	MG	BA	3237	1/1	0.94	0.14	60,60,60,60	0
54	MG	CA	1664	1/1	0.94	0.20	82,82,82,82	0
54	MG	BA	2927	1/1	0.94	0.29	37,37,37,37	0
54	MG	DA	3114	1/1	0.94	0.37	83,83,83,83	0
54	MG	BA	3132	1/1	0.94	0.20	79,79,79,79	0
54	MG	AA	1603	1/1	0.94	0.32	35,35,35,35	0
54	MG	CA	1675	1/1	0.94	0.28	107,107,107,107	0
54	MG	DA	3150	1/1	0.94	0.21	62,62,62,62	0
54	MG	BA	2949	1/1	0.94	0.18	47,47,47,47	0
54	MG	BA	2999	1/1	0.94	0.24	45,45,45,45	0
54	MG	DA	3001	1/1	0.94	0.12	56,56,56,56	0
54	MG	DA	3326	1/1	0.94	0.18	85,85,85,85	0
54	MG	BA	2960	1/1	0.94	0.57	40,40,40,40	0
54	MG	AA	1741	1/1	0.94	0.13	74,74,74,74	0
54	MG	BA	2994	1/1	0.94	0.65	56,56,56,56	0
54	MG	BA	3130	1/1	0.94	0.17	78,78,78,78	0
54	MG	DB	211	1/1	0.94	0.15	109,109,109,109	0
54	MG	BA	3044	1/1	0.94	0.12	64,64,64,64	0
54	MG	BA	3137	1/1	0.94	0.52	54,54,54,54	0
54	MG	CA	1661	1/1	0.94	0.49	92,92,92,92	0
54	MG	AA	1668	1/1	0.94	0.08	90,90,90,90	0
54	MG	DA	3054	1/1	0.94	0.33	75,75,75,75	0
54	MG	CA	1655	1/1	0.94	0.23	80,80,80,80	0
54	MG	AA	1616	1/1	0.94	0.19	63,63,63,63	0
54	MG	DA	3062	1/1	0.94	0.12	65,65,65,65	0
54	MG	AA	1627	1/1	0.94	0.12	85,85,85,85	0
54	MG	CA	1603	1/1	0.94	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1667	1/1	0.94	0.10	67,67,67,67	0
54	MG	DA	3193	1/1	0.94	0.57	51,51,51,51	0
54	MG	CA	1722	1/1	0.94	0.38	108,108,108,108	0
54	MG	CA	1678	1/1	0.94	0.11	107,107,107,107	0
54	MG	DA	3051	1/1	0.94	0.15	89,89,89,89	0
54	MG	CA	1635	1/1	0.94	0.23	67,67,67,67	0
54	MG	DA	3020	1/1	0.94	0.17	63,63,63,63	0
54	MG	AA	1638	1/1	0.94	0.48	63,63,63,63	0
54	MG	CA	1665	1/1	0.94	0.25	89,89,89,89	0
54	MG	DA	2914	1/1	0.94	0.46	27,27,27,27	0
54	MG	DA	3304	1/1	0.94	0.26	59,59,59,59	0
54	MG	DA	3176	1/1	0.94	0.25	83,83,83,83	0
54	MG	BA	3064	1/1	0.95	0.31	40,40,40,40	0
54	MG	AA	1686	1/1	0.95	0.13	72,72,72,72	0
54	MG	CA	1721	1/1	0.95	0.33	101,101,101,101	0
54	MG	CA	1686	1/1	0.95	0.25	60,60,60,60	0
54	MG	DA	3045	1/1	0.95	0.30	48,48,48,48	0
54	MG	BA	3234	1/1	0.95	0.22	61,61,61,61	0
54	MG	BA	2954	1/1	0.95	0.19	52,52,52,52	0
54	MG	DA	2928	1/1	0.95	0.22	43,43,43,43	0
54	MG	DA	3270	1/1	0.95	0.29	81,81,81,81	0
54	MG	DA	3140	1/1	0.95	0.14	67,67,67,67	0
54	MG	BA	3185	1/1	0.95	0.24	56,56,56,56	0
54	MG	CA	1707	1/1	0.95	0.08	104,104,104,104	0
54	MG	BB	215	1/1	0.95	0.19	131,131,131,131	0
54	MG	BA	3227	1/1	0.95	0.15	48,48,48,48	0
54	MG	CA	1730	1/1	0.95	0.08	122,122,122,122	0
54	MG	CA	1716	1/1	0.95	0.23	77,77,77,77	0
54	MG	BA	2916	1/1	0.95	0.43	38,38,38,38	0
54	MG	DA	2957	1/1	0.95	0.09	63,63,63,63	0
54	MG	DA	3058	1/1	0.95	0.11	54,54,54,54	0
54	MG	AA	1708	1/1	0.95	0.15	101,101,101,101	0
54	MG	DA	3106	1/1	0.95	0.37	67,67,67,67	0
54	MG	BA	2909	1/1	0.95	0.41	24,24,24,24	0
54	MG	DB	210	1/1	0.95	0.06	74,74,74,74	0
54	MG	BA	2957	1/1	0.95	0.57	35,35,35,35	0
54	MG	BA	2941	1/1	0.95	0.64	50,50,50,50	0
54	MG	BA	3170	1/1	0.95	0.12	64,64,64,64	0
54	MG	BA	2967	1/1	0.95	0.41	24,24,24,24	0
54	MG	BA	2920	1/1	0.95	0.35	28,28,28,28	0
54	MG	DA	2933	1/1	0.95	0.47	30,30,30,30	0
54	MG	DB	217	1/1	0.95	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2924	1/1	0.95	0.46	47,47,47,47	0
54	MG	DA	3233	1/1	0.95	0.42	57,57,57,57	0
54	MG	BA	3021	1/1	0.95	0.19	60,60,60,60	0
54	MG	DA	2954	1/1	0.95	0.31	28,28,28,28	0
54	MG	CA	1643	1/1	0.95	0.13	58,58,58,58	0
54	MG	DA	3151	1/1	0.95	0.37	82,82,82,82	0
54	MG	DA	3232	1/1	0.95	0.34	39,39,39,39	0
54	MG	BA	2926	1/1	0.95	0.55	31,31,31,31	0
54	MG	DA	2905	1/1	0.95	0.38	9,9,9,9	0
54	MG	CA	1617	1/1	0.95	0.33	90,90,90,90	0
54	MG	DA	3214	1/1	0.95	0.34	46,46,46,46	0
54	MG	DA	2956	1/1	0.95	0.28	45,45,45,45	0
54	MG	BA	2972	1/1	0.95	0.35	49,49,49,49	0
54	MG	AA	1619	1/1	0.95	0.16	80,80,80,80	0
54	MG	BA	3279	1/1	0.95	0.28	77,77,77,77	0
54	MG	CA	1630	1/1	0.95	0.33	70,70,70,70	0
54	MG	DA	2996	1/1	0.95	0.40	43,43,43,43	0
54	MG	BA	3246	1/1	0.95	0.24	73,73,73,73	0
54	MG	DA	2955	1/1	0.95	0.45	40,40,40,40	0
54	MG	BA	2983	1/1	0.95	0.45	62,62,62,62	0
54	MG	BA	2990	1/1	0.95	0.19	54,54,54,54	0
54	MG	DA	3135	1/1	0.95	0.22	65,65,65,65	0
54	MG	CA	1613	1/1	0.95	0.24	87,87,87,87	0
54	MG	DA	3182	1/1	0.95	0.60	86,86,86,86	0
54	MG	AA	1633	1/1	0.95	0.15	73,73,73,73	0
54	MG	BA	2923	1/1	0.95	0.33	29,29,29,29	0
54	MG	AA	1759	1/1	0.95	0.13	81,81,81,81	0
54	MG	BA	2989	1/1	0.95	0.35	53,53,53,53	0
54	MG	BA	3102	1/1	0.95	0.27	69,69,69,69	0
54	MG	BA	3254	1/1	0.95	0.47	81,81,81,81	0
54	MG	AA	1615	1/1	0.95	0.15	42,42,42,42	0
54	MG	DA	3321	1/1	0.95	0.51	30,30,30,30	0
54	MG	DA	2968	1/1	0.95	0.27	56,56,56,56	0
54	MG	DA	2922	1/1	0.95	0.32	7,7,7,7	0
54	MG	AA	1670	1/1	0.95	0.14	85,85,85,85	0
54	MG	DA	3239	1/1	0.95	0.23	42,42,42,42	0
54	MG	BA	2942	1/1	0.95	0.35	22,22,22,22	0
54	MG	BA	2937	1/1	0.95	0.33	36,36,36,36	0
54	MG	BA	3154	1/1	0.95	0.22	89,89,89,89	0
54	MG	DA	2943	1/1	0.95	0.41	32,32,32,32	0
54	MG	BA	3277	1/1	0.95	0.27	71,71,71,71	0
54	MG	DA	2904	1/1	0.95	0.46	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2939	1/1	0.95	0.46	26,26,26,26	0
54	MG	DA	3122	1/1	0.95	0.22	87,87,87,87	0
54	MG	BA	3089	1/1	0.95	0.29	59,59,59,59	0
54	MG	BA	2984	1/1	0.95	0.22	41,41,41,41	0
54	MG	DA	2980	1/1	0.95	0.18	63,63,63,63	0
54	MG	DB	213	1/1	0.95	0.45	63,63,63,63	0
54	MG	AA	1659	1/1	0.96	0.42	51,51,51,51	0
54	MG	BA	3196	1/1	0.96	0.23	51,51,51,51	0
54	MG	DA	3164	1/1	0.96	0.05	88,88,88,88	0
54	MG	AA	1628	1/1	0.96	0.38	62,62,62,62	0
54	MG	AA	1613	1/1	0.96	0.15	47,47,47,47	0
54	MG	BA	3293	1/1	0.96	0.20	86,86,86,86	0
55	ZN	CD	301	1/1	0.96	0.24	131,131,131,131	0
54	MG	DA	3292	1/1	0.96	0.47	33,33,33,33	0
54	MG	CA	1605	1/1	0.96	0.21	56,56,56,56	0
54	MG	AA	1636	1/1	0.96	0.45	76,76,76,76	0
54	MG	DA	2947	1/1	0.96	0.24	40,40,40,40	0
54	MG	DA	3016	1/1	0.96	0.21	74,74,74,74	0
54	MG	CA	1640	1/1	0.96	0.38	69,69,69,69	0
54	MG	BA	2940	1/1	0.96	0.30	29,29,29,29	0
54	MG	CA	1669	1/1	0.96	0.15	66,66,66,66	0
54	MG	AA	1715	1/1	0.96	0.35	63,63,63,63	0
54	MG	DB	201	1/1	0.96	0.24	63,63,63,63	0
54	MG	AA	1648	1/1	0.96	0.40	76,76,76,76	0
54	MG	BA	3179	1/1	0.96	0.48	19,19,19,19	0
54	MG	BA	3010	1/1	0.96	0.15	37,37,37,37	0
54	MG	BA	2981	1/1	0.96	0.16	48,48,48,48	0
54	MG	BA	2908	1/1	0.96	0.47	18,18,18,18	0
54	MG	AA	1601	1/1	0.96	0.44	31,31,31,31	0
54	MG	DA	3197	1/1	0.96	0.34	28,28,28,28	0
55	ZN	CN	101	1/1	0.96	0.10	144,144,144,144	0
54	MG	CA	1652	1/1	0.96	0.43	85,85,85,85	0
54	MG	DA	3213	1/1	0.96	0.20	66,66,66,66	0
54	MG	DA	3073	1/1	0.96	0.10	80,80,80,80	0
54	MG	AA	1611	1/1	0.96	0.27	49,49,49,49	0
54	MG	DA	2985	1/1	0.96	0.37	48,48,48,48	0
54	MG	BA	3024	1/1	0.96	0.53	67,67,67,67	0
54	MG	CA	1673	1/1	0.96	0.15	73,73,73,73	0
54	MG	BA	2907	1/1	0.96	0.26	7,7,7,7	0
54	MG	BA	3070	1/1	0.96	0.24	75,75,75,75	0
54	MG	BA	3120	1/1	0.96	0.29	57,57,57,57	0
54	MG	DA	2901	1/1	0.96	0.46	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3056	1/1	0.96	0.19	48,48,48,48	0
54	MG	BA	2998	1/1	0.96	0.22	46,46,46,46	0
54	MG	DA	2929	1/1	0.96	0.35	39,39,39,39	0
54	MG	BA	3162	1/1	0.96	0.08	94,94,94,94	0
54	MG	DA	3208	1/1	0.96	0.41	49,49,49,49	0
54	MG	CA	1670	1/1	0.96	0.47	128,128,128,128	0
54	MG	DA	3104	1/1	0.96	0.27	99,99,99,99	0
54	MG	BA	3052	1/1	0.96	0.23	56,56,56,56	0
54	MG	AA	1671	1/1	0.96	0.14	114,114,114,114	0
54	MG	BA	3231	1/1	0.96	0.16	22,22,22,22	0
54	MG	AA	1624	1/1	0.96	0.36	67,67,67,67	0
54	MG	BA	3251	1/1	0.96	0.10	64,64,64,64	0
54	MG	DA	3015	1/1	0.96	0.21	74,74,74,74	0
54	MG	DA	3211	1/1	0.96	0.18	38,38,38,38	0
54	MG	AA	1705	1/1	0.96	0.30	92,92,92,92	0
54	MG	CA	1660	1/1	0.96	0.16	100,100,100,100	0
54	MG	DA	2969	1/1	0.96	0.18	42,42,42,42	0
54	MG	BA	3182	1/1	0.96	0.51	20,20,20,20	0
54	MG	BA	3184	1/1	0.96	0.32	42,42,42,42	0
54	MG	AA	1635	1/1	0.96	0.33	68,68,68,68	0
54	MG	AA	1604	1/1	0.96	0.12	57,57,57,57	0
54	MG	BA	3156	1/1	0.96	0.28	80,80,80,80	0
54	MG	DA	3236	1/1	0.96	0.59	63,63,63,63	0
54	MG	AA	1744	1/1	0.96	0.25	82,82,82,82	0
54	MG	BA	3076	1/1	0.96	0.25	68,68,68,68	0
54	MG	DA	3225	1/1	0.96	0.08	80,80,80,80	0
54	MG	BA	3087	1/1	0.96	0.10	69,69,69,69	0
54	MG	BA	3096	1/1	0.96	0.24	65,65,65,65	0
54	MG	DA	2966	1/1	0.96	0.35	70,70,70,70	0
54	MG	DA	2911	1/1	0.96	0.40	7,7,7,7	0
54	MG	DA	3053	1/1	0.96	0.27	61,61,61,61	0
54	MG	BA	3183	1/1	0.96	0.37	27,27,27,27	0
54	MG	AA	1724	1/1	0.96	0.29	85,85,85,85	0
54	MG	DA	3042	1/1	0.96	0.56	79,79,79,79	0
54	MG	DA	3067	1/1	0.96	0.20	63,63,63,63	0
54	MG	DA	3144	1/1	0.96	0.16	72,72,72,72	0
54	MG	DA	3160	1/1	0.96	0.16	71,71,71,71	0
54	MG	DA	2958	1/1	0.96	0.16	2,2,2,2	0
54	MG	DA	3198	1/1	0.96	0.29	26,26,26,26	0
54	MG	CA	1649	1/1	0.96	0.22	80,80,80,80	0
54	MG	BA	2922	1/1	0.97	0.47	25,25,25,25	0
54	MG	DA	2909	1/1	0.97	0.41	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3011	1/1	0.97	0.15	83,83,83,83	0
54	MG	BA	3195	1/1	0.97	0.16	53,53,53,53	0
54	MG	BA	2910	1/1	0.97	0.53	27,27,27,27	0
54	MG	CA	1626	1/1	0.97	0.33	65,65,65,65	0
54	MG	DA	2971	1/1	0.97	0.23	47,47,47,47	0
54	MG	CA	1719	1/1	0.97	0.13	78,78,78,78	0
54	MG	BA	3215	1/1	0.97	0.36	68,68,68,68	0
54	MG	BA	3180	1/1	0.97	0.27	26,26,26,26	0
54	MG	BA	3274	1/1	0.97	0.06	78,78,78,78	0
54	MG	DA	2990	1/1	0.97	0.20	35,35,35,35	0
54	MG	DA	3227	1/1	0.97	0.32	34,34,34,34	0
54	MG	DA	3206	1/1	0.97	0.32	37,37,37,37	0
54	MG	BA	2919	1/1	0.97	0.42	24,24,24,24	0
54	MG	CA	1653	1/1	0.97	0.20	84,84,84,84	0
54	MG	DA	3217	1/1	0.97	0.12	56,56,56,56	0
54	MG	CA	1629	1/1	0.97	0.24	106,106,106,106	0
54	MG	BA	3216	1/1	0.97	0.19	65,65,65,65	0
54	MG	DA	2949	1/1	0.97	0.54	41,41,41,41	0
54	MG	BA	3077	1/1	0.97	0.09	75,75,75,75	0
54	MG	DA	3039	1/1	0.97	0.29	48,48,48,48	0
54	MG	AA	1622	1/1	0.97	0.81	88,88,88,88	0
54	MG	CA	1695	1/1	0.97	0.37	80,80,80,80	0
54	MG	BA	2928	1/1	0.97	0.35	42,42,42,42	0
54	MG	BA	2911	1/1	0.97	0.47	23,23,23,23	0
54	MG	BA	2952	1/1	0.97	0.28	38,38,38,38	0
54	MG	BA	3151	1/1	0.97	0.71	56,56,56,56	0
54	MG	CA	1619	1/1	0.97	0.34	61,61,61,61	0
54	MG	DA	2944	1/1	0.97	0.36	35,35,35,35	0
54	MG	BA	3015	1/1	0.97	0.42	58,58,58,58	0
54	MG	BA	2959	1/1	0.97	0.39	55,55,55,55	0
54	MG	BA	3286	1/1	0.97	0.38	67,67,67,67	0
54	MG	BA	3161	1/1	0.97	0.26	62,62,62,62	0
54	MG	BA	3260	1/1	0.97	0.13	62,62,62,62	0
54	MG	DA	3000	1/1	0.97	0.36	35,35,35,35	0
54	MG	DA	3096	1/1	0.97	0.37	40,40,40,40	0
54	MG	BA	3186	1/1	0.97	0.32	52,52,52,52	0
54	MG	BA	3232	1/1	0.97	0.40	24,24,24,24	0
54	MG	CA	1606	1/1	0.97	0.12	68,68,68,68	0
54	MG	DA	3063	1/1	0.97	0.26	79,79,79,79	0
54	MG	BA	3086	1/1	0.97	0.26	102,102,102,102	0
54	MG	AA	1656	1/1	0.97	0.31	72,72,72,72	0
54	MG	BA	2946	1/1	0.97	0.46	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3331	1/1	0.97	0.19	52,52,52,52	0
54	MG	DA	3252	1/1	0.97	0.10	44,44,44,44	0
54	MG	DA	2926	1/1	0.97	0.23	43,43,43,43	0
54	MG	BA	2904	1/1	0.97	0.39	13,13,13,13	0
54	MG	AA	1710	1/1	0.97	0.26	65,65,65,65	0
54	MG	BA	3053	1/1	0.97	0.20	67,67,67,67	0
54	MG	BA	2943	1/1	0.97	0.37	42,42,42,42	0
54	MG	BA	3233	1/1	0.97	0.23	52,52,52,52	0
54	MG	AA	1736	1/1	0.97	0.13	79,79,79,79	0
54	MG	BA	2913	1/1	0.97	0.33	16,16,16,16	0
54	MG	CA	1712	1/1	0.97	0.11	78,78,78,78	0
54	MG	BA	2938	1/1	0.97	0.20	10,10,10,10	0
54	MG	BB	202	1/1	0.97	0.24	75,75,75,75	0
54	MG	BA	2917	1/1	0.97	0.41	8,8,8,8	0
54	MG	DA	3293	1/1	0.97	0.10	67,67,67,67	0
54	MG	DA	2973	1/1	0.97	0.30	50,50,50,50	0
54	MG	AA	1666	1/1	0.97	0.10	100,100,100,100	0
54	MG	AA	1607	1/1	0.97	0.21	54,54,54,54	0
54	MG	BA	3273	1/1	0.97	0.17	83,83,83,83	0
54	MG	DB	202	1/1	0.98	0.59	64,64,64,64	0
54	MG	CA	1615	1/1	0.98	0.27	51,51,51,51	0
54	MG	BA	2901	1/1	0.98	0.40	23,23,23,23	0
54	MG	DA	3156	1/1	0.98	0.18	78,78,78,78	0
54	MG	AA	1743	1/1	0.98	0.47	83,83,83,83	0
54	MG	BA	2951	1/1	0.98	0.38	28,28,28,28	0
54	MG	BA	3134	1/1	0.98	0.17	64,64,64,64	0
54	MG	BA	3211	1/1	0.98	0.37	59,59,59,59	0
54	MG	DA	3194	1/1	0.98	0.36	10,10,10,10	0
54	MG	BA	3020	1/1	0.98	0.30	62,62,62,62	0
54	MG	BA	3046	1/1	0.98	0.92	87,87,87,87	0
54	MG	BA	3174	1/1	0.98	0.20	84,84,84,84	0
54	MG	BA	3167	1/1	0.98	0.14	50,50,50,50	0
54	MG	DA	2902	1/1	0.98	0.40	10,10,10,10	0
54	MG	DA	2903	1/1	0.98	0.33	7,7,7,7	0
54	MG	AA	1606	1/1	0.98	0.36	53,53,53,53	0
54	MG	DA	3195	1/1	0.98	0.26	51,51,51,51	0
54	MG	BA	3224	1/1	0.98	0.22	45,45,45,45	0
54	MG	BA	3296	1/1	0.98	0.16	47,47,47,47	0
54	MG	BA	3181	1/1	0.98	0.53	22,22,22,22	0
54	MG	DA	3081	1/1	0.98	0.10	71,71,71,71	0
54	MG	BA	2934	1/1	0.98	0.44	28,28,28,28	0
54	MG	BA	3210	1/1	0.98	0.33	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	2923	1/1	0.98	0.23	17,17,17,17	0
54	MG	DA	2908	1/1	0.98	0.26	24,24,24,24	0
54	MG	BA	2956	1/1	0.98	0.46	35,35,35,35	0
54	MG	CA	1659	1/1	0.98	0.38	71,71,71,71	0
54	MG	DA	3183	1/1	0.98	0.09	83,83,83,83	0
54	MG	DA	2907	1/1	0.98	0.47	7,7,7,7	0
54	MG	DA	3075	1/1	0.98	0.23	64,64,64,64	0
54	MG	DA	3328	1/1	0.98	0.10	45,45,45,45	0
54	MG	BA	2918	1/1	0.98	0.35	17,17,17,17	0
54	MG	DA	2997	1/1	0.98	0.17	35,35,35,35	0
54	MG	BA	2945	1/1	0.98	0.22	72,72,72,72	0
54	MG	DA	2906	1/1	0.98	0.41	27,27,27,27	0
54	MG	DA	3255	1/1	0.98	0.15	101,101,101,101	0
54	MG	DA	2961	1/1	0.98	0.15	29,29,29,29	0
54	MG	DA	2962	1/1	0.98	0.38	37,37,37,37	0
54	MG	BA	2974	1/1	0.98	0.20	45,45,45,45	0
54	MG	DA	3044	1/1	0.98	0.08	59,59,59,59	0
54	MG	DA	2937	1/1	0.98	0.55	25,25,25,25	0
54	MG	BA	3214	1/1	0.98	0.41	53,53,53,53	0
54	MG	BA	2947	1/1	0.98	0.30	14,14,14,14	0
54	MG	BA	2933	1/1	0.98	0.30	32,32,32,32	0
54	MG	DA	3203	1/1	0.98	0.23	46,46,46,46	0
54	MG	DA	3048	1/1	0.98	0.09	66,66,66,66	0
54	MG	DA	2919	1/1	0.98	0.28	45,45,45,45	0
54	MG	BA	2977	1/1	0.98	0.28	52,52,52,52	0
54	MG	BA	3304	1/1	0.98	0.06	124,124,124,124	0
54	MG	DA	2930	1/1	0.98	0.15	36,36,36,36	0
54	MG	DA	2910	1/1	0.98	0.30	6,6,6,6	0
54	MG	DA	3102	1/1	0.98	0.20	68,68,68,68	0
54	MG	DA	2921	1/1	0.98	0.42	17,17,17,17	0
54	MG	CA	1644	1/1	0.98	0.45	77,77,77,77	0
54	MG	BA	3203	1/1	0.98	0.19	41,41,41,41	0
54	MG	BA	3264	1/1	0.98	0.14	116,116,116,116	0
54	MG	DA	2976	1/1	0.98	0.30	37,37,37,37	0
54	MG	DA	2984	1/1	0.98	0.20	66,66,66,66	0
54	MG	DA	2924	1/1	0.98	0.48	41,41,41,41	0
54	MG	BA	2953	1/1	0.98	0.16	37,37,37,37	0
54	MG	DA	3219	1/1	0.98	0.29	67,67,67,67	0
54	MG	AA	1672	1/1	0.98	0.46	101,101,101,101	0
54	MG	BA	2950	1/1	0.98	0.18	32,32,32,32	0
54	MG	BA	2932	1/1	0.98	0.26	41,41,41,41	0
54	MG	CA	1734	1/1	0.98	0.15	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3008	1/1	0.98	0.18	57,57,57,57	0
54	MG	DA	3188	1/1	0.98	0.51	9,9,9,9	0
54	MG	BA	3245	1/1	0.98	0.29	54,54,54,54	0
54	MG	BA	2929	1/1	0.98	0.46	37,37,37,37	0
54	MG	BA	2930	1/1	0.98	0.34	34,34,34,34	0
54	MG	AA	1617	1/1	0.98	0.19	77,77,77,77	0
54	MG	CA	1729	1/1	0.98	0.17	98,98,98,98	0
54	MG	BA	2936	1/1	0.98	0.18	43,43,43,43	0
54	MG	DA	3237	1/1	0.98	0.23	87,87,87,87	0
55	ZN	AN	101	1/1	0.98	0.14	120,120,120,120	0
54	MG	AA	1620	1/1	0.98	0.23	56,56,56,56	0
54	MG	BB	204	1/1	0.98	0.12	87,87,87,87	0
54	MG	DA	2912	1/1	0.98	0.45	18,18,18,18	0
54	MG	BA	3198	1/1	0.98	0.20	81,81,81,81	0
54	MG	DA	3190	1/1	0.99	0.44	27,27,27,27	0
54	MG	DA	3167	1/1	0.99	0.16	68,68,68,68	0
54	MG	DA	2931	1/1	0.99	0.25	23,23,23,23	0
54	MG	CA	1690	1/1	0.99	0.52	61,61,61,61	0
54	MG	BA	2903	1/1	0.99	0.39	14,14,14,14	0
54	MG	BA	2925	1/1	0.99	0.27	29,29,29,29	0
54	MG	BA	2902	1/1	0.99	0.46	16,16,16,16	0
54	MG	DA	3204	1/1	0.99	0.14	54,54,54,54	0
54	MG	DA	3191	1/1	0.99	0.48	24,24,24,24	0
54	MG	DA	2917	1/1	0.99	0.25	22,22,22,22	0
54	MG	AA	1730	1/1	0.99	0.09	49,49,49,49	0
54	MG	DA	3123	1/1	0.99	0.08	59,59,59,59	0
54	MG	BA	3247	1/1	0.99	0.15	52,52,52,52	0
54	MG	BA	3153	1/1	0.99	0.30	67,67,67,67	0
55	ZN	AD	301	1/1	0.99	0.27	80,80,80,80	0
54	MG	BA	2965	1/1	0.99	0.27	47,47,47,47	0
54	MG	DA	2918	1/1	0.99	0.35	15,15,15,15	0
54	MG	CA	1602	1/1	0.99	0.09	64,64,64,64	0
54	MG	DA	2951	1/1	0.99	0.18	38,38,38,38	0
54	MG	BA	2906	1/1	1.00	0.22	5,5,5,5	0

6.5 Other polymers ⓘ

There are no such residues in this entry.