



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:40 PM UTC

PDB ID : 4V5D / pdb_00004v5d
Title : Structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, paromomycin, acylated A- and P-site tRNAs, and E-site tRNA.
Authors : Voorhees, R.M.; Weixlbaumer, A.; Loakes, D.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-03-24
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

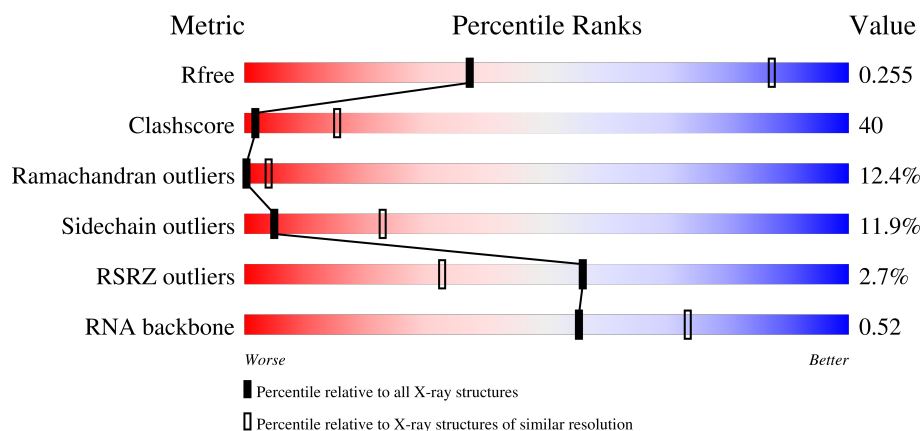
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 of 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	1522	27% 60% 10% ..
1	CA	1522	3% 26% 61% 10% ..
2	AB	256	2% 14% 56% 18% 8%

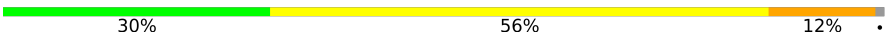
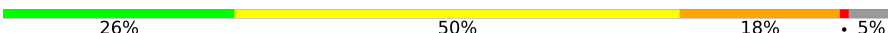
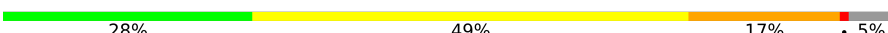
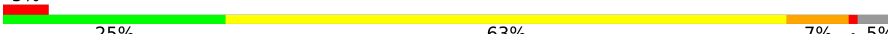
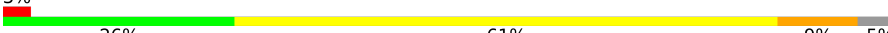
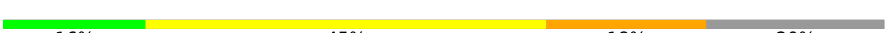
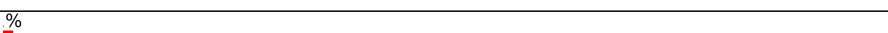
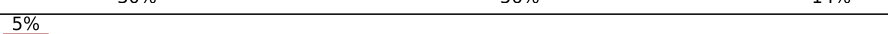
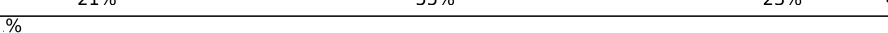
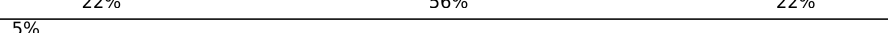
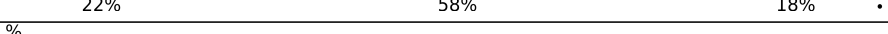
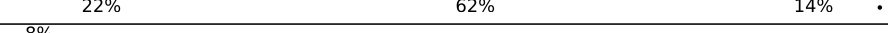
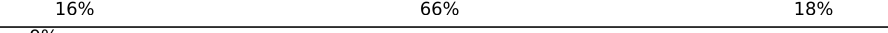
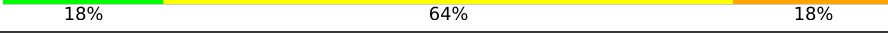
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Mol	Chain	Length	Quality of chain
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	

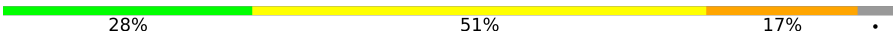
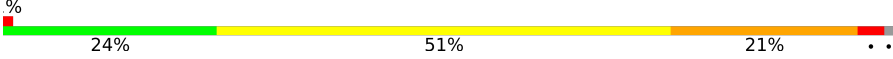
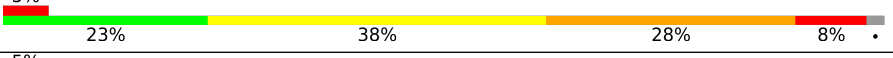
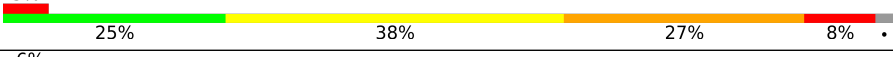
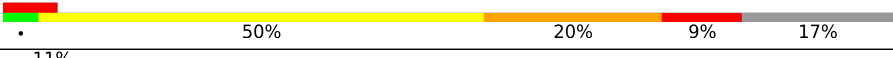
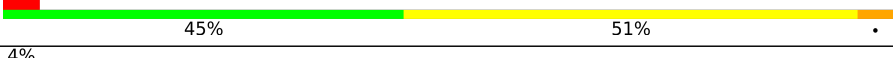
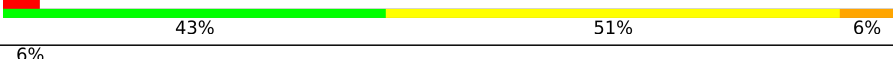
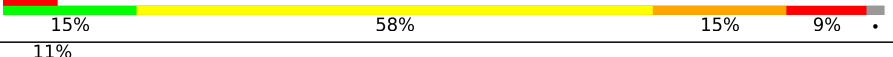
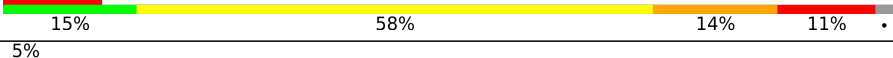
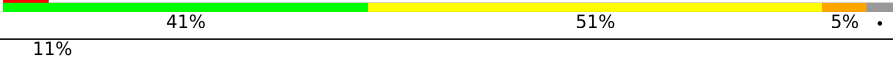
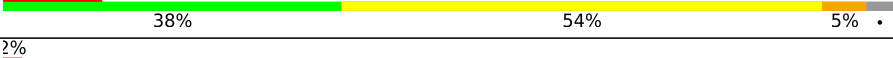
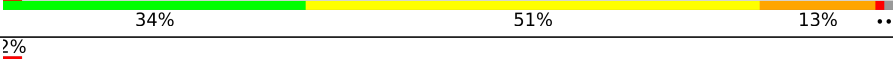
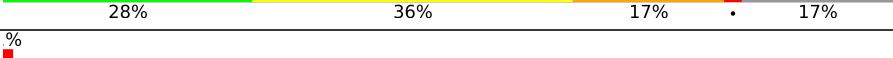
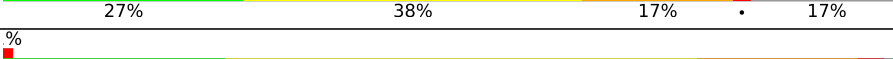
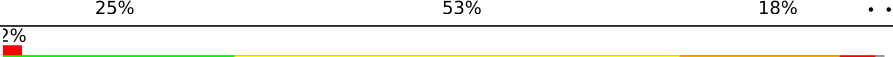
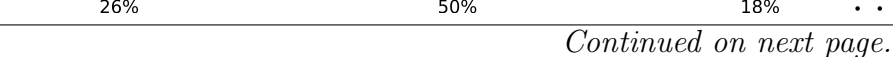
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Mol	Chain	Length	Quality of chain
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AY	77	
22	CV	77	
22	CY	77	
23	AW	76	
23	CW	76	
24	AX	11	
24	CX	11	
25	B0	85	
25	D0	85	
26	B1	98	

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Mol	Chain	Length	Quality of chain
26	D1	98	
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2822	
35	DA	2822	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	

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Mol	Chain	Length	Quality of chain
39	BE	206	
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BN	140	
44	DN	140	
45	BO	122	
45	DO	122	
46	BP	150	
46	DP	150	
47	BQ	141	
47	DQ	141	
48	BR	118	
48	DR	118	
49	BS	112	
49	DS	112	
50	BT	146	
50	DT	146	
51	BU	118	

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Mol	Chain	Length	Quality of chain
51	DU	118	
52	BV	101	
52	DV	101	
53	BW	113	
53	DW	113	
54	BX	96	
54	DX	96	
55	BY	110	
55	DY	110	
56	BZ	206	
56	DZ	206	

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
57	MG	AA	1656	-	-	-	X
57	MG	AA	1737	-	-	-	X
57	MG	AA	1748	-	-	-	X
57	MG	AA	1796	-	-	-	X
57	MG	AL	202	-	-	-	X
57	MG	BA	3138	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3371	-	-	-	X
57	MG	BA	3387	-	-	-	X
57	MG	CA	1656	-	-	-	X
57	MG	CA	1690	-	-	-	X
57	MG	DA	3111	-	-	-	X
57	MG	DA	3127	-	-	-	X
57	MG	DA	3157	-	-	-	X
57	MG	DA	3178	-	-	-	X
57	MG	DA	3183	-	-	-	X
57	MG	DA	3227	-	-	-	X
57	MG	DA	3386	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3389	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 296042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	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	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P AND A-SITE PHE-TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	AY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			
24	CX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
29	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

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

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1140	689	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
42	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	198	Total	Mg	0	0
			198	198		
57	AD	1	Total	Mg	0	0
			1	1		
57	AE	1	Total	Mg	0	0
			1	1		
57	AG	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AI	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	AN	1	Total 1	Mg 1	0	0
57	AV	5	Total 5	Mg 5	0	0
57	AW	8	Total 8	Mg 8	0	0
57	AX	2	Total 2	Mg 2	0	0
57	B0	1	Total 1	Mg 1	0	0
57	B1	1	Total 1	Mg 1	0	0
57	B2	2	Total 2	Mg 2	0	0
57	B5	2	Total 2	Mg 2	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BA	422	Total 422	Mg 422	0	0
57	BB	14	Total 14	Mg 14	0	0
57	BD	2	Total 2	Mg 2	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	BV	1	Total 1	Mg 1	0	0
57	BX	2	Total 2	Mg 2	0	0

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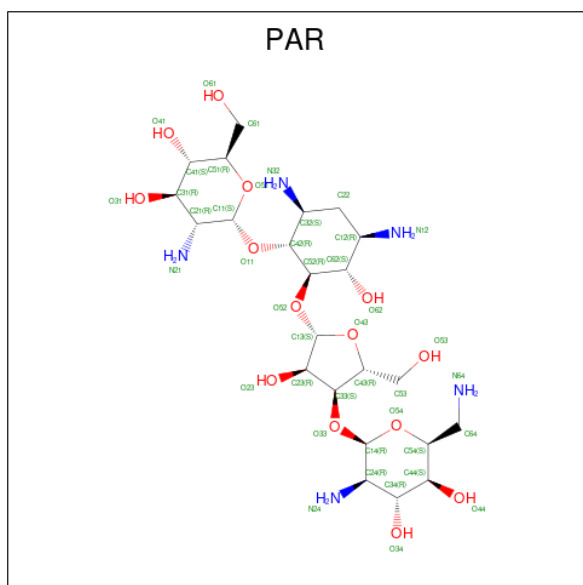
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CA	199	Total 199	Mg 199	0	0
57	CE	1	Total 1	Mg 1	0	0
57	CI	1	Total 1	Mg 1	0	0
57	CL	1	Total 1	Mg 1	0	0
57	CN	1	Total 1	Mg 1	0	0
57	CV	5	Total 5	Mg 5	0	0
57	CW	7	Total 7	Mg 7	0	0
57	CX	3	Total 3	Mg 3	0	0
57	D1	1	Total 1	Mg 1	0	0
57	D2	3	Total 3	Mg 3	0	0
57	D5	2	Total 2	Mg 2	0	0
57	D7	2	Total 2	Mg 2	0	0
57	DA	421	Total 421	Mg 421	0	0
57	DB	13	Total 13	Mg 13	0	0
57	DC	1	Total 1	Mg 1	0	0
57	DD	2	Total 2	Mg 2	0	0
57	DE	1	Total 1	Mg 1	0	0
57	DF	2	Total 2	Mg 2	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DO	1	Total 1	Mg 1	0	0
57	DS	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DV	1	Total	Mg	0	0
			1	1		
57	DX	3	Total	Mg	0	0
			3	3		

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	AA	1	Total	C	N	O	0	0
			42	23	5	14		
58	CA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		

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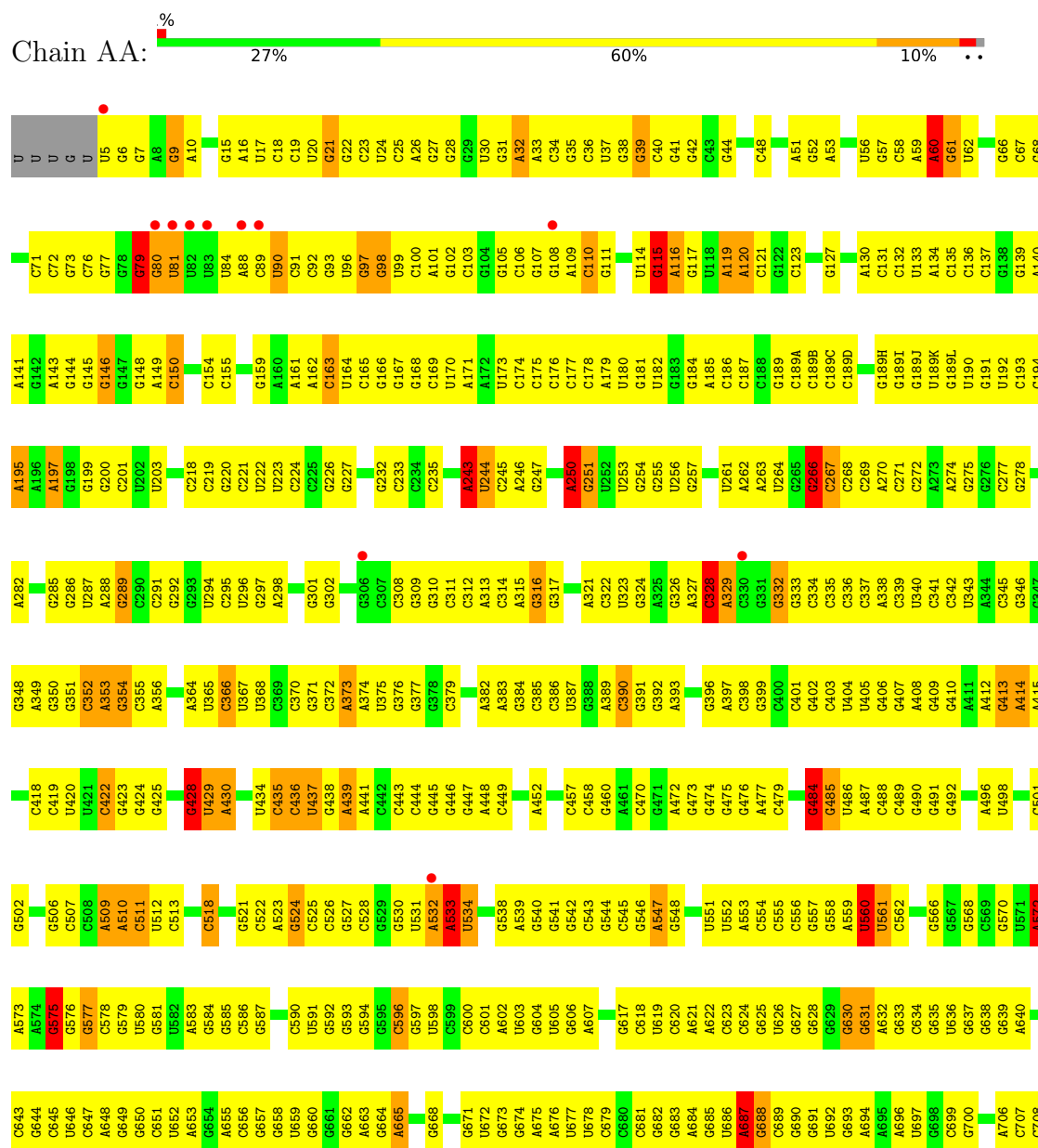
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

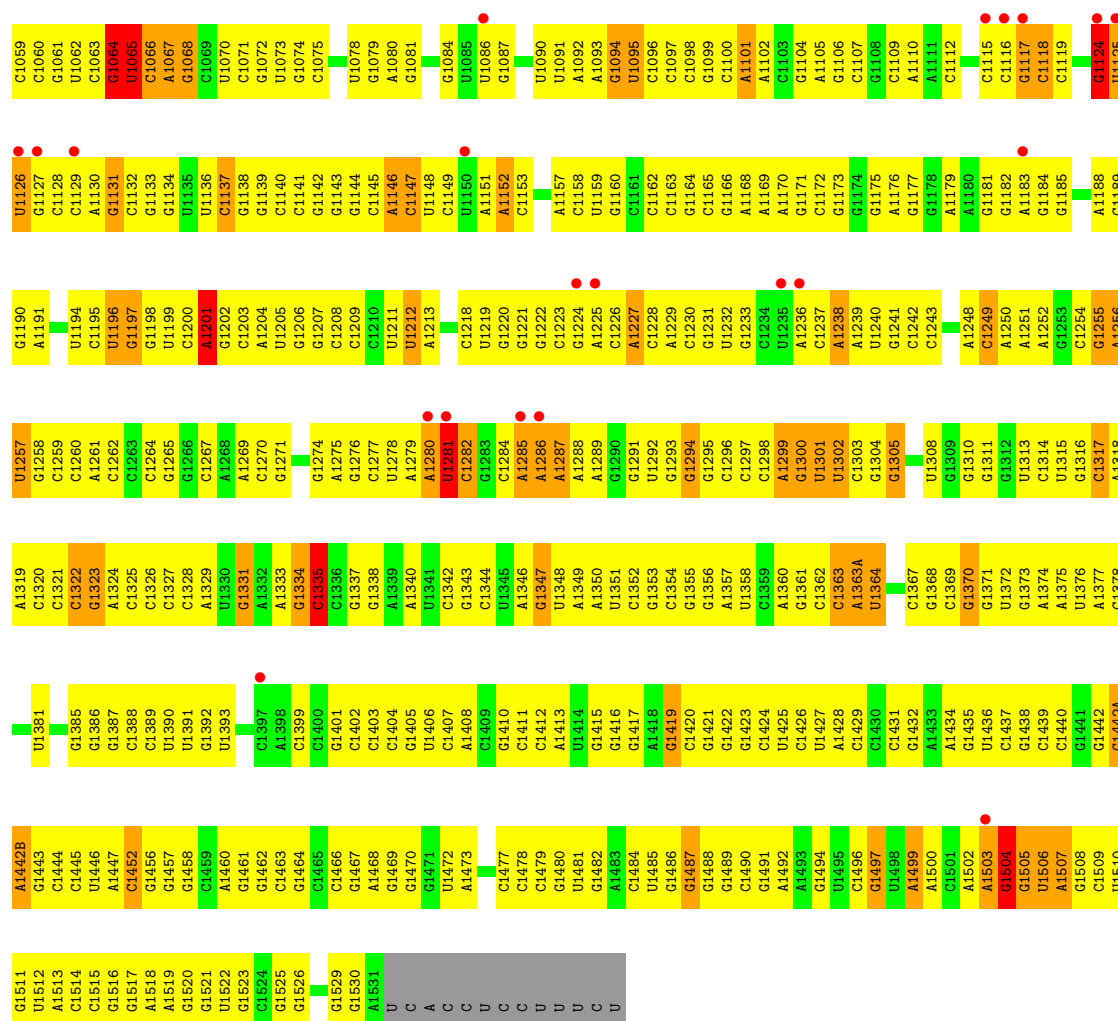
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA

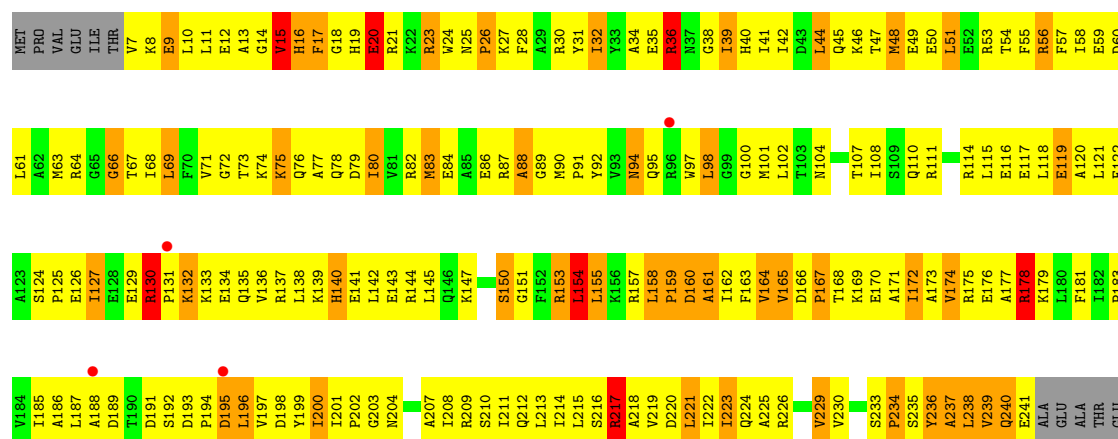
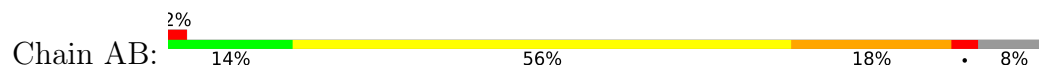




G993	A994	C992	G961	A780	G700	C634	G566	G490	G409	C345	G276	A195	A141	C71	U
A995	C993	G933	C862	A781	G706	G635	G567	G491	G410	G346	C277	A196	G142	C72	U
C995	A935	G934	A863	A782	A706	U636	G568	G492	A411	G347	G278	A197	G143	C73	U
C999	A936	G935	A864	C783	C707	G637	G569		A412	G348		G198	G144	G74	G
U1000	A937	A938	A865	C784	G708	G638	G570	A496	A413	G349	A282	G199	G145	G75	U
A1001	A938	A939	A866		G709	G639	U571	U498	A414	G350	C283	G200	G146	G76	
G1001A	A939	A940	G867	G791	G710	A640	A572	C501	A415	C351	G284	C201	G147	G77	G6
G1002	C940	G941	G868	A792	G711	G641	A573	G502	C418	C352	U287	U202	G148	G78	
G1003	G941	G942	G869	A793	G712	A642	A574	G503	C419	A353	A288	U203	G149	G79	G9
A1004	G942	G943	A794	A794	G713	C643	G575	A509	C420	G354	G289	U204	C150	U81	A10
A1005	U943	U944			G718	G644	G576	A510	U421	C355	A290	C218	C154	U82	
G1006	G944	G945	G875	G797	G718	G645	G577	C511	U422	A356	C291	G219	C155	U83	G15
C1007	G945	G946	G876	G798	U723	G646	G578	U512	G423	U859	G292	G220	C156	U84	A16
G1008	A946	A947			G724	A648	G579	C513	G424	A360	U293	U222	C157	A88	U17
G1009	G947	G948	G877	A802	G725	G649	U580	C514	G425		U294	U223	C158	C89	C18
G1010	C948	C949	A868		G726	G650	U581	G515	G426		C295	C224	C159	U90	G19
A1014	A949	A950	G881	C805	G727	C651	U582	C516	U427	U365	U296	C225	A160	C91	U20
A1015	C951	C952	G882	C806	A728	U652	G584	C517	G428	C366	G297	G226	A161	C92	G21
A1016	U951	U952	C883	A807	G729	A653	G585	C518	U429	U367	A298	G227	C162	C93	G22
G1017	G953	G954	G884		U730		G586	G521	U430	U368		A228	C163	C94	C23
U1020	G955	U956	G885	C811	G731	G657	G587	C522		U369	G301	G232	C164	U96	U24
G1021	U957	U958	G886		G732	G658		A523	U434	C369	G302	G233	C165	G97	U25
G1022	A959	A960	G887	C817	G735	U659	C590	G524	C435	C370	C307	G234	C166	G98	A26
U1025	G961	G962	A892	A818	C736	G660	U591	C525	C436	G371	C308	C235	C167	U99	C25
G1026	A963	A964	C993	A819	C737	G661	G592	C526	U437	A373	G309	G236	C168	U99	G27
G1027	C965	C966	C994	U820	A737	G662	G593	G527	C438	C374	G310	G237	C169	A101	G28
G1028	U961	U962	G995	G821	C738	A663	G594	C528	A439	U375	G311	G238	C170	G102	G29
C1029	C963	C964	G996	G822	G741	G664	U595	G529	A441	G376	C312	G239	C171	C100	
C1030	A965	A966	C997	G823	G742	A665	C596	G530	C442	G377	C313	U244	C172	G107	C34
G1030A	G967	G968	C998	G824	C745	G666	U597	U531	C443	C378	C314	C245	C173	G108	C35
G1030B	A968	A969	C999	G825		G667	C598	A532	C444	C379	A315	C246	C174	G109	C36
A1030D	G970	G971	C999	C826	C748	G668	G599	A533	C445		A316	A247	C175	U109	U37
G1031	A972	A973	A900	U827	G749		C600	U534	G446	A382	G317	G247	C176	C110	G38
G1032	C974	C975	A901	G829	G750	G671	C601	A539	A448	A383	U321	A250	C177	U114	G39
G1033	A976	A977	G902	U830	G754	U672	A602	G540	C449	A384	C322	G251	C178	G115	C40
G1034	C978	C979	U905	U831	G755	G673	U603	G541		C385	U323	G252	C179	G116	C41
A1035	A979	A980	G906	U832	G756	G674	G604	C542	A452	C386	G324	U253	C180	G117	C42
G1036	C981	C982	A907	U833	G757	A675	U605	G543	C457	U387	A325	G254	C181	G118	C43
U1040	A983	A984	C908	U834	G758	G676	A607	G544	C458	C388	G326	G255	C182	U119	C44
A1041	C985	C986	A918	U835	G759	U677	A608	C545	C459	A389	G327	U256	C183	A120	G47
G1042	A987	A988	A919	U836	A759	G678	A609	C546	C460	G391	A328	G257	C184	C121	C48
C1043	U981	U982	U920	G837	G760	G679	G617	A547	A461	C392	C329		C185	G122	
A1044	G982	G983	U921	U838	G763	C681	C618	G548	C470	A393	A329	U261	C186	G123	A51
U1049	A984	A985	G922	G839	G764	G682	U619		G471	G394	C330	G262	C187	C123	G52
G1050	C986	C987	G923	U840	C765	G683	C620	U551	A472	C395	G331	A263	C188	G127	A53
U1051	A986	A987	A923	U841	A766	A684	A621	U552	C473	C396	G332	U264	C189	A130	U56
U1052	C988	C989	G924	U842	G767	G685	A622	G553	C474	A397	G333	G265	C190	C131	C58
G1054	A989	A990	G925	U843	A768	U686	C623	C554	C475	C398	C334	G266	C191	C132	C59
A1055	U982	U983	G926	U844	G769	A687	C624	C555	C476	G399	C335	G267	C192	C133	A60
U1056	A984	A985	G927	U845	G770	G688	G625	C556	A477	C401	C336	C268	C193	C134	G61
G1058	C990	C991	G928	U846	G771	G689	U626	G557	C479	C402	C337	C269	C194	C135	U62
	U991	U992	G929	U847	G772	G690	U627	G558		C403	C338	C270		C136	
	A993	A994	G930	U848	G773	G691	G628	A559	C484	U404	C339	C271		C137	
	C995	C996	C931	U849	G774	U692	G629	U560	C485	U405	C341	C272		G138	G66
					G775	G693	G630	U561	U486	G406	C342	A273		C139	G67
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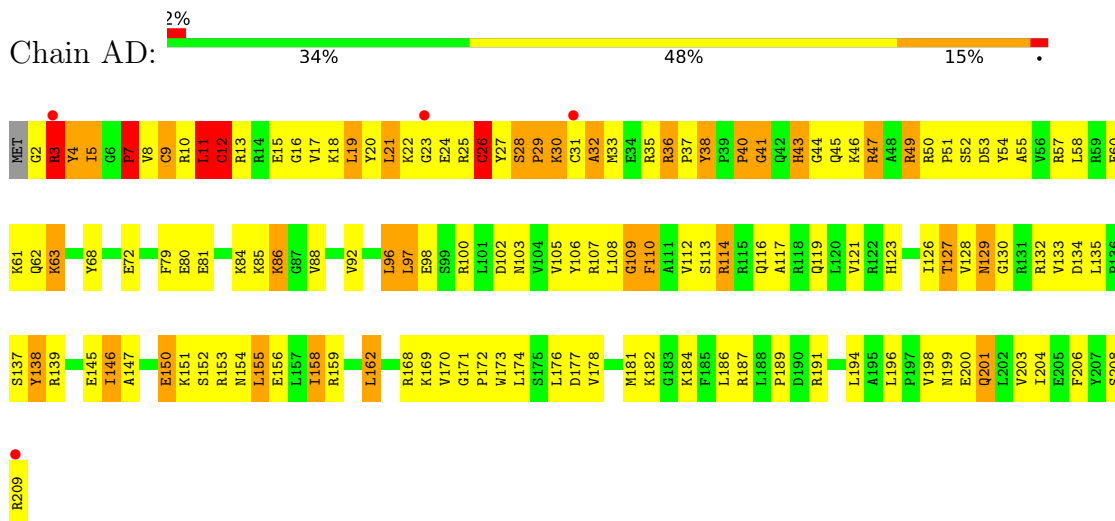


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

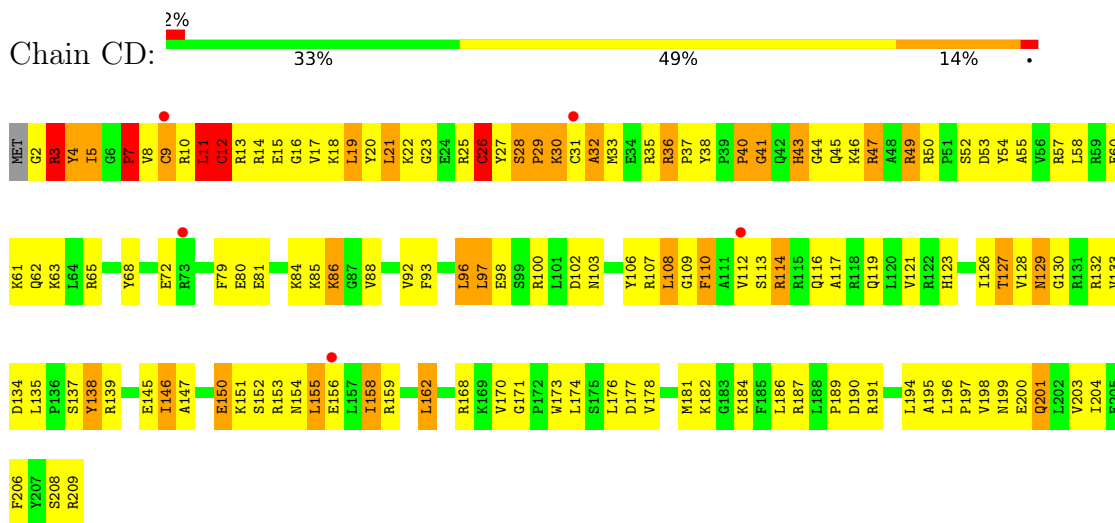


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

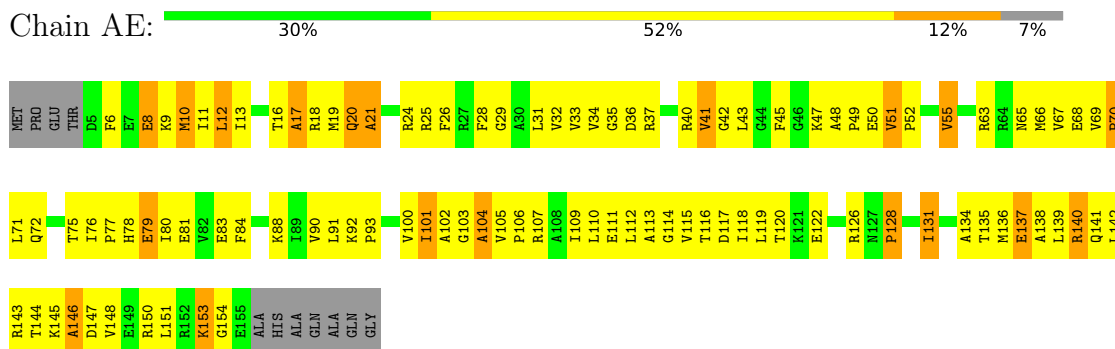
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

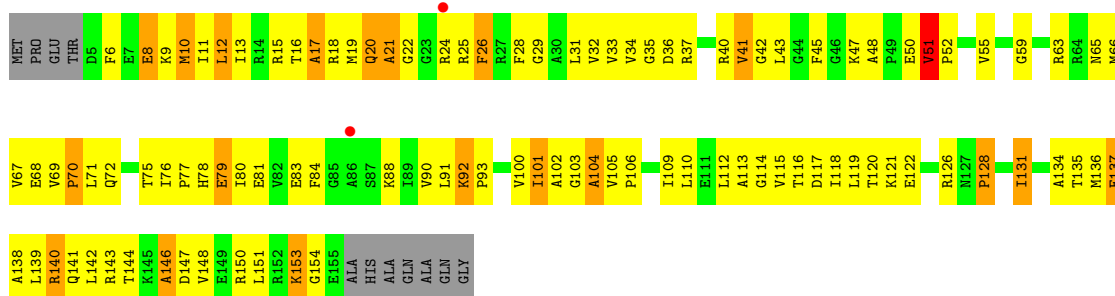


- Molecule 5: 30S RIBOSOMAL PROTEIN S5



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

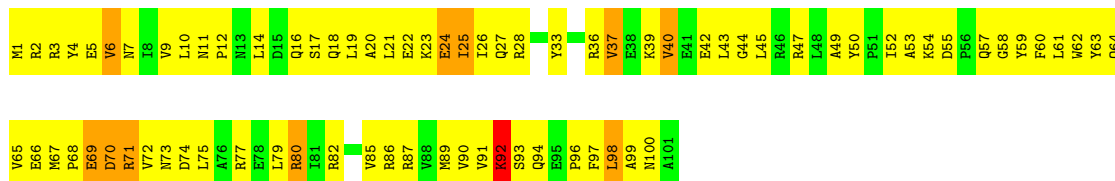




• Molecule 6: 30S RIBOSOMAL PROTEIN S6



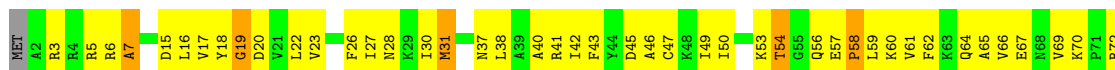
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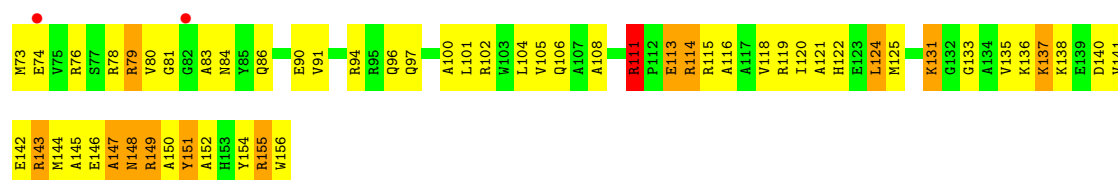


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

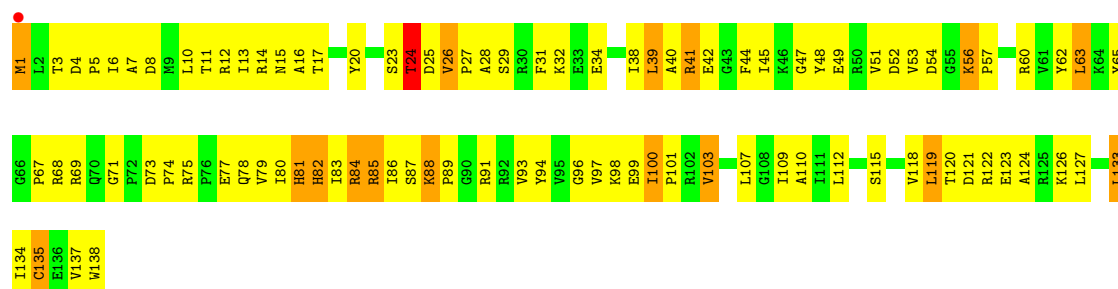


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

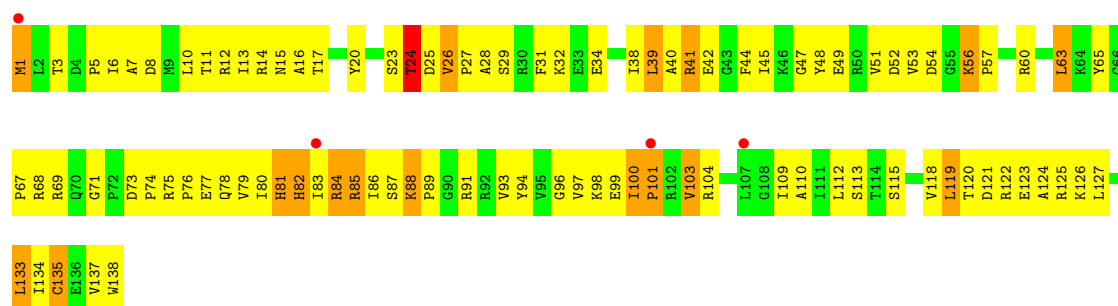




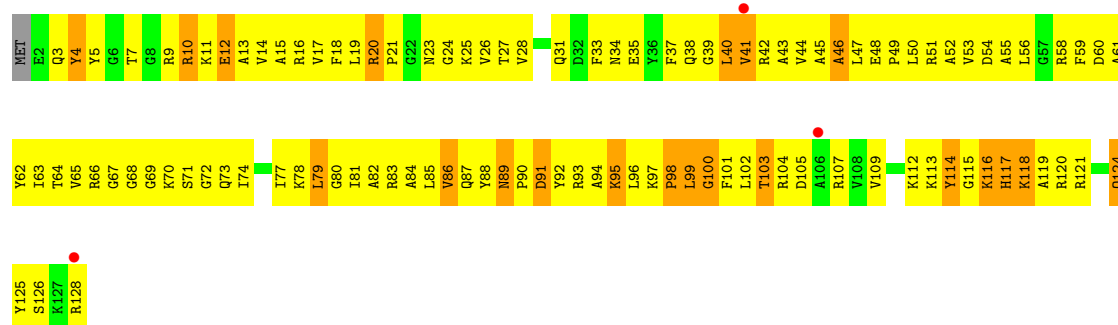
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

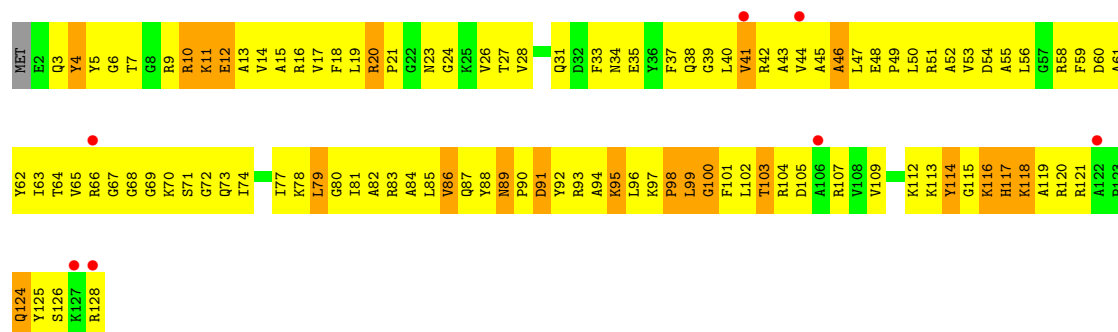


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

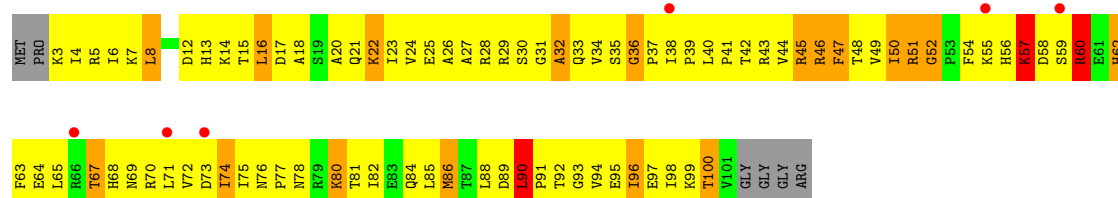
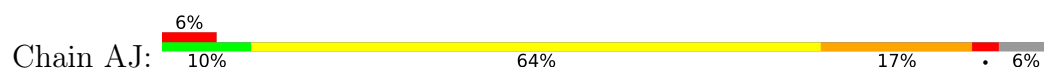


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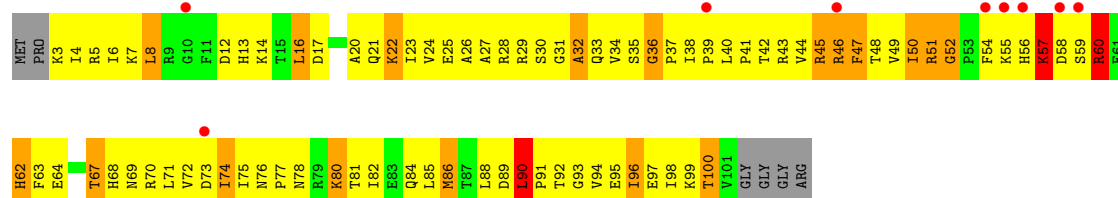
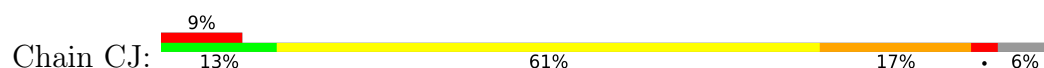




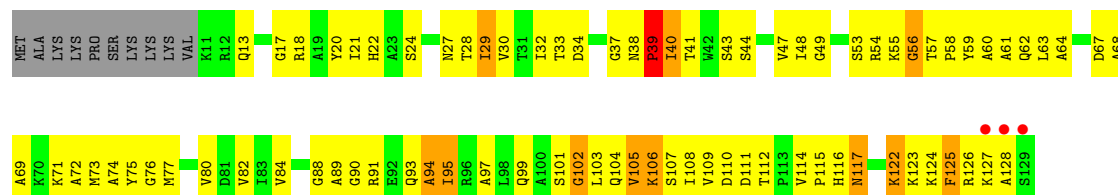
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



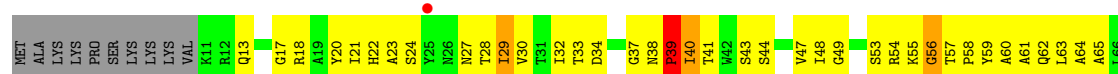
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

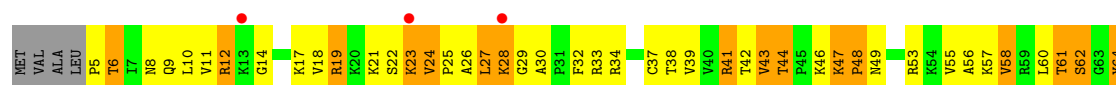




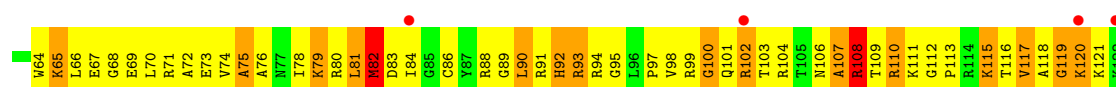
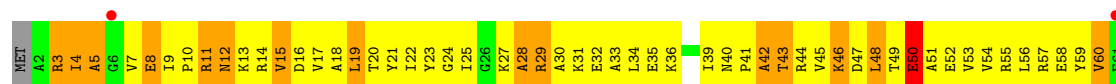
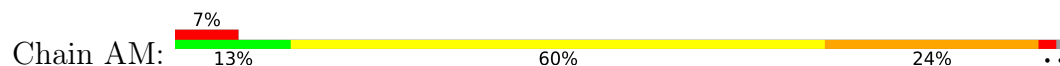
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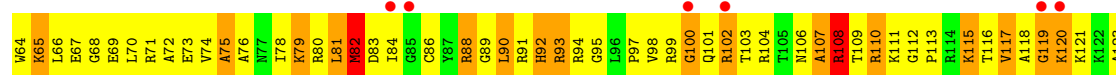
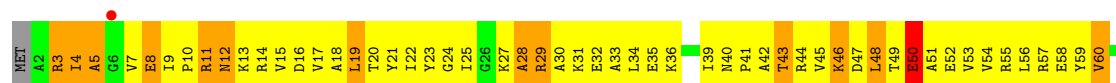
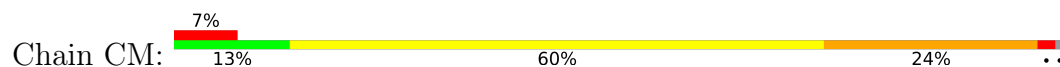
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13





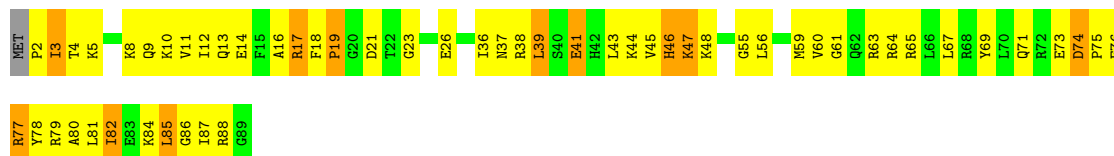
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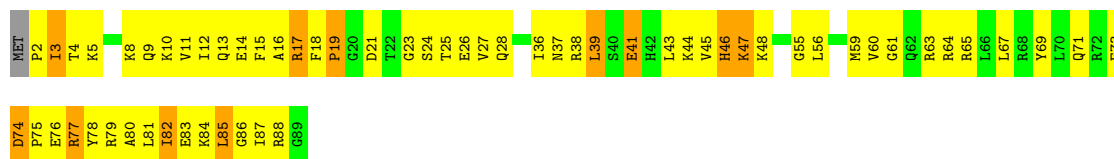
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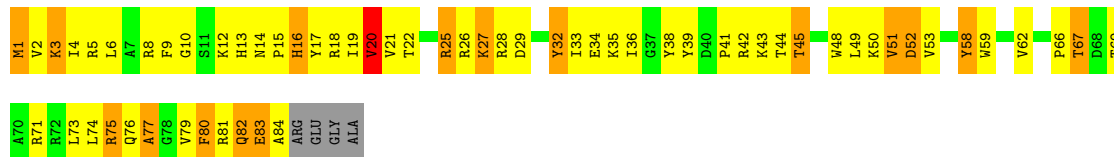
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● Molecule 15: 30S RIBOSOMAL PROTEIN S15

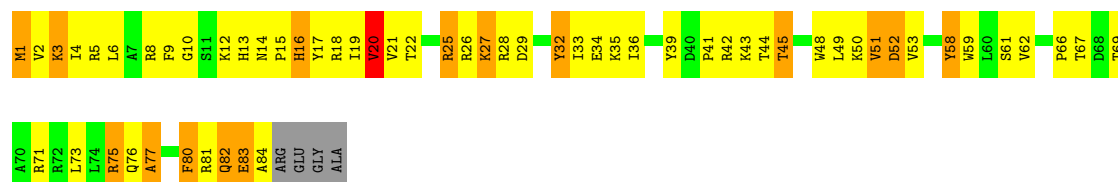


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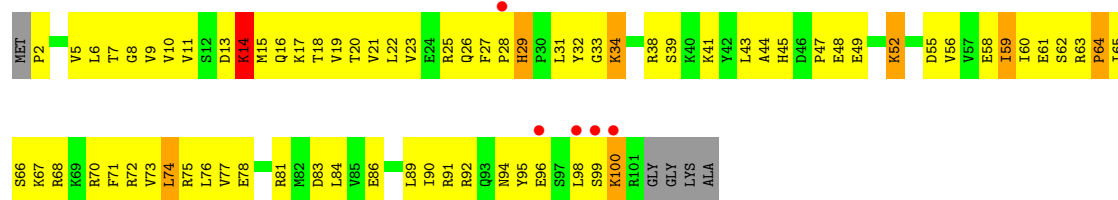


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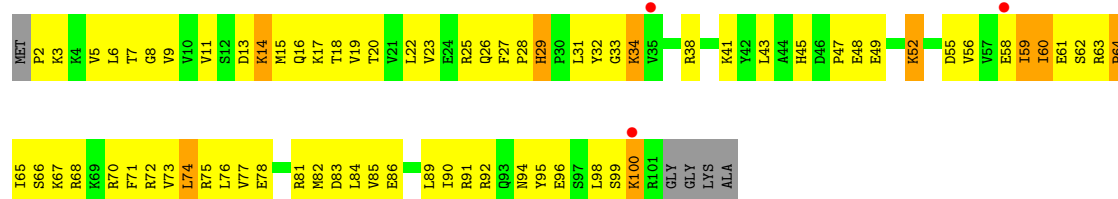




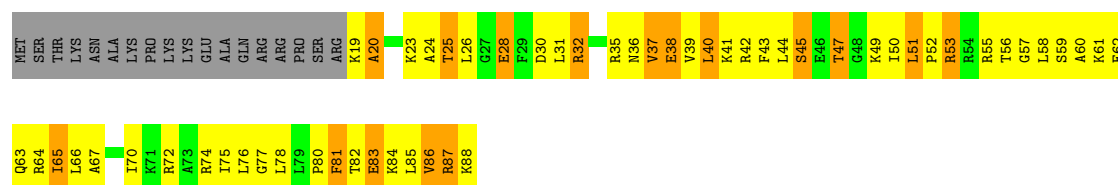
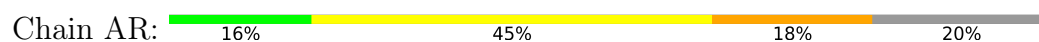
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



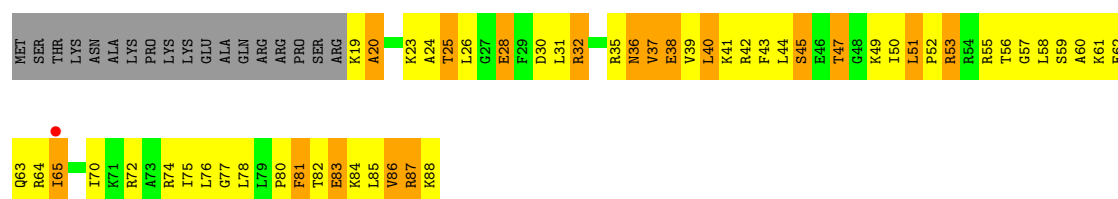
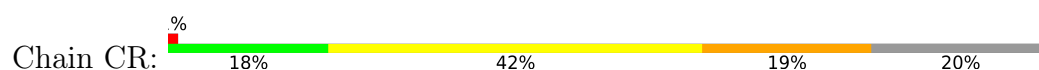
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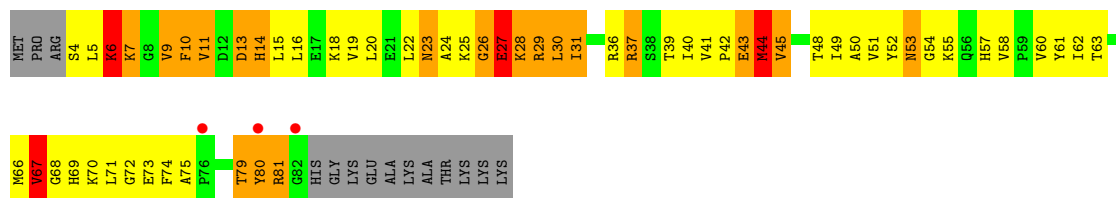
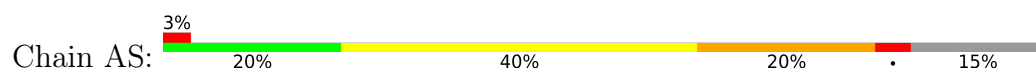
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



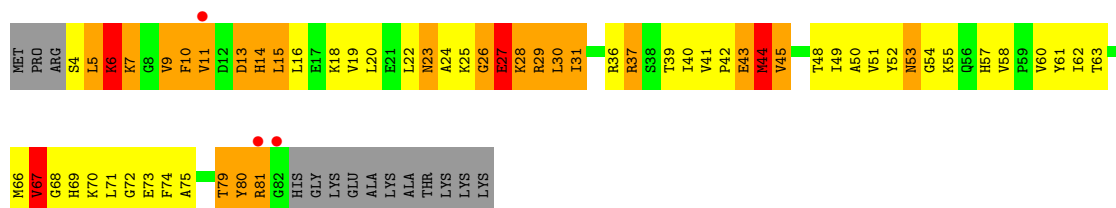
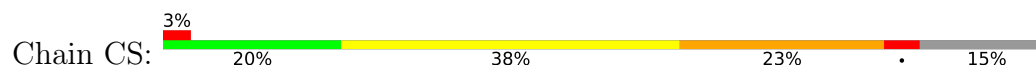
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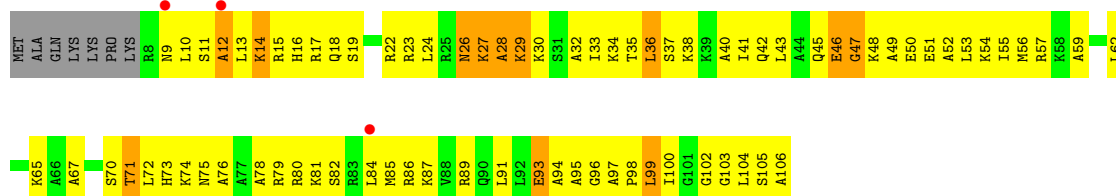
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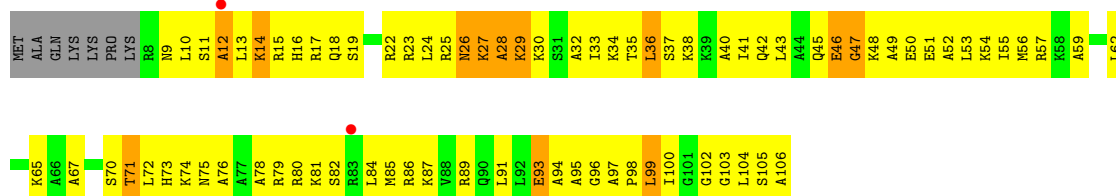
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



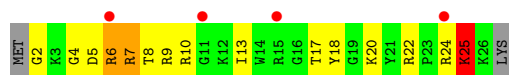
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



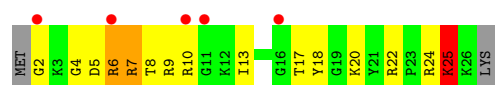
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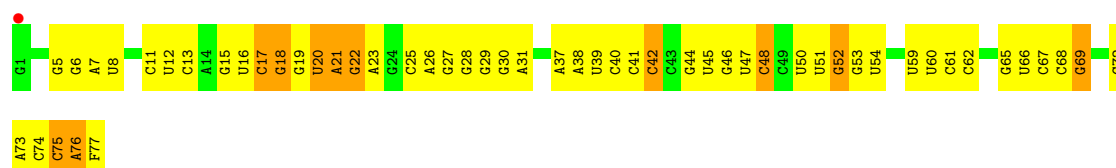
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



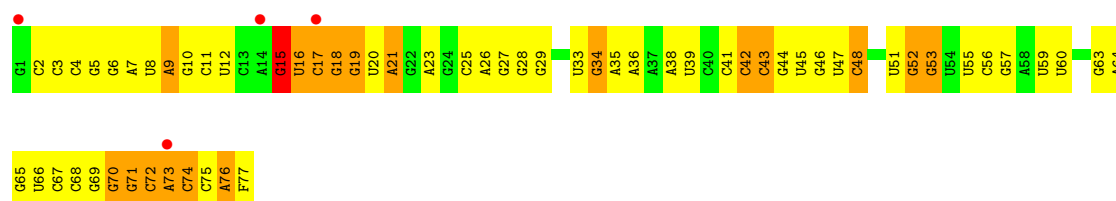
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



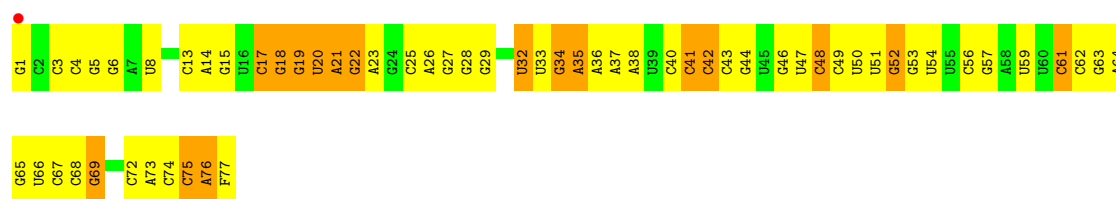
• Molecule 22: P AND A-SITE PHE-TRNA PHE



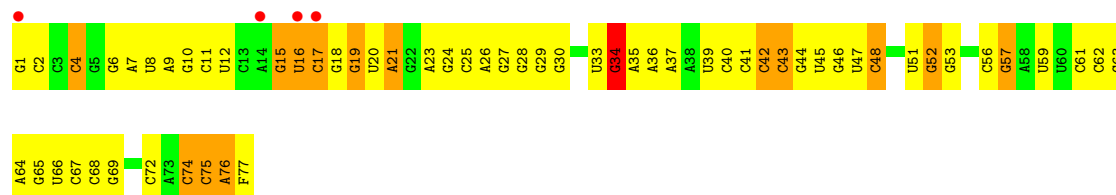
• Molecule 22: P AND A-SITE PHE-TRNA PHE



• Molecule 22: P AND A-SITE PHE-TRNA PHE

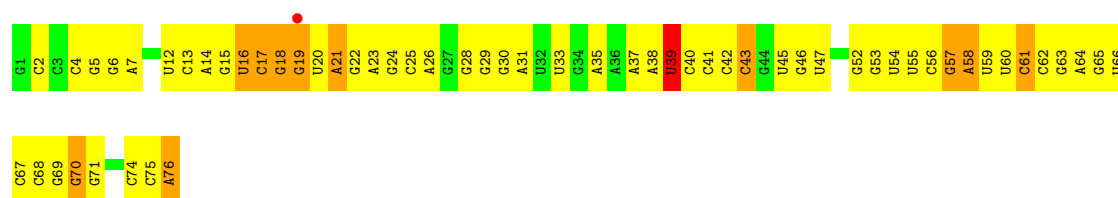


• Molecule 22: P AND A-SITE PHE-TRNA PHE



• Molecule 23: E-SITE TRNA PHE

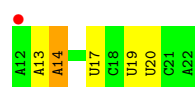




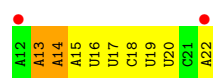
- Molecule 23: E-SITE TRNA PHE



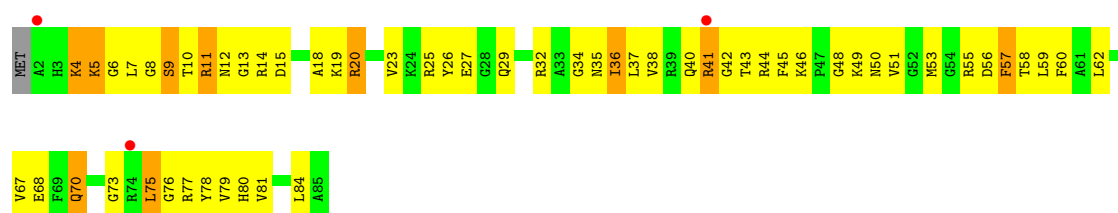
- Molecule 24: MRNA



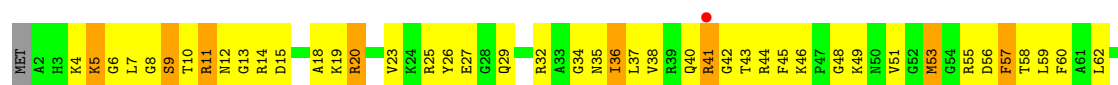
- Molecule 24: MRNA

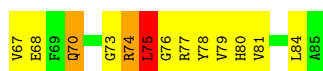


- Molecule 25: 50S RIBOSOMAL PROTEIN L27

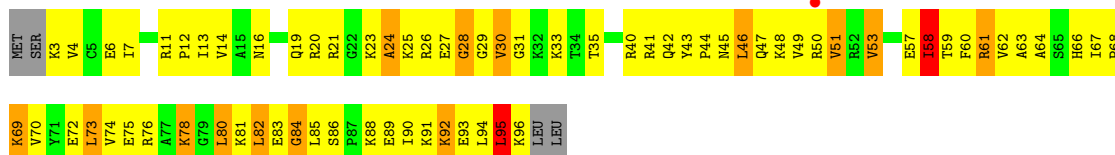


- Molecule 25: 50S RIBOSOMAL PROTEIN L27

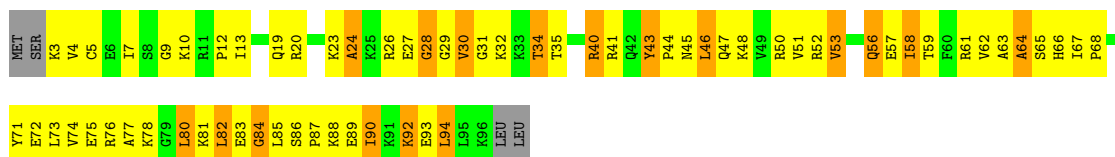




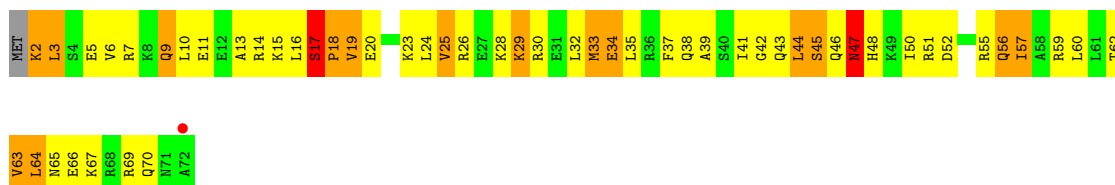
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



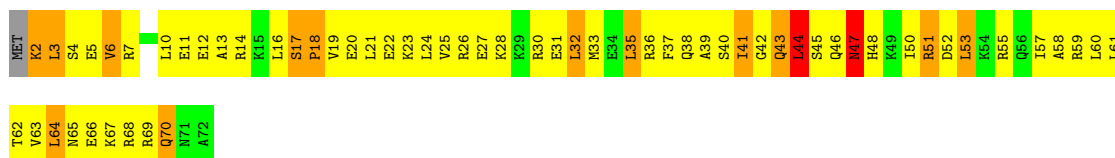
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



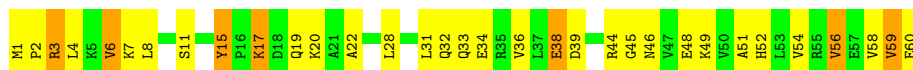
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 27: 50S RIBOSOMAL PROTEIN L29



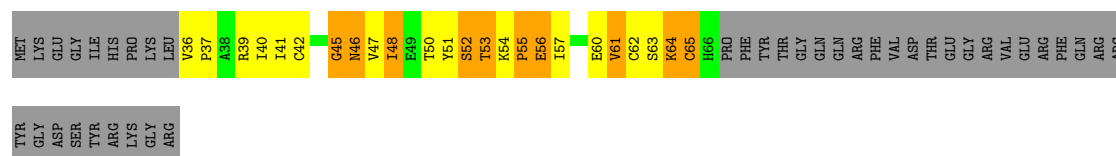
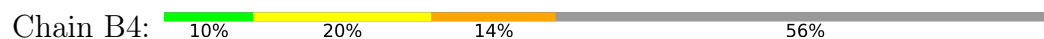
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



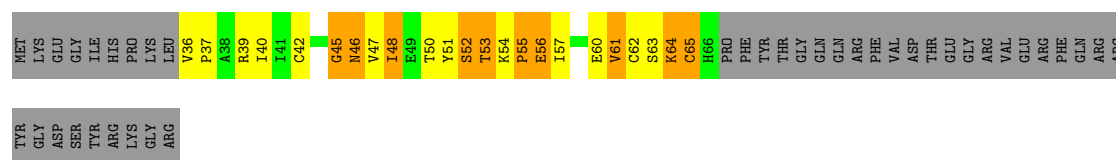
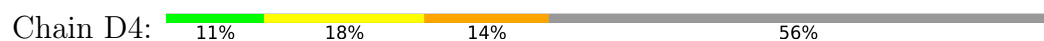
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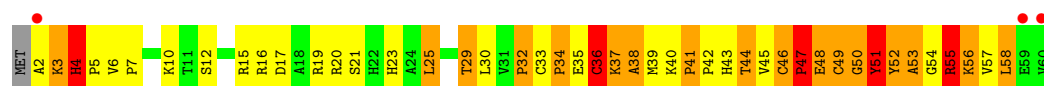
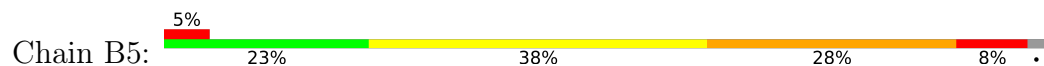
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



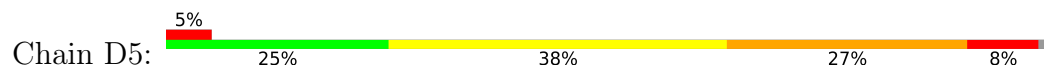
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L33

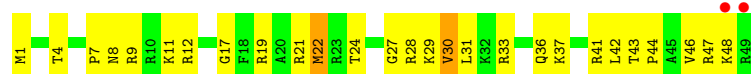


• Molecule 31: 50S RIBOSOMAL PROTEIN L33

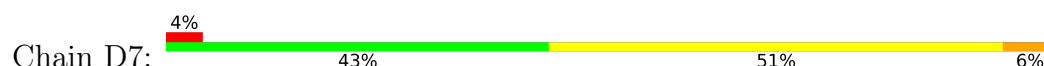




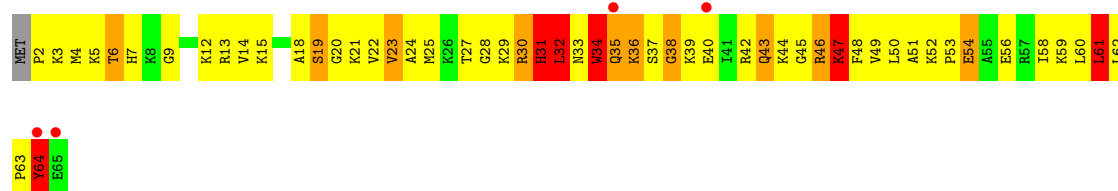
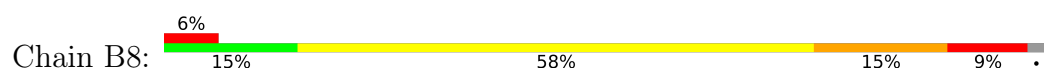
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



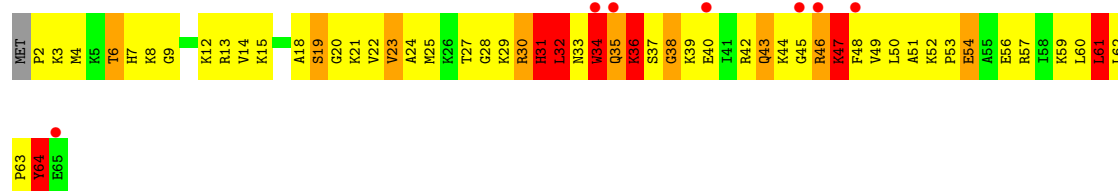
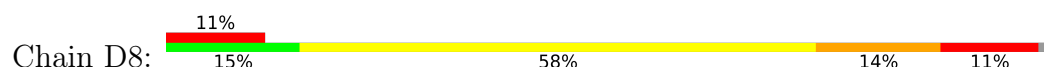
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

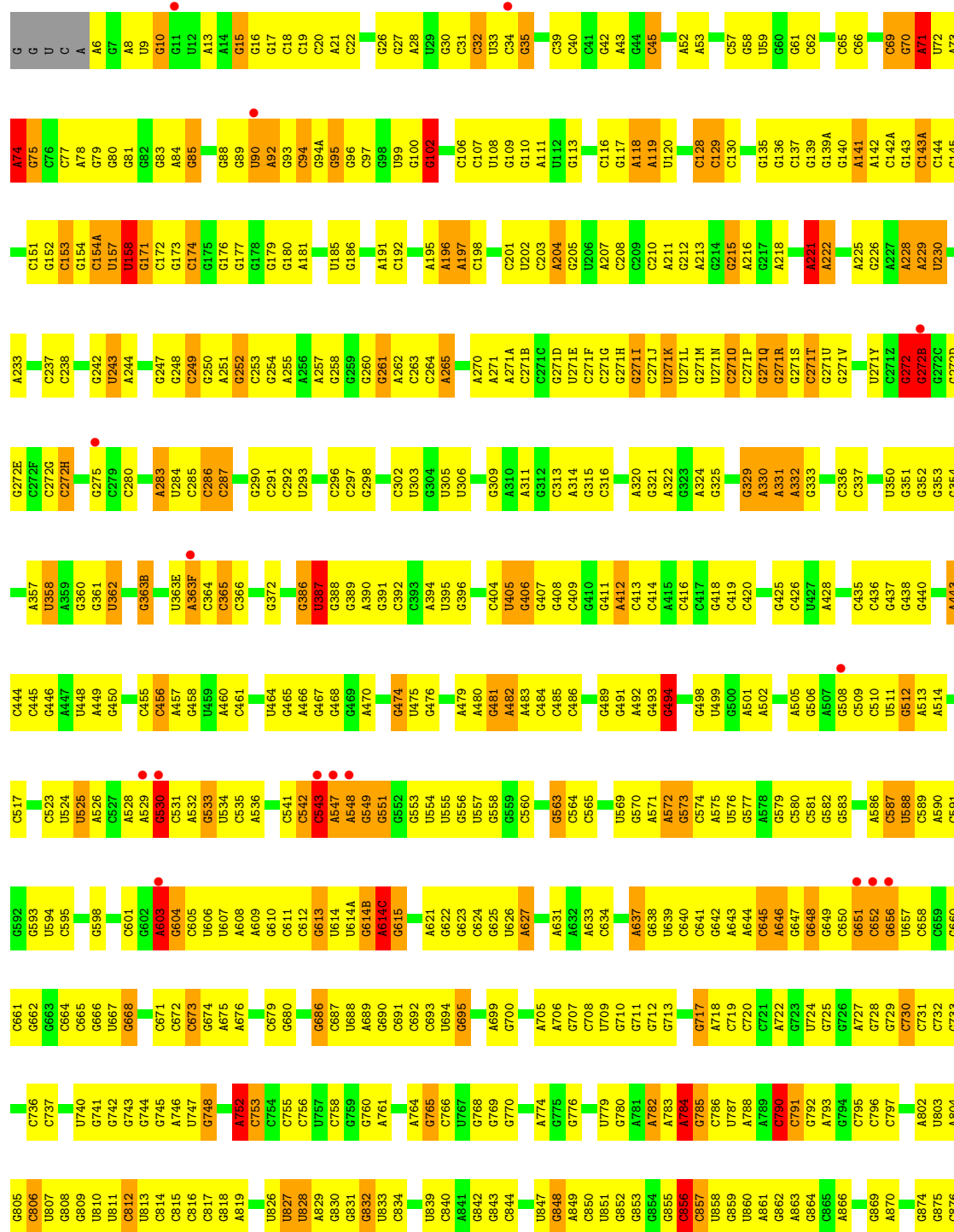


• Molecule 34: 50S RIBOSOMAL PROTEIN L36



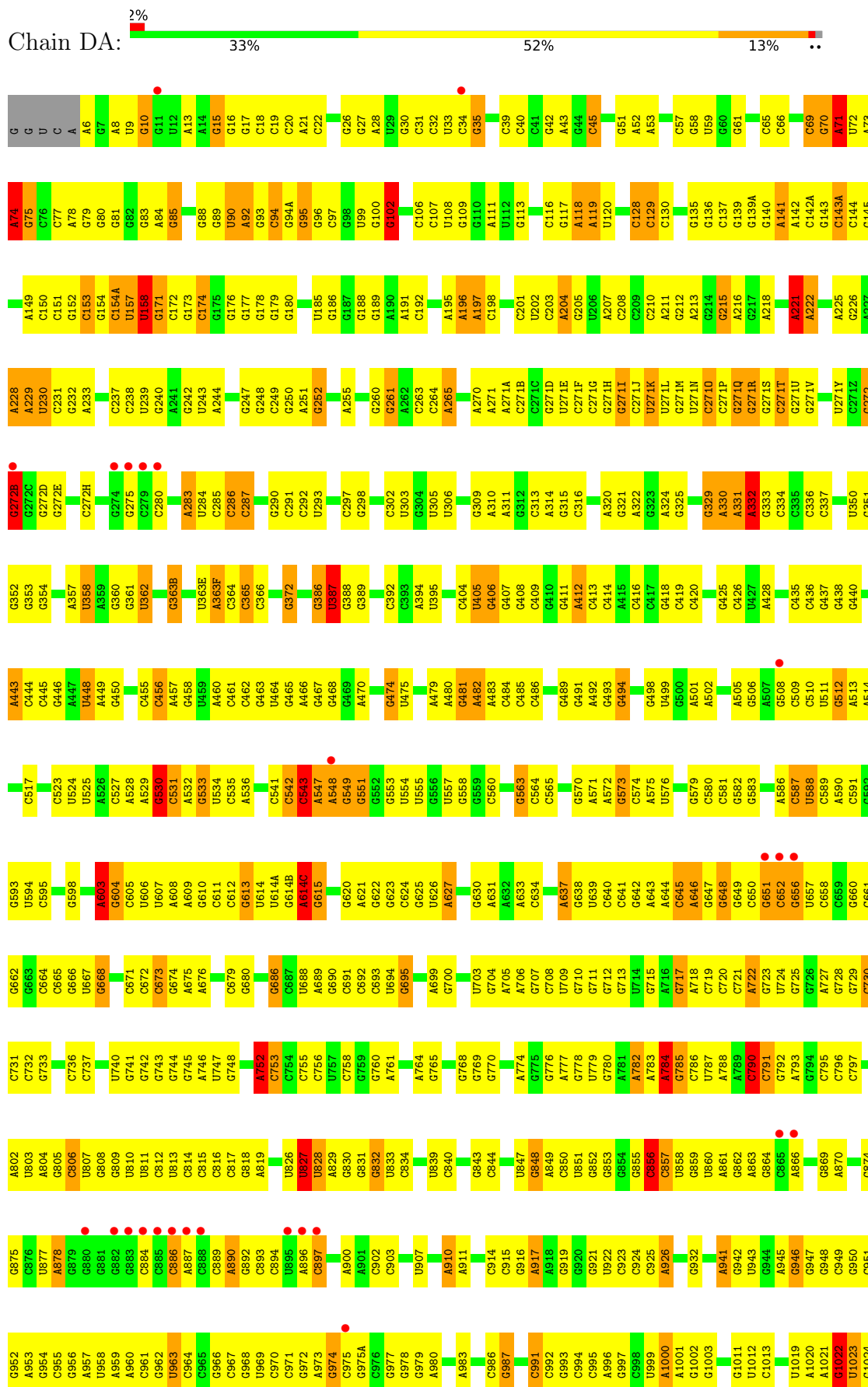


• Molecule 35: 23S RIBOSOMAL RNA

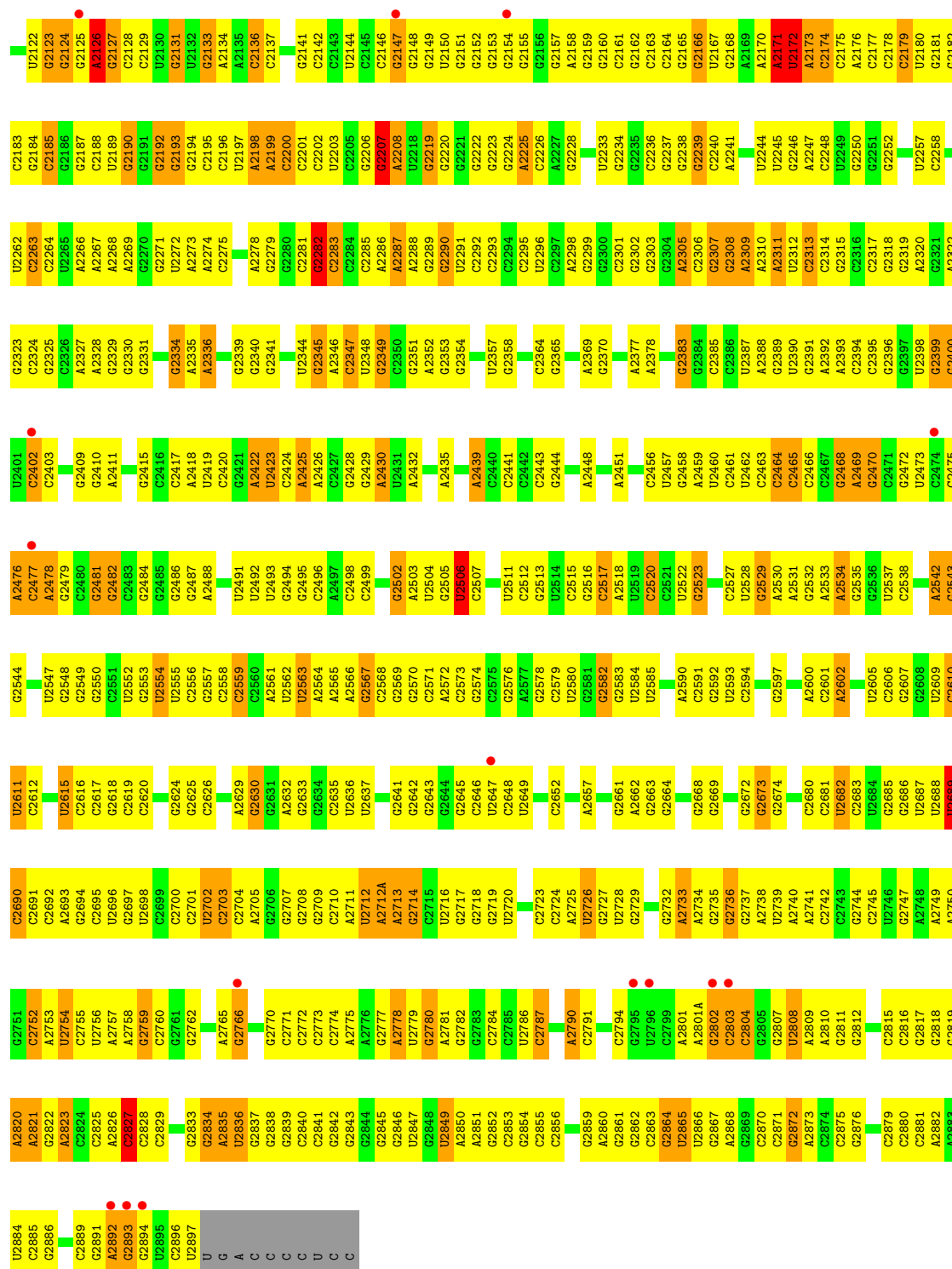


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U1914	G1839	G1772	G1681	C1511	G1447	A1374	C1295	C1222	G1151	U1033	U959	G880
A1915	G1839	A1773	G1682	G1515	G1448	C1375	G1299	C1224	G1153	G1034	C961	G881
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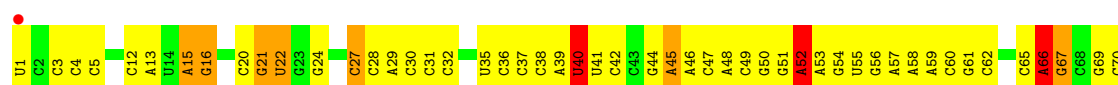






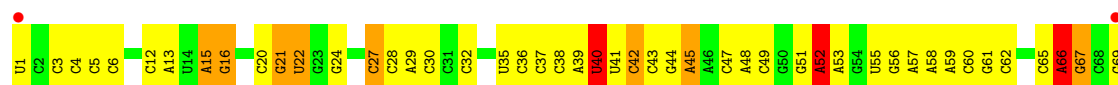


● Molecule 36: 5S RIBOSOMAL RNA

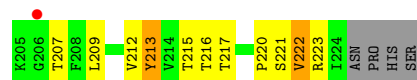
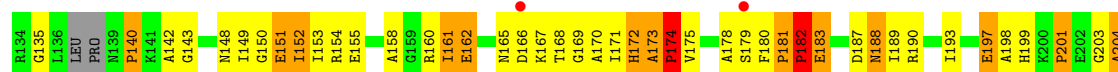
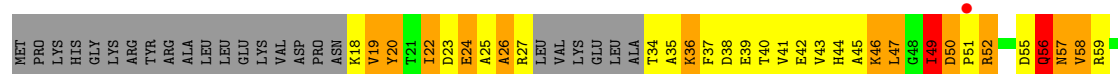




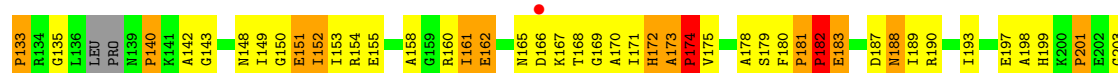
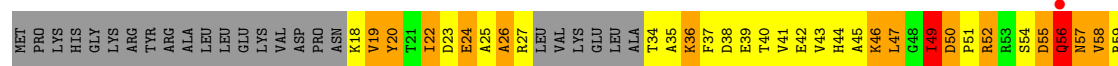
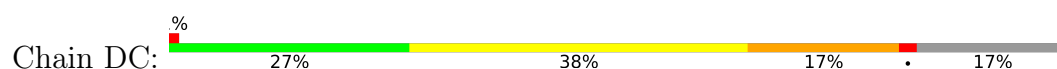
• Molecule 36: 5S RIBOSOMAL RNA



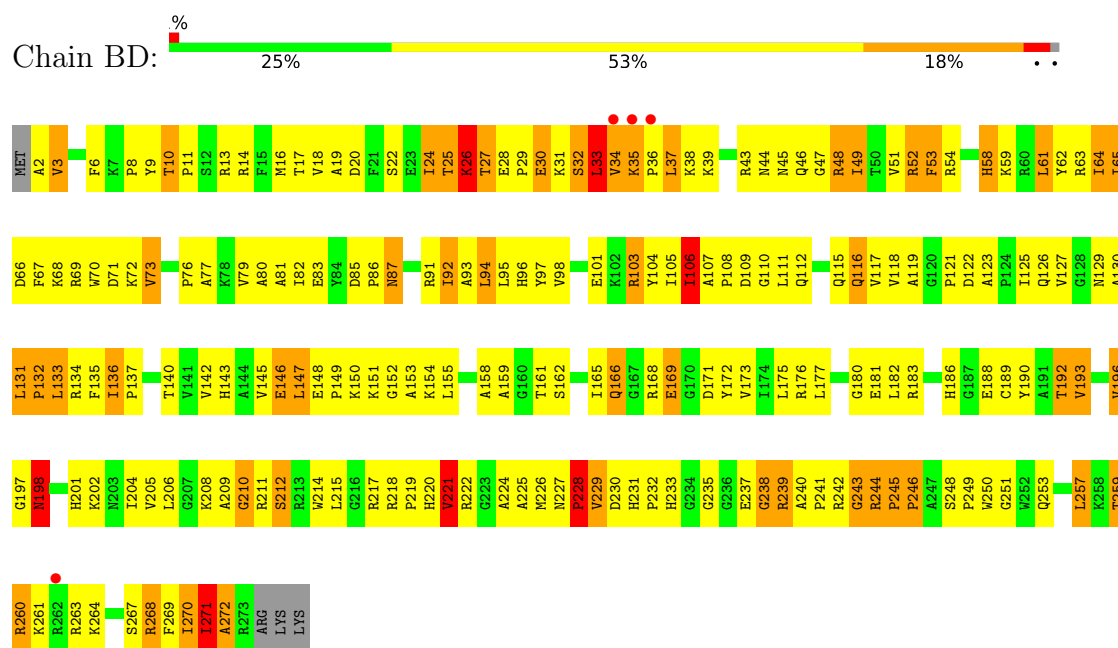
• Molecule 37: 50S RIBOSOMAL PROTEIN L1



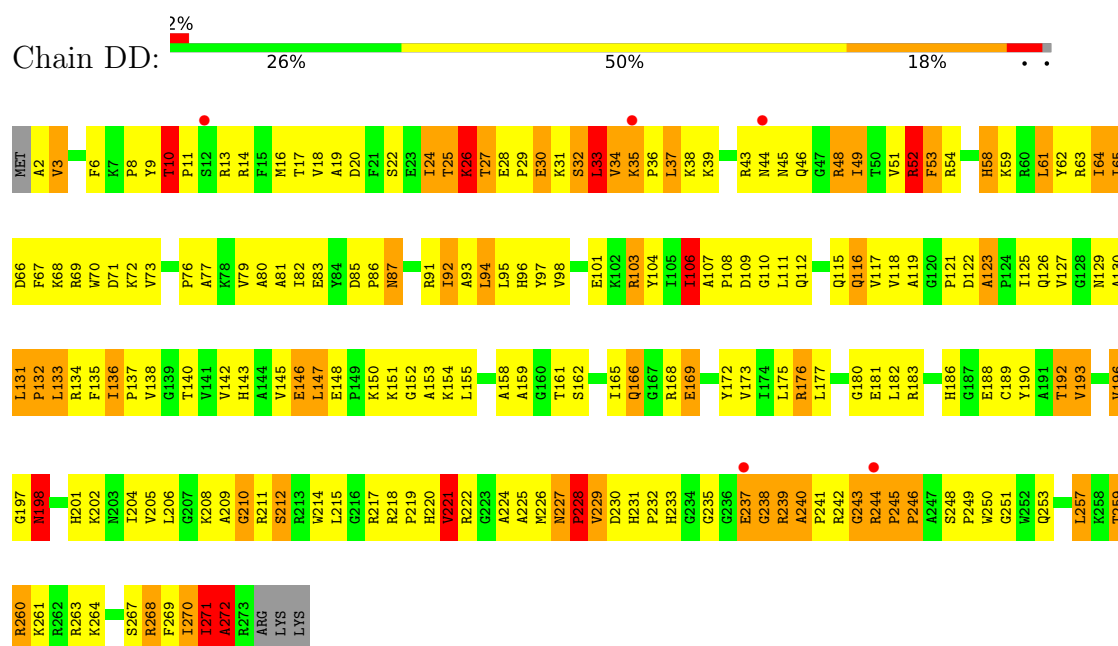
• Molecule 37: 50S RIBOSOMAL PROTEIN L1



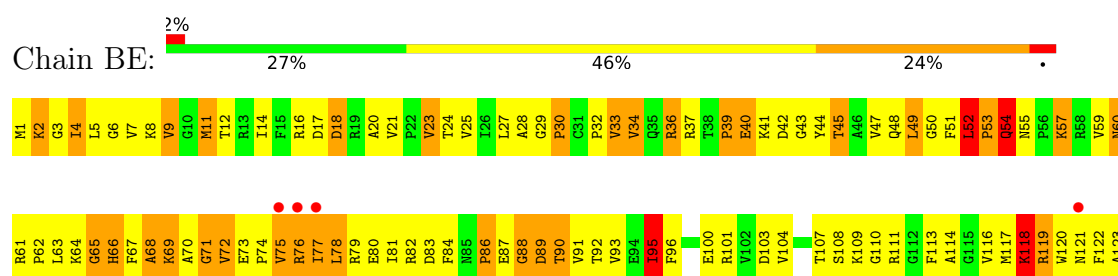
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

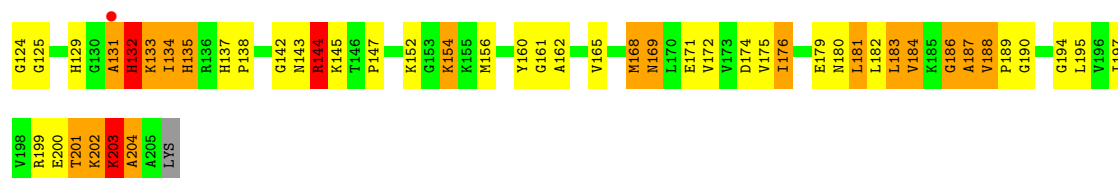


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

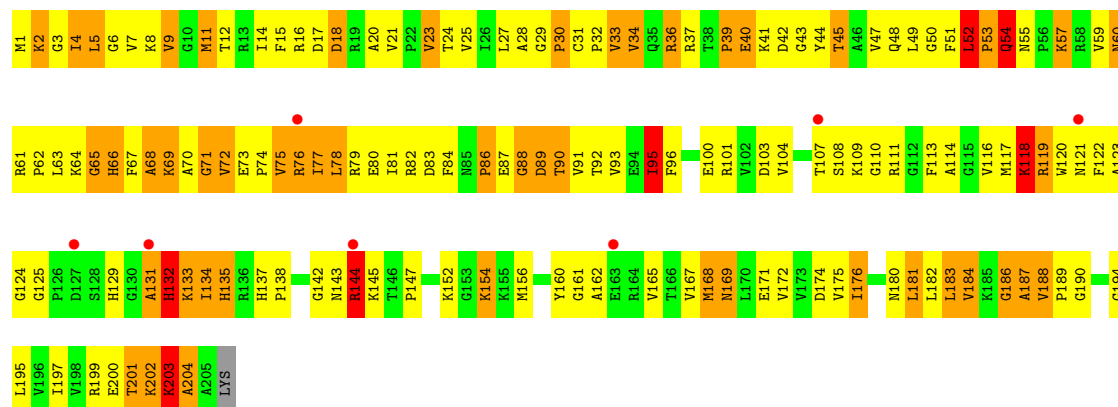


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

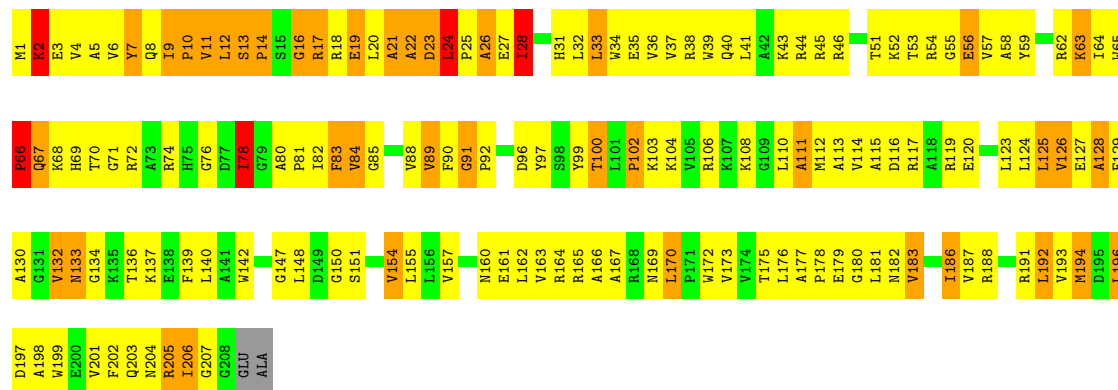
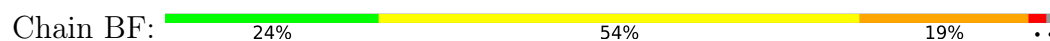




• Molecule 39: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L4

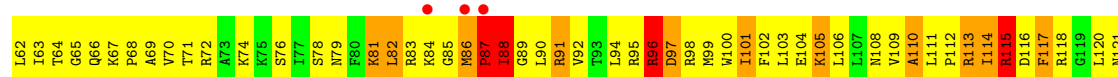
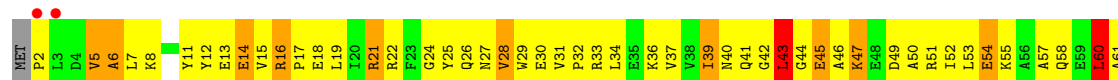


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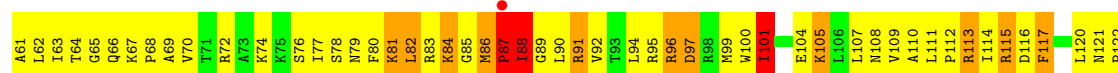
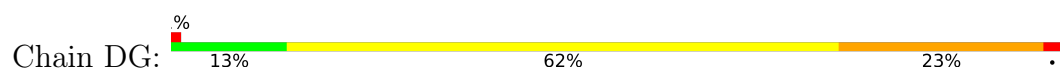




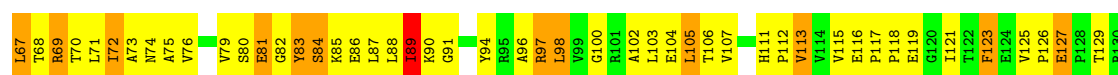
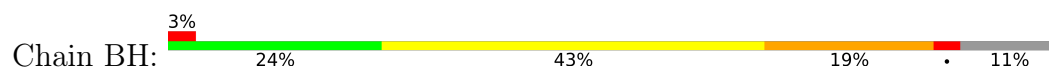
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



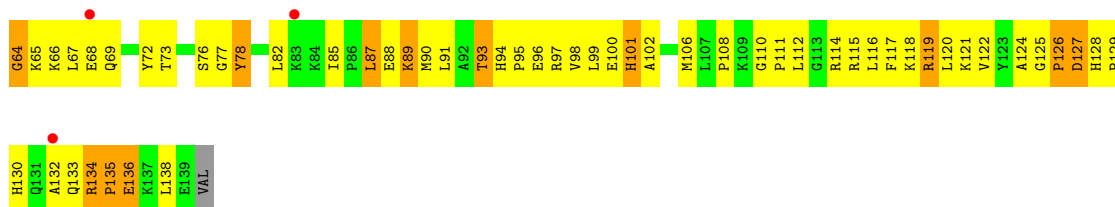
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



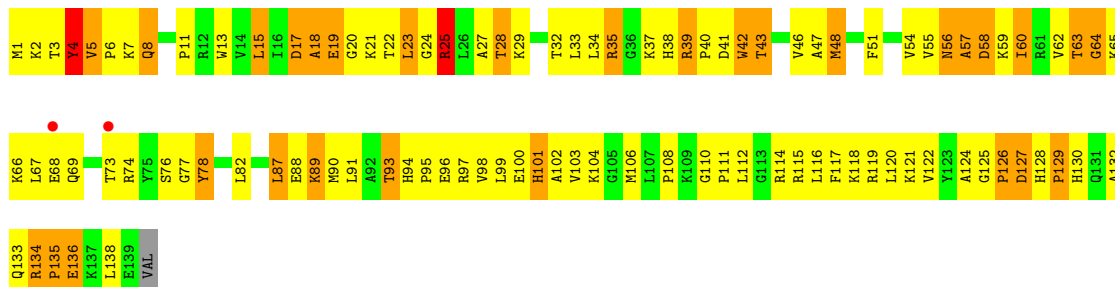
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



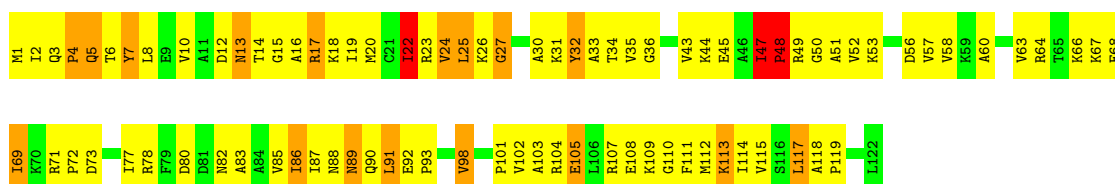
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



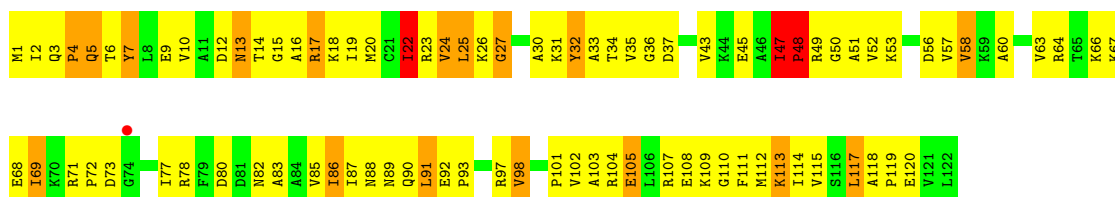
• Molecule 44: 50S RIBOSOMAL PROTEIN L13



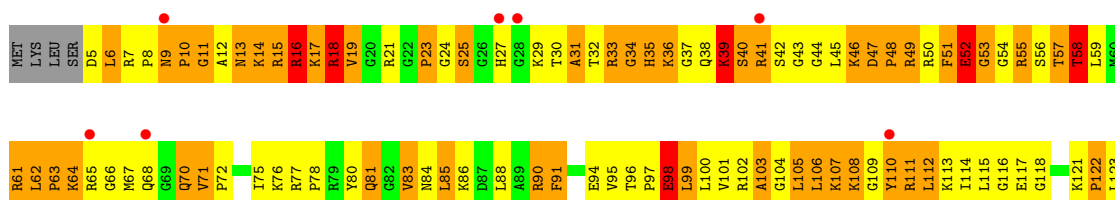
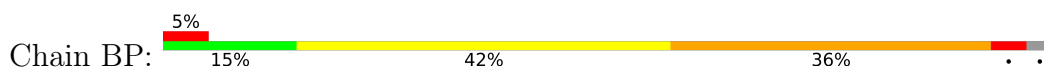
• Molecule 45: 50S RIBOSOMAL PROTEIN L14



• Molecule 45: 50S RIBOSOMAL PROTEIN L14

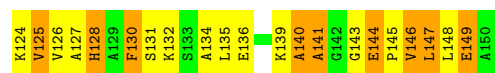
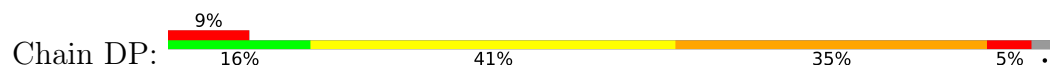


• Molecule 46: 50S RIBOSOMAL PROTEIN L15

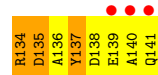




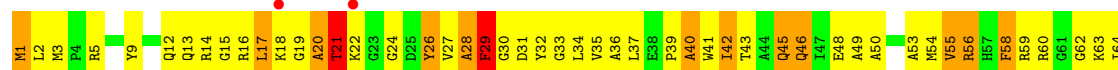
• Molecule 46: 50S RIBOSOMAL PROTEIN L15



• Molecule 47: 50S RIBOSOMAL PROTEIN L16

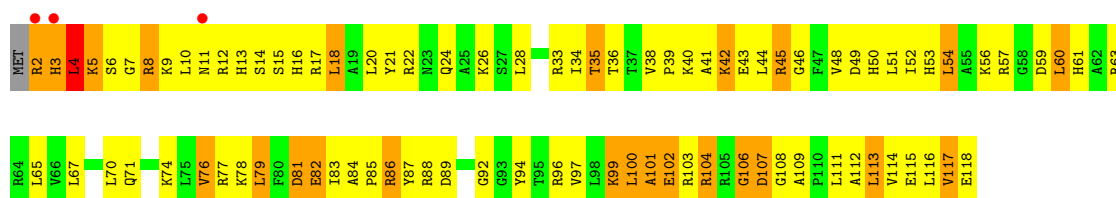


• Molecule 47: 50S RIBOSOMAL PROTEIN L16

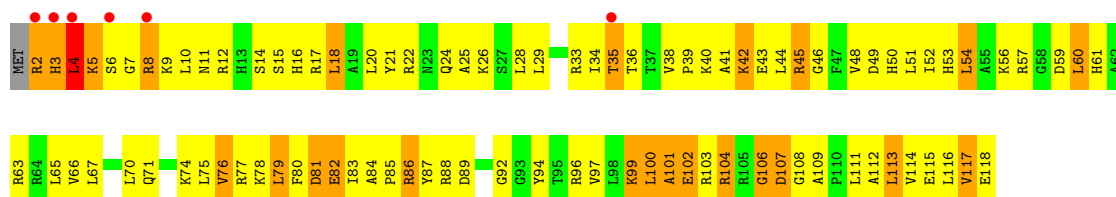


• Molecule 48: 50S RIBOSOMAL PROTEIN L17

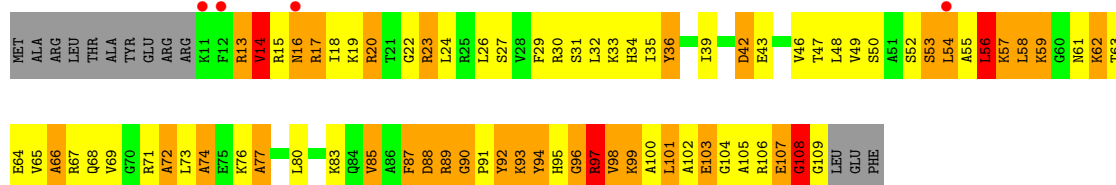
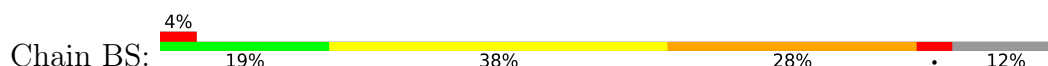




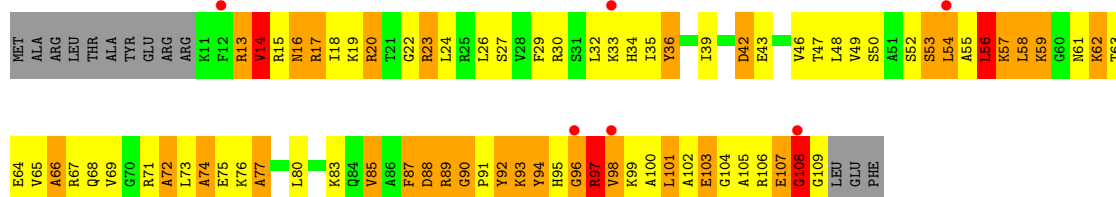
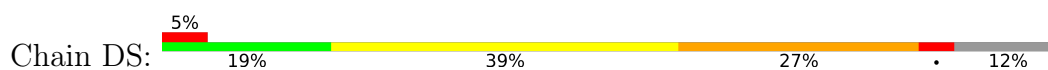
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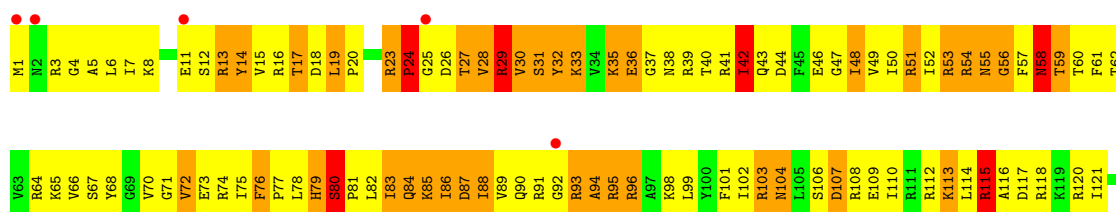
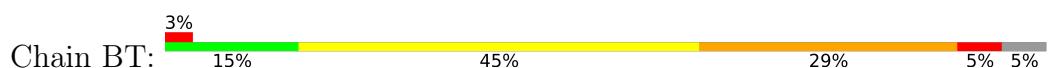
• Molecule 49: 50S RIBOSOMAL PROTEIN L18

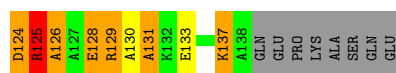


• Molecule 49: 50S RIBOSOMAL PROTEIN L18

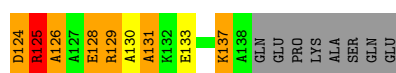
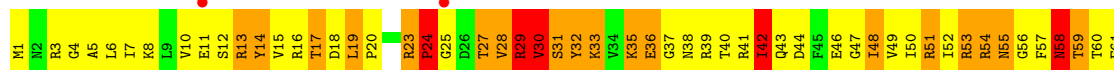
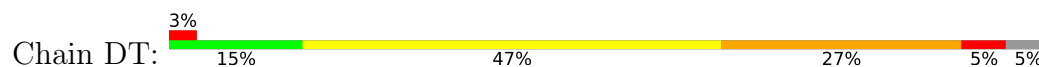


• Molecule 50: 50S RIBOSOMAL PROTEIN L19

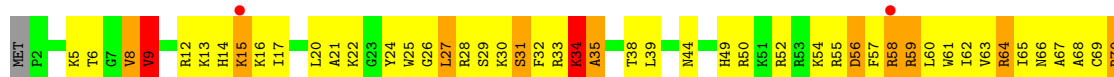




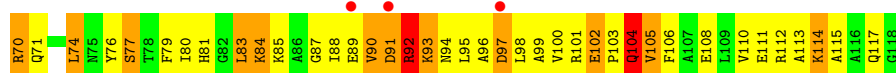
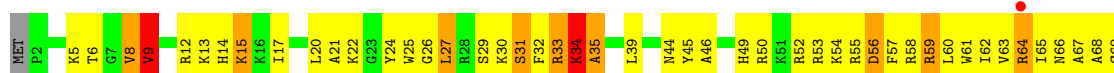
• Molecule 50: 50S RIBOSOMAL PROTEIN L19



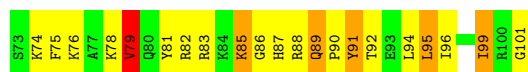
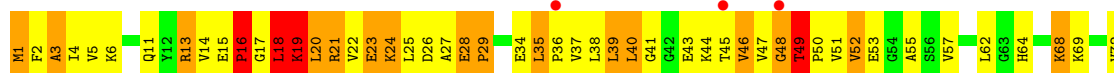
• Molecule 51: 50S RIBOSOMAL PROTEIN L20



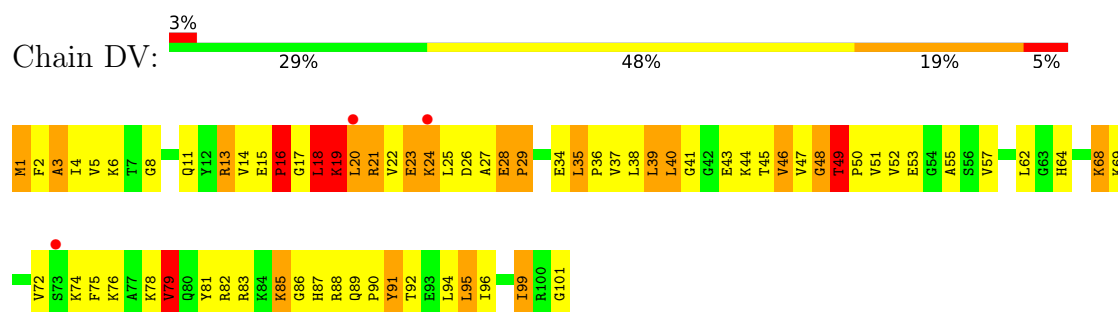
• Molecule 51: 50S RIBOSOMAL PROTEIN L20



• Molecule 52: 50S RIBOSOMAL PROTEIN L21



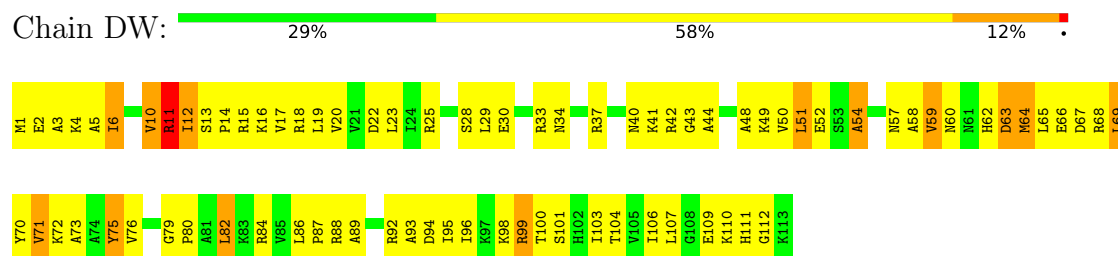
• Molecule 52: 50S RIBOSOMAL PROTEIN L21



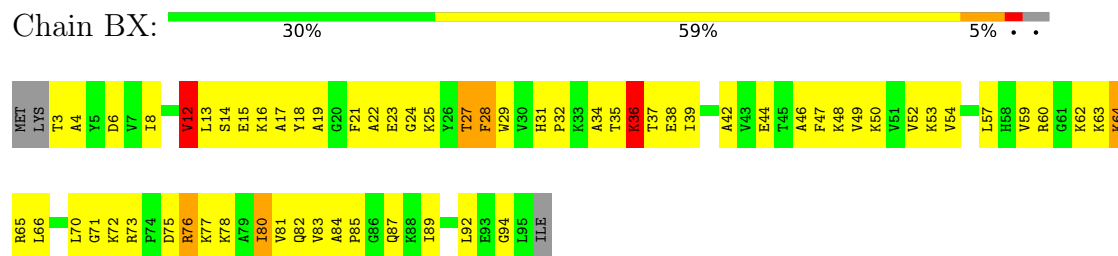
- Molecule 53: 50S RIBOSOMAL PROTEIN L22



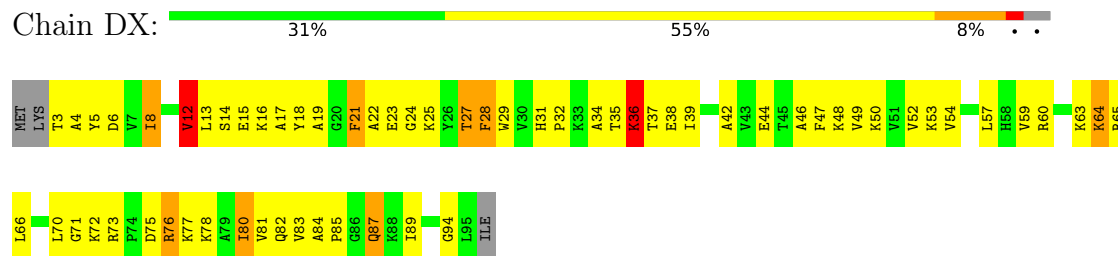
- Molecule 53: 50S RIBOSOMAL PROTEIN L22



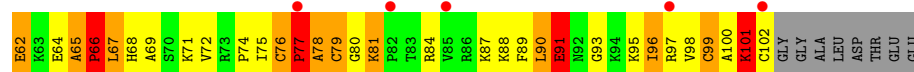
- Molecule 54: 50S RIBOSOMAL PROTEIN L23



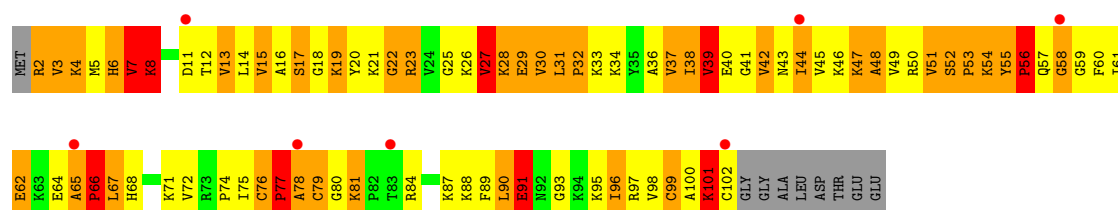
- Molecule 54: 50S RIBOSOMAL PROTEIN L23



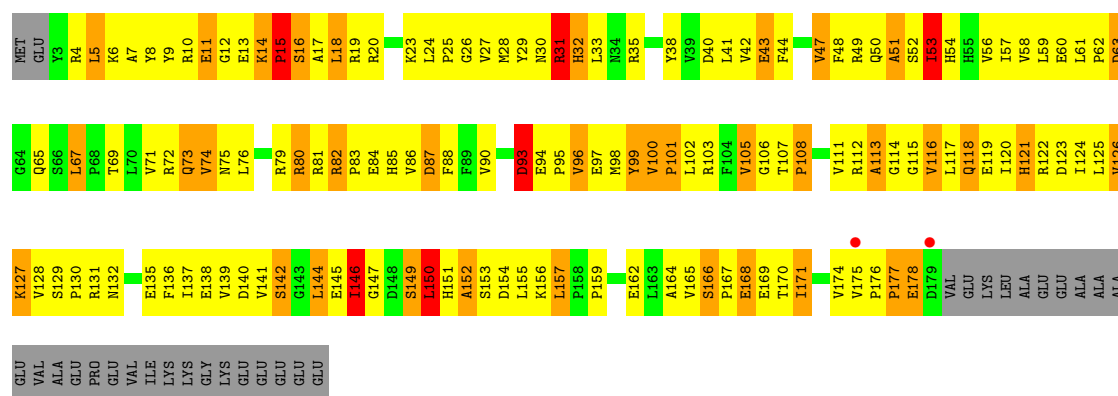
- Molecule 55: 50S RIBOSOMAL PROTEIN L24



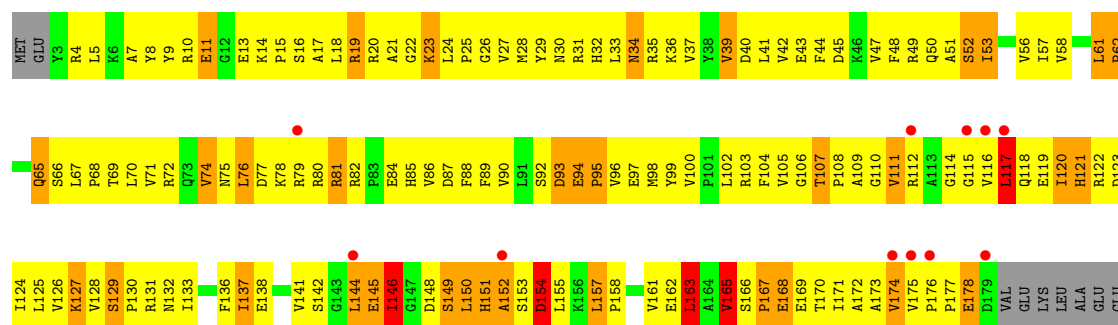
Chain DY:



Chain BZ:



Chain DZ:



ALA
ALA
ALA
GLU
VAL
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.86Å 450.46Å 628.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.50) 99.0 (50.00-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.256 0.208 , 0.255	Depositor DCC
R_{free} test set	36181 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 97.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296042	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: 8AN, PAR, PHA, 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	0.42	0/36190	0.63	37/56486 (0.1%)
1	CA	0.42	0/36190	0.63	36/56486 (0.1%)
2	AB	0.39	1/1936 (0.1%)	0.99	15/2611 (0.6%)
2	CB	0.38	1/1936 (0.1%)	0.98	13/2611 (0.5%)
3	AC	0.41	1/1637 (0.1%)	0.87	3/2207 (0.1%)
3	CC	0.40	1/1637 (0.1%)	0.85	2/2207 (0.1%)
4	AD	0.43	0/1733	1.00	8/2318 (0.3%)
4	CD	0.42	0/1733	1.01	10/2318 (0.4%)
5	AE	0.46	1/1163 (0.1%)	1.00	3/1566 (0.2%)
5	CE	0.44	1/1163 (0.1%)	0.99	4/1566 (0.3%)
6	AF	0.45	0/856	1.03	5/1154 (0.4%)
6	CF	0.42	0/856	1.03	6/1154 (0.5%)
7	AG	0.39	0/1276	0.96	5/1709 (0.3%)
7	CG	0.38	0/1276	0.95	5/1709 (0.3%)
8	AH	0.40	0/1136	1.04	9/1527 (0.6%)
8	CH	0.38	0/1136	1.05	9/1527 (0.6%)
9	AI	0.36	0/1027	0.91	5/1372 (0.4%)
9	CI	0.36	0/1027	0.91	5/1372 (0.4%)
10	AJ	0.46	1/808 (0.1%)	0.93	2/1087 (0.2%)
10	CJ	0.45	1/808 (0.1%)	0.92	2/1087 (0.2%)
11	AK	0.45	0/900	0.98	5/1213 (0.4%)
11	CK	0.42	0/900	0.99	5/1213 (0.4%)
12	AL	0.49	1/987 (0.1%)	1.01	6/1322 (0.5%)
12	CL	0.46	1/987 (0.1%)	1.01	6/1322 (0.5%)
13	AM	0.45	1/996 (0.1%)	1.05	10/1329 (0.8%)
13	CM	0.44	1/996 (0.1%)	1.04	10/1329 (0.8%)
14	AN	0.38	0/501	0.84	1/664 (0.2%)
14	CN	0.37	0/501	0.83	1/664 (0.2%)
15	AO	0.44	0/745	0.91	0/992
15	CO	0.41	0/745	0.91	0/992
16	AP	0.47	1/717 (0.1%)	0.99	5/965 (0.5%)
16	CP	0.47	1/717 (0.1%)	0.99	5/965 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	1/837 (0.1%)	0.89	3/1119 (0.3%)
17	CQ	0.43	1/837 (0.1%)	0.91	3/1119 (0.3%)
18	AR	0.42	0/579	0.90	2/768 (0.3%)
18	CR	0.41	0/579	0.88	2/768 (0.3%)
19	AS	0.46	1/643 (0.2%)	0.98	3/867 (0.3%)
19	CS	0.45	1/643 (0.2%)	0.98	3/867 (0.3%)
20	AT	0.37	0/765	0.99	3/1007 (0.3%)
20	CT	0.36	0/765	0.98	3/1007 (0.3%)
21	AU	0.57	1/213 (0.5%)	0.98	0/279
21	CU	0.56	1/213 (0.5%)	0.97	0/279
22	AV	0.40	0/1784	0.68	0/2780
22	AY	0.50	0/1784	0.68	2/2780 (0.1%)
22	CV	0.39	0/1784	0.64	0/2780
22	CY	0.45	0/1784	0.62	1/2780 (0.0%)
23	AW	0.44	0/1809	0.61	0/2819
23	CW	0.43	0/1809	0.60	0/2819
24	AX	0.43	0/253	0.68	0/391
24	CX	0.42	0/253	0.66	1/391 (0.3%)
25	B0	0.53	0/671	1.05	3/892 (0.3%)
25	D0	0.46	0/671	1.00	3/892 (0.3%)
26	B1	0.61	1/739 (0.1%)	1.18	2/983 (0.2%)
26	D1	0.57	0/739	1.08	2/983 (0.2%)
27	B2	0.56	0/600	1.13	6/793 (0.8%)
27	D2	0.46	0/600	0.94	1/793 (0.1%)
28	B3	0.59	1/473 (0.2%)	1.15	5/636 (0.8%)
28	D3	0.50	1/473 (0.2%)	1.10	5/636 (0.8%)
29	B4	0.61	1/229 (0.4%)	0.97	0/311
29	D4	0.58	1/229 (0.4%)	0.95	0/311
30	B5	0.74	0/473	1.53	11/639 (1.7%)
30	D5	0.61	0/473	1.50	11/639 (1.7%)
31	B6	0.69	1/387 (0.3%)	1.09	2/517 (0.4%)
31	D6	0.65	1/387 (0.3%)	1.07	3/517 (0.6%)
32	B7	0.67	1/427 (0.2%)	1.11	2/563 (0.4%)
32	D7	0.61	1/427 (0.2%)	1.09	3/563 (0.5%)
33	B8	0.75	1/516 (0.2%)	1.42	8/681 (1.2%)
33	D8	0.64	1/516 (0.2%)	1.42	8/681 (1.2%)
34	B9	0.43	0/302	0.87	0/397
34	D9	0.39	0/302	0.88	0/397
35	BA	0.48	4/67716 (0.0%)	0.72	70/105718 (0.1%)
35	DA	0.44	3/67716 (0.0%)	0.70	60/105718 (0.1%)
36	BB	0.44	0/2853	0.73	3/4451 (0.1%)
36	DB	0.40	0/2853	0.70	3/4451 (0.1%)
37	BC	0.54	1/1143 (0.1%)	1.06	11/1552 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.55	1/1145 (0.1%)	1.07	11/1556 (0.7%)
38	BD	0.65	0/2155	1.21	16/2907 (0.6%)
38	DD	0.58	1/2155 (0.0%)	1.19	20/2907 (0.7%)
39	BE	0.63	1/1597 (0.1%)	1.19	14/2155 (0.6%)
39	DE	0.52	1/1597 (0.1%)	1.16	15/2155 (0.7%)
40	BF	0.59	1/1659 (0.1%)	1.13	16/2246 (0.7%)
40	DF	0.51	1/1659 (0.1%)	1.09	11/2246 (0.5%)
41	BG	0.51	0/1498	1.16	13/2013 (0.6%)
41	DG	0.47	0/1498	1.14	16/2013 (0.8%)
42	BH	0.55	1/1246 (0.1%)	1.16	10/1684 (0.6%)
42	DH	0.46	1/1246 (0.1%)	1.12	10/1684 (0.6%)
43	BI	0.50	1/1147 (0.1%)	1.04	7/1553 (0.5%)
43	DI	0.47	1/1147 (0.1%)	1.02	7/1553 (0.5%)
44	BN	0.60	1/1132 (0.1%)	1.20	10/1527 (0.7%)
44	DN	0.49	1/1132 (0.1%)	1.16	10/1527 (0.7%)
45	BO	0.59	0/943	1.06	6/1269 (0.5%)
45	DO	0.48	0/943	1.02	7/1269 (0.6%)
46	BP	0.64	0/1131	1.40	18/1504 (1.2%)
46	DP	0.55	0/1131	1.36	19/1504 (1.3%)
47	BQ	0.54	0/1143	1.05	6/1527 (0.4%)
47	DQ	0.48	0/1143	1.04	5/1527 (0.3%)
48	BR	0.59	0/974	1.11	4/1302 (0.3%)
48	DR	0.51	0/974	1.07	5/1302 (0.4%)
49	BS	0.59	1/779 (0.1%)	1.12	6/1038 (0.6%)
49	DS	0.51	1/779 (0.1%)	1.09	5/1038 (0.5%)
50	BT	0.55	1/1156 (0.1%)	1.24	23/1544 (1.5%)
50	DT	0.49	1/1156 (0.1%)	1.22	21/1544 (1.4%)
51	BU	0.63	0/975	1.36	12/1297 (0.9%)
51	DU	0.51	0/975	1.29	10/1297 (0.8%)
52	BV	0.56	0/790	1.02	3/1057 (0.3%)
52	DV	0.44	0/790	0.99	3/1057 (0.3%)
53	BW	0.63	0/907	1.10	6/1216 (0.5%)
53	DW	0.54	0/907	1.07	7/1216 (0.6%)
54	BX	0.61	1/740 (0.1%)	1.03	1/995 (0.1%)
54	DX	0.54	1/740 (0.1%)	1.02	1/995 (0.1%)
55	BY	0.71	1/789 (0.1%)	1.26	12/1053 (1.1%)
55	DY	0.64	1/789 (0.1%)	1.24	11/1053 (1.0%)
56	BZ	0.54	1/1436 (0.1%)	1.11	14/1951 (0.7%)
56	DZ	0.46	1/1436 (0.1%)	1.04	9/1951 (0.5%)
All	All	0.46	61/320004 (0.0%)	0.81	886/478610 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	10
1	CA	0	8
23	AW	0	2
35	BA	4	39
35	DA	3	33
36	BB	0	3
36	DB	0	3
All	All	7	98

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	652	C	O5'-C5'	7.12	1.53	1.42
35	BA	656	G	O5'-C5'	7.03	1.53	1.42
35	BA	652	C	C3'-O3'	6.81	1.53	1.43
35	DA	656	G	O5'-C5'	6.78	1.52	1.42
35	DA	652	C	O5'-C5'	6.75	1.52	1.42

The worst 5 of 886 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	BU	34	LYS	N-CA-C	-18.54	93.49	114.62
51	DU	34	LYS	N-CA-C	-18.42	93.62	114.62
33	D8	32	LEU	N-CA-C	-15.40	93.96	111.82
33	B8	32	LEU	N-CA-C	-14.93	94.50	111.82
35	BA	283	A	C2'-C3'-O3'	13.79	130.18	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	283	A	C3'
35	BA	1378	A	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'
35	DA	283	A	C3'

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	484	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	Sidechain
1	AA	9	G	Sidechain

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	32329	0	16315	1274	0
1	CA	32329	0	16312	1270	0
2	AB	1901	0	1951	298	0
2	CB	1901	0	1951	298	0
3	AC	1613	0	1677	255	0
3	CC	1613	0	1677	259	0
4	AD	1703	0	1762	175	0
4	CD	1703	0	1763	175	0
5	AE	1147	0	1207	144	0
5	CE	1147	0	1207	138	0
6	AF	843	0	857	105	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	120	0
8	AH	1116	0	1177	130	0
8	CH	1116	0	1177	133	0
9	AI	1011	0	1041	174	0
9	CI	1011	0	1041	174	0
10	AJ	795	0	840	179	0
10	CJ	795	0	840	177	0
11	AK	885	0	904	106	0
11	CK	885	0	904	103	0
12	AL	971	0	1057	132	0
12	CL	971	0	1057	131	0
13	AM	988	0	1056	179	0
13	CM	988	0	1056	175	0
14	AN	492	0	529	77	0
14	CN	492	0	529	77	0
15	AO	734	0	771	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	82	0
16	AP	701	0	720	84	0
16	CP	701	0	720	81	0
17	AQ	824	0	891	94	0
17	CQ	824	0	891	90	0
18	AR	574	0	644	83	0
18	CR	574	0	644	89	0
19	AS	630	0	652	109	0
19	CS	630	0	652	103	0
20	AT	763	0	861	104	0
20	CT	763	0	861	106	0
21	AU	209	0	221	17	0
21	CU	209	0	221	19	0
22	AV	1630	0	831	65	0
22	AY	1630	0	831	84	0
22	CV	1630	0	831	78	0
22	CY	1630	0	831	71	0
23	AW	1619	0	822	95	0
23	CW	1619	0	821	95	0
24	AX	227	0	119	7	0
24	CX	227	0	118	11	0
25	B0	662	0	688	83	0
25	D0	662	0	688	83	0
26	B1	732	0	808	99	0
26	D1	732	0	808	95	0
27	B2	598	0	653	62	0
27	D2	598	0	653	96	0
28	B3	468	0	523	32	0
28	D3	468	0	523	32	0
29	B4	226	0	229	44	0
29	D4	226	0	229	37	0
30	B5	459	0	480	93	0
30	D5	459	0	480	90	0
31	B6	381	0	390	108	0
31	D6	381	0	390	107	0
32	B7	419	0	467	30	0
32	D7	419	0	467	30	0
33	B8	508	0	576	105	0
33	D8	508	0	576	103	0
34	B9	299	0	325	29	0
34	D9	299	0	325	31	0
35	BA	60459	0	30474	2068	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	60459	0	30478	2074	0
36	BB	2551	0	1294	105	0
36	DB	2551	0	1294	88	0
37	BC	1140	0	863	131	0
37	DC	1142	0	865	133	0
38	BD	2105	0	2182	335	0
38	DD	2105	0	2182	327	0
39	BE	1564	0	1629	263	0
39	DE	1564	0	1629	266	0
40	BF	1624	0	1677	222	0
40	DF	1624	0	1677	220	0
41	BG	1474	0	1534	273	0
41	DG	1474	0	1534	276	0
42	BH	1223	0	1282	179	0
42	DH	1223	0	1282	176	0
43	BI	1132	0	1218	200	0
43	DI	1132	0	1218	204	0
44	BN	1105	0	1180	150	0
44	DN	1105	0	1180	148	0
45	BO	933	0	996	132	0
45	DO	933	0	996	131	0
46	BP	1114	0	1187	290	0
46	DP	1114	0	1187	287	0
47	BQ	1122	0	1179	178	0
47	DQ	1122	0	1179	177	0
48	BR	960	0	1021	145	0
48	DR	960	0	1021	145	0
49	BS	771	0	832	156	0
49	DS	771	0	832	150	0
50	BT	1142	0	1202	251	0
50	DT	1142	0	1202	237	0
51	BU	958	0	1015	168	0
51	DU	958	0	1015	166	0
52	BV	779	0	852	163	0
52	DV	779	0	852	162	0
53	BW	896	0	953	94	0
53	DW	896	0	953	97	0
54	BX	726	0	778	90	0
54	DX	726	0	778	91	0
55	BY	776	0	870	191	0
55	DY	776	0	870	196	0
56	BZ	1404	0	1432	241	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DZ	1404	0	1432	248	0
57	AA	198	0	0	0	0
57	AD	1	0	0	0	0
57	AE	1	0	0	0	0
57	AG	1	0	0	0	0
57	AI	1	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AV	5	0	0	0	0
57	AW	8	0	0	0	0
57	AX	2	0	0	0	0
57	B0	1	0	0	0	0
57	B1	1	0	0	0	0
57	B2	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	422	0	0	0	0
57	BB	14	0	0	0	0
57	BD	2	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	1	0
57	BV	1	0	0	0	0
57	BX	2	0	0	0	0
57	CA	199	0	0	0	0
57	CE	1	0	0	0	0
57	CI	1	0	0	0	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CV	5	0	0	0	0
57	CW	7	0	0	0	0
57	CX	3	0	0	0	0
57	D1	1	0	0	0	0
57	D2	3	0	0	0	0
57	D5	2	0	0	0	0
57	D7	2	0	0	0	0
57	DA	421	0	0	0	0
57	DB	13	0	0	0	0
57	DC	1	0	0	0	0
57	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DE	1	0	0	0	0
57	DF	2	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DS	1	0	0	0	0
57	DV	1	0	0	0	0
57	DX	3	0	0	0	0
58	AA	42	0	45	2	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D9	1	0	0	0	0
All	All	296042	0	199734	19777	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

The worst 5 of 19777 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)
54:BX:63:LYS:HE3	54:BX:72:LYS:HE3	1.23	1.21
56:DZ:53:ILE:HG23	56:DZ:71:VAL:HG23	1.21	1.18
46:DP:59:LEU:HA	46:DP:61:ARG:CZ	1.73	1.18
35:BA:2334:G:H21	49:BS:18:ILE:HD11	1.09	1.17
35:DA:925:C:H2'	35:DA:926:A:H5''	1.27	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	138 (59%)	63 (27%)	32 (14%)	0	3
2	CB	233/256 (91%)	138 (59%)	62 (27%)	33 (14%)	0	3
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	0	6
3	CC	205/239 (86%)	128 (62%)	56 (27%)	21 (10%)	0	6
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	0	7
4	CD	206/209 (99%)	150 (73%)	38 (18%)	18 (9%)	0	7
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	1	9
5	CE	149/162 (92%)	115 (77%)	22 (15%)	12 (8%)	1	8
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	1	15
6	CF	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	1	15
7	AG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	2	20
7	CG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	2	20
8	AH	136/138 (99%)	107 (79%)	25 (18%)	4 (3%)	3	26
8	CH	136/138 (99%)	108 (79%)	24 (18%)	4 (3%)	3	26
9	AI	121/128 (94%)	85 (70%)	23 (19%)	13 (11%)	0	5
9	CI	121/128 (94%)	83 (69%)	26 (22%)	12 (10%)	0	6
10	AJ	97/105 (92%)	62 (64%)	25 (26%)	10 (10%)	0	5
10	CJ	97/105 (92%)	63 (65%)	24 (25%)	10 (10%)	0	5
11	AK	117/129 (91%)	86 (74%)	26 (22%)	5 (4%)	2	18
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	2	18
12	AL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	5
12	CL	123/135 (91%)	83 (68%)	26 (21%)	14 (11%)	0	5
13	AM	117/126 (93%)	67 (57%)	30 (26%)	20 (17%)	0	2
13	CM	117/126 (93%)	67 (57%)	31 (26%)	19 (16%)	0	2
14	AN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	3
14	CN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	3
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	0	6
15	CO	86/89 (97%)	57 (66%)	21 (24%)	8 (9%)	0	6
16	AP	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	4	29
16	CP	82/88 (93%)	59 (72%)	21 (26%)	2 (2%)	4	29
17	AQ	98/105 (93%)	74 (76%)	20 (20%)	4 (4%)	2	19
17	CQ	98/105 (93%)	76 (78%)	19 (19%)	3 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	41 (60%)	14 (21%)	13 (19%)	0	1
18	CR	68/88 (77%)	41 (60%)	13 (19%)	14 (21%)	0	1
19	AS	77/93 (83%)	49 (64%)	16 (21%)	12 (16%)	0	2
19	CS	77/93 (83%)	49 (64%)	15 (20%)	13 (17%)	0	2
20	AT	97/106 (92%)	69 (71%)	18 (19%)	10 (10%)	0	5
20	CT	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	0	5
21	AU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	0	7
21	CU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	0	7
25	B0	82/85 (96%)	65 (79%)	14 (17%)	3 (4%)	2	21
25	D0	82/85 (96%)	61 (74%)	17 (21%)	4 (5%)	1	16
26	B1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	0	5
26	D1	92/98 (94%)	66 (72%)	18 (20%)	8 (9%)	0	7
27	B2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	0	6
27	D2	69/72 (96%)	37 (54%)	23 (33%)	9 (13%)	0	3
28	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	1	14
28	D3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	1	14
29	B4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
29	D4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
30	B5	57/60 (95%)	38 (67%)	8 (14%)	11 (19%)	0	1
30	D5	57/60 (95%)	39 (68%)	6 (10%)	12 (21%)	0	1
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
31	D6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	3
33	D8	62/65 (95%)	43 (69%)	10 (16%)	9 (14%)	0	3
34	B9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
34	D9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
37	BC	183/229 (80%)	81 (44%)	47 (26%)	55 (30%)	0	0
37	DC	183/229 (80%)	82 (45%)	47 (26%)	54 (30%)	0	0
38	BD	270/276 (98%)	208 (77%)	38 (14%)	24 (9%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	205 (76%)	38 (14%)	27 (10%)	0	6
39	BE	203/206 (98%)	130 (64%)	40 (20%)	33 (16%)	0	2
39	DE	203/206 (98%)	127 (63%)	44 (22%)	32 (16%)	0	2
40	BF	206/210 (98%)	142 (69%)	35 (17%)	29 (14%)	0	3
40	DF	206/210 (98%)	143 (69%)	35 (17%)	28 (14%)	0	3
41	BG	177/182 (97%)	107 (60%)	50 (28%)	20 (11%)	0	5
41	DG	177/182 (97%)	108 (61%)	45 (25%)	24 (14%)	0	3
42	BH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	2
42	DH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	2
43	BI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	2
43	DI	144/148 (97%)	85 (59%)	37 (26%)	22 (15%)	0	2
44	BN	137/140 (98%)	90 (66%)	30 (22%)	17 (12%)	0	4
44	DN	137/140 (98%)	91 (66%)	29 (21%)	17 (12%)	0	4
45	BO	120/122 (98%)	91 (76%)	21 (18%)	8 (7%)	1	11
45	DO	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	11
46	BP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
46	DP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
47	BQ	139/141 (99%)	107 (77%)	24 (17%)	8 (6%)	1	13
47	DQ	139/141 (99%)	106 (76%)	23 (16%)	10 (7%)	1	9
48	BR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	4
48	DR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	4
49	BS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	0
49	DS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	0
50	BT	136/146 (93%)	82 (60%)	26 (19%)	28 (21%)	0	1
50	DT	136/146 (93%)	81 (60%)	27 (20%)	28 (21%)	0	1
51	BU	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	1	12
51	DU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	8
52	BV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	2
52	DV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	2
53	BW	111/113 (98%)	87 (78%)	15 (14%)	9 (8%)	1	8
53	DW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BX	91/96 (95%)	74 (81%)	14 (15%)	3 (3%)	3	23
54	DX	91/96 (95%)	74 (81%)	13 (14%)	4 (4%)	2	17
55	BY	99/110 (90%)	37 (37%)	30 (30%)	32 (32%)	0	0
55	DY	99/110 (90%)	35 (35%)	32 (32%)	32 (32%)	0	0
56	BZ	175/206 (85%)	113 (65%)	38 (22%)	24 (14%)	0	3
56	DZ	175/206 (85%)	103 (59%)	45 (26%)	27 (15%)	0	2
All	All	11670/12592 (93%)	7783 (67%)	2440 (21%)	1447 (12%)	0	4

5 of 1447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	88	ALA
2	AB	154	LEU
2	AB	165	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	181 (90%)	21 (10%)	7	27
2	CB	202/220 (92%)	183 (91%)	19 (9%)	8	31
3	AC	160/188 (85%)	151 (94%)	9 (6%)	19	46
3	CC	160/188 (85%)	151 (94%)	9 (6%)	19	46
4	AD	180/181 (99%)	159 (88%)	21 (12%)	5	24
4	CD	180/181 (99%)	161 (89%)	19 (11%)	6	27
5	AE	115/123 (94%)	108 (94%)	7 (6%)	17	43
5	CE	115/123 (94%)	108 (94%)	7 (6%)	17	43
6	AF	90/90 (100%)	85 (94%)	5 (6%)	19	46
6	CF	90/90 (100%)	84 (93%)	6 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	116 (92%)	10 (8%)	11	36
7	CG	126/127 (99%)	116 (92%)	10 (8%)	11	36
8	AH	119/119 (100%)	107 (90%)	12 (10%)	7	28
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7	28
9	AI	98/99 (99%)	89 (91%)	9 (9%)	8	32
9	CI	98/99 (99%)	89 (91%)	9 (9%)	8	32
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	22
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	22
11	AK	90/99 (91%)	85 (94%)	5 (6%)	19	46
11	CK	90/99 (91%)	86 (96%)	4 (4%)	25	51
12	AL	104/111 (94%)	94 (90%)	10 (10%)	8	30
12	CL	104/111 (94%)	93 (89%)	11 (11%)	6	27
13	AM	99/101 (98%)	89 (90%)	10 (10%)	7	28
13	CM	99/101 (98%)	89 (90%)	10 (10%)	7	28
14	AN	49/50 (98%)	46 (94%)	3 (6%)	17	43
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	43
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	28
15	CO	79/80 (99%)	71 (90%)	8 (10%)	7	28
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3	16
16	CP	72/74 (97%)	62 (86%)	10 (14%)	3	19
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	16	42
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	16	42
18	AR	61/77 (79%)	55 (90%)	6 (10%)	7	30
18	CR	61/77 (79%)	55 (90%)	6 (10%)	7	30
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2	14
19	CS	69/80 (86%)	57 (83%)	12 (17%)	2	11
20	AT	76/82 (93%)	72 (95%)	4 (5%)	20	47
20	CT	76/82 (93%)	72 (95%)	4 (5%)	20	47
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	47
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	47
25	B0	66/67 (98%)	60 (91%)	6 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	6	27
26	B1	78/83 (94%)	66 (85%)	12 (15%)	2	16
26	D1	78/83 (94%)	65 (83%)	13 (17%)	2	13
27	B2	66/67 (98%)	55 (83%)	11 (17%)	2	13
27	D2	66/67 (98%)	58 (88%)	8 (12%)	5	22
28	B3	51/52 (98%)	48 (94%)	3 (6%)	18	44
28	D3	51/52 (98%)	48 (94%)	3 (6%)	18	44
29	B4	27/63 (43%)	24 (89%)	3 (11%)	6	25
29	D4	27/63 (43%)	24 (89%)	3 (11%)	6	25
30	B5	51/52 (98%)	42 (82%)	9 (18%)	2	11
30	D5	51/52 (98%)	42 (82%)	9 (18%)	2	11
31	B6	43/52 (83%)	33 (77%)	10 (23%)	1	5
31	D6	43/52 (83%)	32 (74%)	11 (26%)	0	3
32	B7	41/42 (98%)	35 (85%)	6 (15%)	3	17
32	D7	41/42 (98%)	35 (85%)	6 (15%)	3	17
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	12
33	D8	53/55 (96%)	43 (81%)	10 (19%)	1	9
34	B9	33/34 (97%)	30 (91%)	3 (9%)	9	32
34	D9	33/34 (97%)	30 (91%)	3 (9%)	9	32
37	BC	61/181 (34%)	52 (85%)	9 (15%)	3	17
37	DC	61/181 (34%)	52 (85%)	9 (15%)	3	17
38	BD	213/218 (98%)	178 (84%)	35 (16%)	2	14
38	DD	213/218 (98%)	178 (84%)	35 (16%)	2	14
39	BE	165/166 (99%)	141 (86%)	24 (14%)	3	17
39	DE	165/166 (99%)	140 (85%)	25 (15%)	3	16
40	BF	165/166 (99%)	145 (88%)	20 (12%)	5	22
40	DF	165/166 (99%)	146 (88%)	19 (12%)	5	24
41	BG	155/156 (99%)	132 (85%)	23 (15%)	3	17
41	DG	155/156 (99%)	135 (87%)	20 (13%)	4	21
42	BH	132/148 (89%)	119 (90%)	13 (10%)	7	30
42	DH	132/148 (89%)	120 (91%)	12 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	114 (93%)	8 (7%)	15	41
43	DI	122/124 (98%)	114 (93%)	8 (7%)	15	41
44	BN	117/119 (98%)	99 (85%)	18 (15%)	2	16
44	DN	117/119 (98%)	99 (85%)	18 (15%)	2	16
45	BO	100/100 (100%)	85 (85%)	15 (15%)	3	17
45	DO	100/100 (100%)	86 (86%)	14 (14%)	3	19
46	BP	112/116 (97%)	94 (84%)	18 (16%)	2	14
46	DP	112/116 (97%)	95 (85%)	17 (15%)	3	16
47	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	16
47	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	14
48	BR	100/101 (99%)	87 (87%)	13 (13%)	4	21
48	DR	100/101 (99%)	87 (87%)	13 (13%)	4	21
49	BS	77/88 (88%)	67 (87%)	10 (13%)	4	21
49	DS	77/88 (88%)	67 (87%)	10 (13%)	4	21
50	BT	120/127 (94%)	102 (85%)	18 (15%)	3	17
50	DT	120/127 (94%)	101 (84%)	19 (16%)	2	15
51	BU	92/94 (98%)	78 (85%)	14 (15%)	3	16
51	DU	92/94 (98%)	78 (85%)	14 (15%)	3	16
52	BV	82/82 (100%)	65 (79%)	17 (21%)	1	6
52	DV	82/82 (100%)	66 (80%)	16 (20%)	1	8
53	BW	91/92 (99%)	83 (91%)	8 (9%)	9	32
53	DW	91/92 (99%)	83 (91%)	8 (9%)	9	32
54	BX	74/78 (95%)	66 (89%)	8 (11%)	6	26
54	DX	74/78 (95%)	65 (88%)	9 (12%)	5	22
55	BY	84/91 (92%)	67 (80%)	17 (20%)	1	7
55	DY	84/91 (92%)	67 (80%)	17 (20%)	1	7
56	BZ	155/179 (87%)	134 (86%)	21 (14%)	4	20
56	DZ	155/179 (87%)	135 (87%)	20 (13%)	4	21
All	All	9654/10432 (92%)	8505 (88%)	1149 (12%)	5	23

5 of 1149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	DG	91	ARG
56	DZ	163	LEU
43	DI	118	LYS
41	DG	88	ILE
49	DS	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 324 such sidechains are listed below:

Mol	Chain	Res	Type
25	D0	35	ASN
43	DI	43	ASN
27	D2	46	GLN
38	DD	166	GLN
47	DQ	141	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	217 (14%)	29 (1%)
1	CA	1503/1522 (98%)	218 (14%)	29 (1%)
22	AV	74/77 (96%)	15 (20%)	0
22	AY	74/77 (96%)	20 (27%)	1 (1%)
22	CV	74/77 (96%)	19 (25%)	1 (1%)
22	CY	74/77 (96%)	20 (27%)	1 (1%)
23	AW	75/76 (98%)	13 (17%)	0
23	CW	75/76 (98%)	15 (20%)	0
24	AX	10/11 (90%)	1 (10%)	0
24	CX	10/11 (90%)	2 (20%)	0
35	BA	2806/2822 (99%)	519 (18%)	55 (1%)
35	DA	2806/2822 (99%)	517 (18%)	53 (1%)
36	BB	118/122 (96%)	13 (11%)	1 (0%)
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9320/9414 (99%)	1602 (17%)	171 (1%)

5 of 1602 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	AA	48	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	CV	34	G
35	DA	1532	C
35	DA	128	C
35	DA	603	A
35	DA	1912	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	PHA	AV	77	22	10,11,11	0.67	0	8,13,13	0.36	0
22	8AN	CY	76	35,22	21,24,25	0.70	1 (4%)	26,35,38	0.40	0
22	8AN	CV	76	57,22	21,24,25	0.90	1 (4%)	26,35,38	0.54	1 (3%)
22	8AN	AV	76	57,22	21,24,25	0.88	1 (4%)	26,35,38	0.60	1 (3%)
22	8AN	AY	76	35,22	21,24,25	0.92	1 (4%)	26,35,38	0.38	0
22	PHA	CY	77	22	10,11,11	1.24	0	8,13,13	0.40	0
22	PHA	AY	77	22	10,11,11	0.71	0	8,13,13	0.45	0
22	PHA	CV	77	22	10,11,11	0.69	0	8,13,13	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHA	AV	77	22	-	0/5/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	8AN	CY	76	35,22	-	0/7/25/26	0/3/3/3
22	8AN	CV	76	57,22	-	1/7/25/26	0/3/3/3
22	8AN	AV	76	57,22	-	1/7/25/26	0/3/3/3
22	8AN	AY	76	35,22	-	0/7/25/26	0/3/3/3
22	PHA	CY	77	22	-	2/5/6/6	0/1/1/1
22	PHA	AY	77	22	-	3/5/6/6	0/1/1/1
22	PHA	CV	77	22	-	0/5/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AY	76	8AN	C3'-N3'	-3.69	1.41	1.47
22	AV	76	8AN	C3'-N3'	-3.64	1.41	1.47
22	CV	76	8AN	C3'-N3'	-3.46	1.42	1.47
22	CY	76	8AN	C3'-N3'	-2.78	1.43	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	76	8AN	O4'-C4'-C3'	2.15	107.35	104.22
22	CV	76	8AN	O4'-C4'-C3'	2.12	107.31	104.22

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AV	76	8AN	C4'-C5'-O5'-P
22	AY	77	PHA	O-C-CA-CB
22	CV	76	8AN	C4'-C5'-O5'-P
22	CY	77	PHA	C-CA-CB-CG
22	CY	77	PHA	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	77	PHA	1	0
22	CY	76	8AN	2	0
22	CV	76	8AN	2	0
22	AV	76	8AN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AY	76	8AN	3	0
22	CY	77	PHA	4	0
22	AY	77	PHA	5	0
22	CV	77	PHA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1354 ligands modelled in this entry, 1352 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	CA	1800	-	44,45,45	1.67	10 (22%)	63,67,67	1.26	8 (12%)
58	PAR	AA	1799	-	44,45,45	1.92	13 (29%)	63,67,67	1.37	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	CA	1800	-	-	4/18/94/94	0/4/4/4
58	PAR	AA	1799	-	-	3/18/94/94	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	1799	PAR	C31-C21	5.15	1.60	1.53
58	AA	1799	PAR	C11-C21	4.36	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1800	PAR	O54-C14	3.56	1.51	1.41
58	AA	1799	PAR	C34-C24	3.34	1.57	1.53
58	CA	1800	PAR	C34-C24	3.30	1.57	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	1799	PAR	O33-C14-C24	4.23	115.00	108.08
58	AA	1799	PAR	O11-C11-C21	4.16	114.89	108.08
58	CA	1800	PAR	C14-O54-C54	3.72	120.99	113.72
58	AA	1799	PAR	O54-C54-C64	3.70	113.19	106.07
58	CA	1800	PAR	O54-C54-C64	3.65	113.09	106.07

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

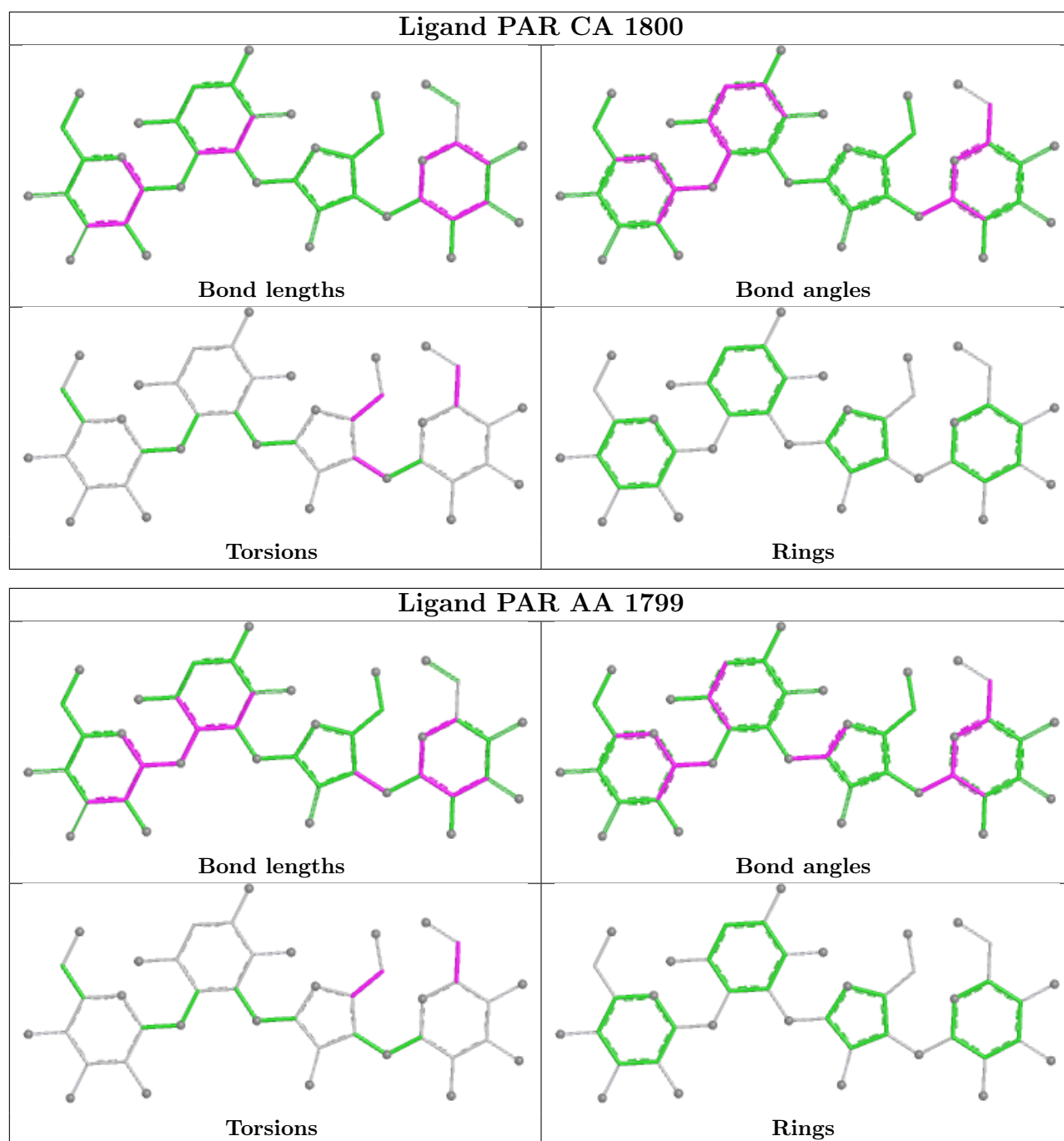
Mol	Chain	Res	Type	Atoms
58	AA	1799	PAR	O43-C43-C53-O53
58	AA	1799	PAR	C44-C54-C64-N64
58	CA	1800	PAR	O43-C43-C53-O53
58	AA	1799	PAR	C33-C43-C53-O53
58	CA	1800	PAR	C33-C43-C53-O53

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	1800	PAR	2	0
58	AA	1799	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
9	AI	2
9	CI	2
31	D6	1
31	B6	1
41	BG	1
41	DG	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	4.60
1	B6	46:HIS	C	47:THR	N	4.59
1	BG	112:PRO	C	113:ARG	N	3.80
1	DG	112:PRO	C	113:ARG	N	3.77
1	CM	69:GLU	C	70:LEU	N	3.15

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	1504/1522 (98%)	0.11	21 (1%) 73 48	47, 104, 183, 200	0
1	CA	1504/1522 (98%)	0.34	41 (2%) 56 33	69, 117, 189, 200	0
2	AB	235/256 (91%)	0.12	4 (1%) 69 43	73, 131, 181, 200	0
2	CB	235/256 (91%)	0.11	4 (1%) 69 43	85, 154, 189, 200	0
3	AC	207/239 (86%)	0.03	1 (0%) 87 68	71, 116, 160, 200	0
3	CC	207/239 (86%)	0.15	1 (0%) 87 68	87, 139, 180, 200	0
4	AD	208/209 (99%)	0.20	4 (1%) 66 41	60, 110, 153, 185	0
4	CD	208/209 (99%)	0.05	5 (2%) 59 35	58, 101, 142, 180	0
5	AE	151/162 (93%)	-0.24	0 100 100	52, 101, 144, 174	0
5	CE	151/162 (93%)	0.20	2 (1%) 75 50	66, 119, 168, 200	0
6	AF	101/101 (100%)	-0.20	0 100 100	56, 96, 142, 181	0
6	CF	101/101 (100%)	-0.20	0 100 100	51, 107, 147, 196	0
7	AG	155/156 (99%)	0.12	2 (1%) 75 50	65, 117, 166, 200	0
7	CG	155/156 (99%)	0.11	2 (1%) 75 50	80, 129, 161, 182	0
8	AH	138/138 (100%)	0.00	1 (0%) 84 63	62, 106, 140, 174	0
8	CH	138/138 (100%)	0.21	4 (2%) 53 31	82, 122, 160, 195	0
9	AI	127/128 (99%)	0.26	3 (2%) 59 35	79, 136, 176, 200	0
9	CI	127/128 (99%)	0.47	7 (5%) 30 18	96, 145, 188, 200	0
10	AJ	99/105 (94%)	0.56	6 (6%) 27 16	65, 140, 184, 200	0
10	CJ	99/105 (94%)	0.64	9 (9%) 15 10	70, 153, 195, 200	0
11	AK	119/129 (92%)	0.07	3 (2%) 58 35	62, 99, 159, 198	0
11	CK	119/129 (92%)	0.15	5 (4%) 40 22	74, 111, 155, 184	0
12	AL	125/135 (92%)	0.04	0 100 100	51, 91, 144, 190	0
12	CL	125/135 (92%)	0.46	6 (4%) 35 19	59, 113, 161, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.27	9 (7%)	21	14	75, 120, 163, 200	0
13	CM	125/126 (99%)	0.44	9 (7%)	21	14	77, 137, 184, 200	0
14	AN	60/61 (98%)	0.39	4 (6%)	24	15	50, 109, 147, 200	0
14	CN	60/61 (98%)	0.85	7 (11%)	9	6	89, 135, 183, 200	0
15	AO	88/89 (98%)	0.15	0	100	100	55, 100, 144, 162	0
15	CO	88/89 (98%)	0.01	0	100	100	69, 108, 154, 182	0
16	AP	84/88 (95%)	0.20	0	100	100	78, 107, 147, 184	0
16	CP	84/88 (95%)	0.11	0	100	100	61, 100, 150, 179	0
17	AQ	100/105 (95%)	0.28	5 (5%)	34	19	82, 109, 150, 181	0
17	CQ	100/105 (95%)	0.22	3 (3%)	52	30	71, 115, 153, 167	0
18	AR	70/88 (79%)	-0.26	0	100	100	59, 96, 139, 169	0
18	CR	70/88 (79%)	0.07	1 (1%)	73	48	66, 111, 152, 173	0
19	AS	79/93 (84%)	0.25	3 (3%)	44	24	82, 122, 176, 200	0
19	CS	79/93 (84%)	0.27	3 (3%)	44	24	91, 145, 188, 200	0
20	AT	99/106 (93%)	0.31	3 (3%)	52	30	77, 120, 170, 195	0
20	CT	99/106 (93%)	0.26	2 (2%)	65	39	67, 116, 174, 200	0
21	AU	25/27 (92%)	1.14	4 (16%)	5	4	80, 119, 154, 178	0
21	CU	25/27 (92%)	1.30	5 (20%)	3	3	79, 141, 171, 185	0
22	AV	75/77 (97%)	0.13	1 (1%)	75	50	55, 121, 158, 197	0
22	AY	75/77 (97%)	0.54	4 (5%)	32	18	49, 162, 196, 200	0
22	CV	75/77 (97%)	0.19	1 (1%)	75	50	64, 144, 178, 192	0
22	CY	75/77 (97%)	0.51	4 (5%)	32	18	84, 181, 199, 200	0
23	AW	76/76 (100%)	0.36	1 (1%)	75	50	99, 173, 199, 200	0
23	CW	76/76 (100%)	0.26	6 (7%)	18	12	117, 178, 200, 200	0
24	AX	11/11 (100%)	0.41	1 (9%)	15	10	68, 116, 146, 168	0
24	CX	11/11 (100%)	0.70	2 (18%)	3	4	87, 126, 158, 159	0
25	B0	84/85 (98%)	-0.07	3 (3%)	46	25	30, 62, 111, 143	0
25	D0	84/85 (98%)	0.30	1 (1%)	76	52	58, 106, 148, 178	0
26	B1	94/98 (95%)	-0.01	1 (1%)	78	54	37, 68, 129, 162	0
26	D1	94/98 (95%)	-0.07	0	100	100	38, 79, 131, 166	0
27	B2	71/72 (98%)	0.01	1 (1%)	73	48	40, 80, 141, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.12	0 100 100	62, 97, 150, 182	0
28	B3	60/60 (100%)	-0.15	0 100 100	30, 67, 112, 190	0
28	D3	60/60 (100%)	0.24	1 (1%) 69 43	65, 124, 163, 200	0
29	B4	31/71 (43%)	0.31	0 100 100	67, 132, 172, 182	0
29	D4	31/71 (43%)	0.29	0 100 100	105, 142, 184, 197	0
30	B5	59/60 (98%)	0.16	3 (5%) 33 19	37, 60, 164, 200	0
30	D5	59/60 (98%)	0.31	3 (5%) 33 19	52, 88, 175, 191	0
31	B6	45/54 (83%)	0.63	3 (6%) 24 15	57, 113, 166, 174	0
31	D6	45/54 (83%)	0.79	6 (13%) 7 6	92, 138, 175, 200	0
32	B7	49/49 (100%)	0.01	2 (4%) 41 22	25, 53, 112, 194	0
32	D7	49/49 (100%)	0.02	2 (4%) 41 22	41, 67, 119, 181	0
33	B8	64/65 (98%)	0.29	4 (6%) 26 15	25, 69, 131, 198	0
33	D8	64/65 (98%)	0.69	7 (10%) 10 7	45, 92, 149, 183	0
34	B9	36/37 (97%)	0.58	2 (5%) 30 17	70, 99, 142, 153	0
34	D9	36/37 (97%)	1.23	4 (11%) 10 7	120, 159, 194, 200	0
35	BA	2807/2822 (99%)	-0.13	59 (2%) 63 38	35, 64, 176, 200	0
35	DA	2807/2822 (99%)	0.17	54 (1%) 66 41	44, 93, 186, 200	0
36	BB	119/122 (97%)	-0.03	6 (5%) 34 19	57, 81, 135, 179	0
36	DB	119/122 (97%)	0.32	3 (2%) 58 35	90, 129, 183, 197	0
37	BC	191/229 (83%)	0.43	4 (2%) 63 38	115, 175, 200, 200	0
37	DC	191/229 (83%)	0.32	2 (1%) 79 56	113, 172, 200, 200	0
38	BD	272/276 (98%)	-0.15	4 (1%) 72 47	33, 62, 106, 186	0
38	DD	272/276 (98%)	-0.07	5 (1%) 67 42	40, 76, 114, 158	0
39	BE	205/206 (99%)	-0.01	5 (2%) 59 35	28, 65, 151, 200	0
39	DE	205/206 (99%)	0.43	7 (3%) 48 27	53, 105, 162, 193	0
40	BF	208/210 (99%)	-0.17	0 100 100	26, 65, 154, 194	0
40	DF	208/210 (99%)	0.08	2 (0%) 79 56	41, 91, 166, 200	0
41	BG	181/182 (99%)	0.10	6 (3%) 49 28	57, 99, 158, 197	0
41	DG	181/182 (99%)	0.05	2 (1%) 78 54	78, 120, 160, 182	0
42	BH	160/180 (88%)	0.13	5 (3%) 51 29	44, 94, 160, 199	0
42	DH	160/180 (88%)	0.58	10 (6%) 26 15	107, 169, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.91	21 (14%) 6 5	48, 154, 200, 200	0
43	DI	146/148 (98%)	0.40	8 (5%) 30 18	74, 126, 175, 200	0
44	BN	139/140 (99%)	-0.01	5 (3%) 46 25	33, 68, 138, 187	0
44	DN	139/140 (99%)	0.33	2 (1%) 73 48	75, 116, 173, 200	0
45	BO	122/122 (100%)	-0.30	0 100 100	30, 69, 107, 139	0
45	DO	122/122 (100%)	0.15	1 (0%) 82 60	59, 105, 137, 156	0
46	BP	146/150 (97%)	0.42	7 (4%) 35 19	25, 84, 158, 188	0
46	DP	146/150 (97%)	0.51	13 (8%) 15 10	51, 108, 169, 200	0
47	BQ	141/141 (100%)	-0.02	4 (2%) 55 32	41, 69, 130, 200	0
47	DQ	141/141 (100%)	0.42	6 (4%) 40 21	66, 115, 166, 200	0
48	BR	117/118 (99%)	-0.17	3 (2%) 57 33	21, 62, 114, 165	0
48	DR	117/118 (99%)	0.21	6 (5%) 33 19	37, 89, 131, 173	0
49	BS	99/112 (88%)	0.34	4 (4%) 42 23	43, 83, 138, 181	0
49	DS	99/112 (88%)	0.76	6 (6%) 27 16	80, 128, 179, 200	0
50	BT	138/146 (94%)	0.20	5 (3%) 46 25	40, 86, 164, 195	0
50	DT	138/146 (94%)	0.39	5 (3%) 46 25	74, 116, 173, 200	0
51	BU	117/118 (99%)	-0.15	3 (2%) 57 33	23, 55, 106, 158	0
51	DU	117/118 (99%)	0.32	4 (3%) 48 27	56, 101, 167, 200	0
52	BV	101/101 (100%)	0.04	3 (2%) 52 30	29, 76, 135, 200	0
52	DV	101/101 (100%)	0.31	3 (2%) 52 30	55, 135, 177, 200	0
53	BW	113/113 (100%)	-0.29	0 100 100	26, 55, 122, 200	0
53	DW	113/113 (100%)	-0.17	0 100 100	50, 80, 140, 194	0
54	BX	93/96 (96%)	-0.18	0 100 100	41, 66, 106, 157	0
54	DX	93/96 (96%)	-0.18	0 100 100	42, 86, 118, 150	0
55	BY	101/110 (91%)	0.59	9 (8%) 15 10	42, 88, 178, 200	0
55	DY	101/110 (91%)	0.70	7 (6%) 23 14	49, 107, 181, 200	0
56	BZ	177/206 (85%)	0.07	2 (1%) 78 54	40, 107, 185, 200	0
56	DZ	177/206 (85%)	0.44	11 (6%) 26 16	96, 152, 198, 200	0
All	All	21244/22006 (96%)	0.15	564 (2%) 56 33	21, 102, 183, 200	0

The worst 5 of 564 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	AK	129	SER	8.6
19	CS	82	GLY	8.6
56	DZ	175	VAL	8.3
43	BI	88	ILE	8.0
43	BI	92	VAL	7.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
22	PHA	CV	77	11/11	0.89	0.35	121,125,131,132	0
22	8AN	CY	76	22/23	0.93	0.13	29,48,67,71	0
22	PHA	AV	77	11/11	0.93	0.28	121,125,131,132	0
22	PHA	CY	77	11/11	0.93	0.21	42,44,48,152	0
22	8AN	CV	76	22/23	0.95	0.10	12,58,100,116	0
22	8AN	AY	76	22/23	0.95	0.11	29,48,67,71	0
22	8AN	AV	76	22/23	0.96	0.09	12,58,100,116	0
22	PHA	AY	77	11/11	0.97	0.19	42,44,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	AA	1682	1/1	-0.14	0.20	131,131,131,131	0
57	MG	CV	104	1/1	-0.11	0.23	163,163,163,163	0
57	MG	CA	1673	1/1	-0.01	0.25	128,128,128,128	1
57	MG	BA	3314	1/1	0.01	0.36	92,92,92,92	1
57	MG	DA	3370	1/1	0.08	0.29	92,92,92,92	0
57	MG	BA	3349	1/1	0.09	0.27	94,94,94,94	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1705	1/1	0.09	0.25	150,150,150,150	0
57	MG	AA	1741	1/1	0.15	0.34	124,124,124,124	0
57	MG	AA	1737	1/1	0.16	0.48	136,136,136,136	0
57	MG	DA	3300	1/1	0.17	0.28	95,95,95,95	0
57	MG	CA	1690	1/1	0.19	0.44	110,110,110,110	0
57	MG	DA	3128	1/1	0.20	0.33	73,73,73,73	1
57	MG	CW	107	1/1	0.26	0.17	113,113,113,113	1
57	MG	CA	1752	1/1	0.30	0.17	112,112,112,112	1
57	MG	AV	104	1/1	0.32	0.20	127,127,127,127	0
57	MG	DA	3399	1/1	0.33	0.16	119,119,119,119	0
57	MG	CA	1622	1/1	0.34	0.36	117,117,117,117	0
57	MG	DB	213	1/1	0.35	0.24	93,93,93,93	0
57	MG	CA	1728	1/1	0.38	0.30	101,101,101,101	0
57	MG	BA	3177	1/1	0.39	0.32	112,112,112,112	0
57	MG	CA	1691	1/1	0.40	0.31	110,110,110,110	0
57	MG	DA	3419	1/1	0.41	0.25	115,115,115,115	0
57	MG	BA	3337	1/1	0.42	0.21	162,162,162,162	0
57	MG	DA	3321	1/1	0.42	0.30	126,126,126,126	0
57	MG	AA	1748	1/1	0.44	0.84	144,144,144,144	1
57	MG	DA	3196	1/1	0.44	0.19	96,96,96,96	0
57	MG	CA	1688	1/1	0.46	0.39	15,15,15,15	1
57	MG	CA	1655	1/1	0.46	0.20	94,94,94,94	1
57	MG	DA	3284	1/1	0.46	0.26	74,74,74,74	0
57	MG	DA	3392	1/1	0.47	0.15	107,107,107,107	0
57	MG	AA	1672	1/1	0.48	0.26	125,125,125,125	1
57	MG	AA	1783	1/1	0.48	0.25	105,105,105,105	0
57	MG	DS	201	1/1	0.48	0.13	74,74,74,74	1
57	MG	DA	3152	1/1	0.49	0.32	82,82,82,82	0
57	MG	CA	1640	1/1	0.50	0.28	121,121,121,121	0
57	MG	DA	3314	1/1	0.50	0.22	141,141,141,141	0
57	MG	BA	3186	1/1	0.50	0.18	144,144,144,144	0
57	MG	DA	3354	1/1	0.50	0.29	84,84,84,84	0
57	MG	BA	3196	1/1	0.50	0.46	130,130,130,130	1
57	MG	DA	3139	1/1	0.51	0.29	112,112,112,112	0
57	MG	DA	3296	1/1	0.51	0.18	138,138,138,138	0
57	MG	DA	3420	1/1	0.51	0.17	137,137,137,137	1
57	MG	CA	1683	1/1	0.51	0.30	110,110,110,110	0
57	MG	AA	1622	1/1	0.51	0.31	135,135,135,135	0
57	MG	AV	103	1/1	0.52	0.27	81,81,81,81	0
57	MG	AA	1661	1/1	0.52	0.23	84,84,84,84	0
57	MG	DA	3228	1/1	0.53	0.24	83,83,83,83	0
57	MG	DA	3276	1/1	0.53	0.28	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1761	1/1	0.53	0.39	122,122,122,122	0
57	MG	DB	211	1/1	0.53	0.16	119,119,119,119	0
57	MG	BA	3162	1/1	0.53	0.13	79,79,79,79	0
57	MG	CA	1649	1/1	0.53	0.31	95,95,95,95	0
57	MG	BA	3311	1/1	0.54	0.12	74,74,74,74	1
57	MG	CA	1701	1/1	0.54	0.34	93,93,93,93	0
57	MG	AA	1744	1/1	0.54	0.33	84,84,84,84	0
57	MG	AA	1727	1/1	0.55	0.25	54,54,54,54	1
57	MG	BA	3195	1/1	0.55	0.40	79,79,79,79	0
57	MG	BA	3101	1/1	0.55	0.31	72,72,72,72	1
57	MG	AW	106	1/1	0.56	0.20	102,102,102,102	1
57	MG	AA	1777	1/1	0.56	0.31	141,141,141,141	0
57	MG	CA	1602	1/1	0.56	0.32	101,101,101,101	0
57	MG	CA	1656	1/1	0.56	0.41	120,120,120,120	0
57	MG	AA	1657	1/1	0.56	0.37	121,121,121,121	0
57	MG	DA	3325	1/1	0.57	0.23	83,83,83,83	1
57	MG	AL	202	1/1	0.57	0.51	165,165,165,165	0
57	MG	AA	1704	1/1	0.57	0.17	103,103,103,103	0
57	MG	DA	3315	1/1	0.57	0.18	85,85,85,85	1
57	MG	AA	1720	1/1	0.57	0.19	137,137,137,137	0
57	MG	DA	3188	1/1	0.58	0.28	111,111,111,111	0
57	MG	CA	1727	1/1	0.58	0.34	139,139,139,139	0
57	MG	CA	1625	1/1	0.58	0.21	96,96,96,96	0
57	MG	AA	1650	1/1	0.58	0.21	99,99,99,99	0
57	MG	CA	1725	1/1	0.58	0.28	116,116,116,116	1
57	MG	AA	1656	1/1	0.59	0.40	97,97,97,97	0
57	MG	CA	1766	1/1	0.59	0.15	96,96,96,96	0
57	MG	DO	201	1/1	0.59	0.20	85,85,85,85	0
57	MG	DA	3338	1/1	0.59	0.16	74,74,74,74	0
57	MG	DA	3183	1/1	0.60	0.43	96,96,96,96	0
57	MG	DA	3413	1/1	0.60	0.17	84,84,84,84	0
57	MG	CA	1729	1/1	0.60	0.21	70,70,70,70	1
57	MG	DA	3397	1/1	0.60	0.25	101,101,101,101	0
57	MG	DB	203	1/1	0.61	0.14	33,33,33,33	1
57	MG	CA	1643	1/1	0.61	0.16	157,157,157,157	0
57	MG	DA	3210	1/1	0.61	0.28	96,96,96,96	0
57	MG	CA	1716	1/1	0.61	0.27	68,68,68,68	1
57	MG	BA	3313	1/1	0.61	0.20	162,162,162,162	0
57	MG	CW	102	1/1	0.62	0.17	112,112,112,112	0
57	MG	AA	1683	1/1	0.62	0.14	101,101,101,101	0
57	MG	DA	3197	1/1	0.62	0.37	106,106,106,106	0
57	MG	DA	3166	1/1	0.62	0.26	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3216	1/1	0.62	0.22	80,80,80,80	0
57	MG	DA	3369	1/1	0.62	0.32	112,112,112,112	0
57	MG	BA	3371	1/1	0.63	0.44	101,101,101,101	0
57	MG	DA	3349	1/1	0.63	0.20	41,41,41,41	1
57	MG	BA	3373	1/1	0.63	0.18	83,83,83,83	1
57	MG	AA	1781	1/1	0.63	0.29	63,63,63,63	0
57	MG	CA	1662	1/1	0.64	0.36	80,80,80,80	0
57	MG	BA	3224	1/1	0.64	0.15	91,91,91,91	0
57	MG	BA	3254	1/1	0.64	0.18	44,44,44,44	0
57	MG	BA	3309	1/1	0.64	0.11	112,112,112,112	1
57	MG	AA	1796	1/1	0.64	0.41	121,121,121,121	0
57	MG	AW	102	1/1	0.64	0.15	135,135,135,135	0
57	MG	DA	3213	1/1	0.64	0.27	89,89,89,89	0
57	MG	BA	3158	1/1	0.64	0.17	55,55,55,55	0
57	MG	CA	1775	1/1	0.65	0.20	79,79,79,79	0
57	MG	CA	1754	1/1	0.65	0.39	105,105,105,105	1
57	MG	CA	1606	1/1	0.65	0.24	78,78,78,78	0
57	MG	DA	3324	1/1	0.66	0.18	64,64,64,64	1
57	MG	AW	104	1/1	0.66	0.22	60,60,60,60	1
57	MG	CA	1665	1/1	0.66	0.10	68,68,68,68	0
57	MG	AV	105	1/1	0.66	0.35	89,89,89,89	0
57	MG	CA	1726	1/1	0.66	0.27	104,104,104,104	1
57	MG	DA	3367	1/1	0.66	0.32	108,108,108,108	0
57	MG	BA	3047	1/1	0.66	0.33	72,72,72,72	0
57	MG	DA	3253	1/1	0.66	0.20	86,86,86,86	1
57	MG	DA	3389	1/1	0.66	0.42	113,113,113,113	0
57	MG	DA	3266	1/1	0.66	0.16	84,84,84,84	0
57	MG	DA	3247	1/1	0.67	0.16	61,61,61,61	0
57	MG	CA	1757	1/1	0.67	0.38	128,128,128,128	0
57	MG	DA	3318	1/1	0.67	0.09	138,138,138,138	0
57	MG	CA	1623	1/1	0.67	0.21	71,71,71,71	0
57	MG	CA	1771	1/1	0.67	0.34	98,98,98,98	0
57	MG	AW	107	1/1	0.67	0.13	101,101,101,101	0
57	MG	AA	1689	1/1	0.67	0.28	118,118,118,118	0
57	MG	BA	3421	1/1	0.67	0.14	110,110,110,110	1
57	MG	AA	1743	1/1	0.68	0.13	86,86,86,86	0
57	MG	CA	1698	1/1	0.68	0.25	86,86,86,86	0
57	MG	CW	106	1/1	0.68	0.16	86,86,86,86	1
57	MG	DA	3289	1/1	0.68	0.24	74,74,74,74	0
57	MG	CA	1721	1/1	0.68	0.08	97,97,97,97	0
57	MG	DA	3111	1/1	0.68	0.47	111,111,111,111	0
57	MG	AA	1798	1/1	0.68	0.32	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1733	1/1	0.68	0.14	81,81,81,81	1
57	MG	CA	1750	1/1	0.68	0.39	77,77,77,77	1
57	MG	CA	1793	1/1	0.68	0.38	100,100,100,100	1
57	MG	DA	3270	1/1	0.69	0.32	87,87,87,87	0
57	MG	CA	1684	1/1	0.69	0.16	94,94,94,94	0
57	MG	DA	3195	1/1	0.69	0.12	89,89,89,89	0
57	MG	CA	1762	1/1	0.69	0.24	84,84,84,84	0
57	MG	BA	3354	1/1	0.69	0.26	129,129,129,129	0
57	MG	AA	1731	1/1	0.69	0.21	73,73,73,73	1
57	MG	CA	1610	1/1	0.70	0.17	88,88,88,88	0
57	MG	CA	1611	1/1	0.70	0.24	110,110,110,110	0
57	MG	BA	3150	1/1	0.70	0.27	64,64,64,64	0
57	MG	BA	3352	1/1	0.70	0.37	23,23,23,23	1
57	MG	DA	3340	1/1	0.70	0.25	98,98,98,98	1
57	MG	DA	3048	1/1	0.70	0.17	61,61,61,61	0
57	MG	DA	3421	1/1	0.70	0.15	168,168,168,168	0
57	MG	BB	206	1/1	0.70	0.18	105,105,105,105	0
57	MG	AA	1770	1/1	0.70	0.22	163,163,163,163	0
57	MG	AA	1734	1/1	0.70	0.28	102,102,102,102	0
57	MG	CA	1709	1/1	0.70	0.12	73,73,73,73	0
57	MG	CA	1746	1/1	0.70	0.16	91,91,91,91	0
57	MG	DX	102	1/1	0.70	0.14	126,126,126,126	0
57	MG	DA	3157	1/1	0.71	0.44	79,79,79,79	0
57	MG	AA	1701	1/1	0.71	0.27	92,92,92,92	0
57	MG	CA	1668	1/1	0.71	0.22	99,99,99,99	0
57	MG	DA	3402	1/1	0.71	0.20	125,125,125,125	0
57	MG	DA	3412	1/1	0.71	0.24	74,74,74,74	0
57	MG	CA	1739	1/1	0.71	0.21	128,128,128,128	0
57	MG	BA	3312	1/1	0.71	0.12	102,102,102,102	0
57	MG	DA	3279	1/1	0.71	0.31	49,49,49,49	1
57	MG	DA	3108	1/1	0.71	0.30	83,83,83,83	0
57	MG	BA	3250	1/1	0.71	0.23	76,76,76,76	0
57	MG	DB	207	1/1	0.71	0.13	49,49,49,49	1
57	MG	CA	1783	1/1	0.71	0.27	105,105,105,105	0
57	MG	AW	108	1/1	0.71	0.13	82,82,82,82	1
57	MG	DA	3217	1/1	0.71	0.18	62,62,62,62	0
57	MG	DA	3376	1/1	0.71	0.23	110,110,110,110	0
57	MG	BA	3160	1/1	0.71	0.25	74,74,74,74	0
57	MG	D2	602	1/1	0.72	0.17	99,99,99,99	0
57	MG	AG	201	1/1	0.72	0.20	80,80,80,80	0
57	MG	DA	3198	1/1	0.72	0.24	58,58,58,58	1
57	MG	BA	3342	1/1	0.72	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	BA	3310	1/1	0.72	0.15	102,102,102,102	1
57	MG	BA	3420	1/1	0.72	0.18	78,78,78,78	0
57	MG	DA	3192	1/1	0.72	0.40	74,74,74,74	0
57	MG	DA	3229	1/1	0.72	0.21	92,92,92,92	0
57	MG	DA	3342	1/1	0.72	0.38	90,90,90,90	0
57	MG	AA	1641	1/1	0.72	0.22	83,83,83,83	0
57	MG	DA	3353	1/1	0.72	0.23	107,107,107,107	0
57	MG	AA	1723	1/1	0.73	0.38	79,79,79,79	1
57	MG	DA	3287	1/1	0.73	0.11	148,148,148,148	0
57	MG	AA	1666	1/1	0.73	0.16	93,93,93,93	0
57	MG	DA	3293	1/1	0.73	0.25	74,74,74,74	0
57	MG	CA	1648	1/1	0.73	0.20	83,83,83,83	0
57	MG	BA	3249	1/1	0.73	0.23	114,114,114,114	0
57	MG	BA	3339	1/1	0.73	0.34	125,125,125,125	1
57	MG	CA	1720	1/1	0.73	0.27	89,89,89,89	0
57	MG	CA	1694	1/1	0.73	0.23	116,116,116,116	0
57	MG	DA	3319	1/1	0.73	0.38	102,102,102,102	1
57	MG	CV	103	1/1	0.74	0.28	74,74,74,74	0
57	MG	AA	1739	1/1	0.74	0.27	115,115,115,115	0
57	MG	CA	1630	1/1	0.74	0.14	84,84,84,84	0
57	MG	CA	1745	1/1	0.74	0.24	115,115,115,115	0
57	MG	CA	1767	1/1	0.74	0.10	97,97,97,97	0
57	MG	DA	3285	1/1	0.74	0.13	71,71,71,71	0
57	MG	DA	3178	1/1	0.74	0.41	88,88,88,88	0
57	MG	DA	3222	1/1	0.74	0.29	95,95,95,95	0
57	MG	AA	1763	1/1	0.74	0.12	62,62,62,62	0
57	MG	DB	202	1/1	0.74	0.17	113,113,113,113	0
57	MG	CA	1612	1/1	0.74	0.17	91,91,91,91	0
57	MG	AA	1708	1/1	0.74	0.31	72,72,72,72	0
57	MG	DA	3311	1/1	0.74	0.08	65,65,65,65	1
57	MG	DA	3250	1/1	0.74	0.26	63,63,63,63	1
57	MG	DA	3251	1/1	0.74	0.12	96,96,96,96	0
57	MG	DA	3386	1/1	0.74	0.46	115,115,115,115	0
57	MG	AA	1742	1/1	0.74	0.21	100,100,100,100	0
57	MG	AA	1757	1/1	0.75	0.32	87,87,87,87	1
57	MG	AA	1740	1/1	0.75	0.21	87,87,87,87	0
57	MG	BA	3221	1/1	0.75	0.34	80,80,80,80	1
57	MG	DB	209	1/1	0.75	0.36	7,7,7,7	1
57	MG	CA	1680	1/1	0.75	0.34	94,94,94,94	0
57	MG	AA	1648	1/1	0.75	0.21	87,87,87,87	0
57	MG	CA	1777	1/1	0.75	0.30	135,135,135,135	0
57	MG	AA	1655	1/1	0.75	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1759	1/1	0.75	0.21	67,67,67,67	1
57	MG	BA	3405	1/1	0.76	0.27	164,164,164,164	1
57	MG	CA	1687	1/1	0.76	0.14	84,84,84,84	0
57	MG	DA	3172	1/1	0.76	0.13	58,58,58,58	0
57	MG	DA	3317	1/1	0.76	0.14	55,55,55,55	1
57	MG	AA	1706	1/1	0.76	0.17	108,108,108,108	0
57	MG	BA	3251	1/1	0.76	0.28	136,136,136,136	1
57	MG	CA	1661	1/1	0.76	0.21	56,56,56,56	0
57	MG	CA	1761	1/1	0.76	0.13	74,74,74,74	0
57	MG	BB	202	1/1	0.76	0.22	92,92,92,92	0
57	MG	DA	3272	1/1	0.76	0.20	108,108,108,108	0
57	MG	BB	204	1/1	0.76	0.14	106,106,106,106	0
57	MG	BA	3100	1/1	0.76	0.15	49,49,49,49	0
57	MG	CA	1735	1/1	0.76	0.26	90,90,90,90	0
57	MG	DA	3127	1/1	0.76	0.44	67,67,67,67	0
57	MG	BA	3296	1/1	0.76	0.23	66,66,66,66	0
57	MG	BA	3241	1/1	0.76	0.34	70,70,70,70	0
57	MG	AA	1686	1/1	0.76	0.30	104,104,104,104	0
57	MG	DA	3226	1/1	0.76	0.10	88,88,88,88	0
57	MG	DA	3372	1/1	0.76	0.23	120,120,120,120	1
57	MG	DA	3227	1/1	0.76	0.62	136,136,136,136	0
57	MG	DA	3263	1/1	0.77	0.37	69,69,69,69	0
57	MG	DA	3264	1/1	0.77	0.11	96,96,96,96	0
57	MG	BA	3279	1/1	0.77	0.11	53,53,53,53	0
57	MG	AA	1746	1/1	0.77	0.38	95,95,95,95	0
57	MG	DA	3202	1/1	0.77	0.36	73,73,73,73	0
57	MG	DA	3404	1/1	0.77	0.10	97,97,97,97	1
57	MG	DA	3136	1/1	0.77	0.35	63,63,63,63	0
57	MG	BA	3387	1/1	0.77	0.57	119,119,119,119	0
57	MG	AW	105	1/1	0.77	0.14	154,154,154,154	1
57	MG	BA	3416	1/1	0.77	0.34	93,93,93,93	0
57	MG	CA	1617	1/1	0.77	0.11	81,81,81,81	0
57	MG	AA	1794	1/1	0.77	0.14	126,126,126,126	0
57	MG	CA	1696	1/1	0.77	0.39	108,108,108,108	0
57	MG	AA	1671	1/1	0.77	0.23	73,73,73,73	0
57	MG	DA	3042	1/1	0.77	0.20	89,89,89,89	0
57	MG	AA	1677	1/1	0.77	0.21	89,89,89,89	0
57	MG	DA	3312	1/1	0.77	0.13	56,56,56,56	1
57	MG	DA	3373	1/1	0.77	0.12	98,98,98,98	0
57	MG	AA	1717	1/1	0.77	0.29	61,61,61,61	0
57	MG	BA	3367	1/1	0.77	0.12	1,1,1,1	1
57	MG	AA	1635	1/1	0.78	0.15	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1685	1/1	0.78	0.09	62,62,62,62	0
57	MG	BA	3297	1/1	0.78	0.23	77,77,77,77	0
57	MG	DA	3252	1/1	0.78	0.12	95,95,95,95	0
57	MG	AA	1621	1/1	0.78	0.16	50,50,50,50	0
57	MG	DA	3256	1/1	0.78	0.16	79,79,79,79	0
57	MG	BA	3248	1/1	0.78	0.21	50,50,50,50	1
57	MG	DA	3002	1/1	0.78	0.18	69,69,69,69	0
57	MG	CA	1666	1/1	0.78	0.23	87,87,87,87	0
57	MG	BA	3263	1/1	0.78	0.23	77,77,77,77	0
57	MG	DA	3087	1/1	0.78	0.24	84,84,84,84	0
57	MG	BA	3274	1/1	0.78	0.36	85,85,85,85	0
57	MG	AA	1603	1/1	0.78	0.13	84,84,84,84	0
57	MG	DA	3281	1/1	0.78	0.10	52,52,52,52	0
57	MG	BA	3285	1/1	0.78	0.33	89,89,89,89	0
57	MG	DA	3246	1/1	0.78	0.17	97,97,97,97	0
57	MG	CA	1770	1/1	0.79	0.22	94,94,94,94	0
57	MG	CA	1647	1/1	0.79	0.19	68,68,68,68	0
57	MG	AA	1613	1/1	0.79	0.15	81,81,81,81	0
57	MG	CA	1722	1/1	0.79	0.27	121,121,121,121	0
57	MG	AA	1705	1/1	0.79	0.28	63,63,63,63	0
57	MG	CA	1674	1/1	0.79	0.24	63,63,63,63	1
57	MG	DA	3243	1/1	0.79	0.35	76,76,76,76	0
57	MG	DA	3122	1/1	0.79	0.33	77,77,77,77	0
57	MG	BA	3264	1/1	0.79	0.14	58,58,58,58	0
57	MG	CA	1682	1/1	0.79	0.23	90,90,90,90	0
57	MG	CA	1609	1/1	0.79	0.27	61,61,61,61	0
57	MG	BA	3273	1/1	0.79	0.13	75,75,75,75	0
57	MG	BA	3383	1/1	0.79	0.08	101,101,101,101	0
57	MG	AA	1786	1/1	0.79	0.27	108,108,108,108	0
57	MG	DA	3345	1/1	0.79	0.28	43,43,43,43	1
57	MG	BA	3393	1/1	0.80	0.23	74,74,74,74	0
57	MG	BA	3138	1/1	0.80	0.41	124,124,124,124	0
57	MG	DA	3301	1/1	0.80	0.38	84,84,84,84	0
57	MG	AA	1690	1/1	0.80	0.11	81,81,81,81	0
57	MG	DA	3383	1/1	0.80	0.14	67,67,67,67	0
57	MG	CA	1734	1/1	0.80	0.35	67,67,67,67	0
57	MG	DA	3182	1/1	0.80	0.35	60,60,60,60	0
57	MG	BA	3200	1/1	0.80	0.19	52,52,52,52	0
57	MG	DA	3011	1/1	0.80	0.18	52,52,52,52	0
57	MG	AA	1715	1/1	0.80	0.30	39,39,39,39	1
57	MG	AA	1607	1/1	0.80	0.25	64,64,64,64	0
57	MG	AA	1684	1/1	0.80	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1681	1/1	0.80	0.21	86,86,86,86	0
57	MG	CA	1779	1/1	0.80	0.12	115,115,115,115	0
57	MG	DA	3329	1/1	0.80	0.26	140,140,140,140	0
57	MG	DA	3121	1/1	0.80	0.22	83,83,83,83	0
57	MG	CA	1780	1/1	0.80	0.17	32,32,32,32	1
57	MG	BA	3179	1/1	0.80	0.82	117,117,117,117	0
57	MG	DA	3344	1/1	0.80	0.18	64,64,64,64	0
57	MG	CA	1788	1/1	0.80	0.10	75,75,75,75	0
57	MG	BA	3318	1/1	0.80	0.18	70,70,70,70	1
57	MG	DA	3351	1/1	0.80	0.11	94,94,94,94	0
57	MG	CA	1756	1/1	0.80	0.18	53,53,53,53	0
57	MG	DA	3151	1/1	0.80	0.18	57,57,57,57	1
57	MG	AA	1640	1/1	0.80	0.32	76,76,76,76	0
57	MG	DA	3154	1/1	0.80	0.13	60,60,60,60	0
57	MG	BA	3415	1/1	0.81	0.24	77,77,77,77	0
57	MG	CA	1736	1/1	0.81	0.20	73,73,73,73	0
57	MG	DA	3379	1/1	0.81	0.34	105,105,105,105	0
57	MG	CA	1657	1/1	0.81	0.20	86,86,86,86	0
57	MG	DA	3384	1/1	0.81	0.16	115,115,115,115	0
57	MG	DA	3072	1/1	0.81	0.20	94,94,94,94	0
57	MG	BA	3270	1/1	0.81	0.13	76,76,76,76	0
57	MG	AA	1629	1/1	0.81	0.15	62,62,62,62	0
57	MG	DA	3219	1/1	0.81	0.19	99,99,99,99	0
57	MG	BA	3155	1/1	0.81	0.50	116,116,116,116	0
57	MG	DA	3400	1/1	0.81	0.27	77,77,77,77	0
57	MG	DA	3119	1/1	0.81	0.21	86,86,86,86	0
57	MG	CA	1795	1/1	0.81	0.20	78,78,78,78	0
57	MG	DA	3408	1/1	0.81	0.20	44,44,44,44	0
57	MG	AA	1795	1/1	0.82	0.44	128,128,128,128	0
57	MG	DA	3327	1/1	0.82	0.37	64,64,64,64	1
57	MG	BA	3353	1/1	0.82	0.28	79,79,79,79	0
57	MG	DA	3051	1/1	0.82	0.22	75,75,75,75	0
57	MG	DA	3282	1/1	0.82	0.13	50,50,50,50	0
57	MG	DA	3068	1/1	0.82	0.13	98,98,98,98	0
57	MG	CA	1678	1/1	0.82	0.41	94,94,94,94	0
57	MG	AA	1762	1/1	0.82	0.11	80,80,80,80	1
57	MG	DA	3106	1/1	0.82	0.31	78,78,78,78	0
57	MG	AA	1602	1/1	0.82	0.26	97,97,97,97	0
57	MG	DA	3248	1/1	0.82	0.18	90,90,90,90	0
57	MG	BA	3057	1/1	0.82	0.34	85,85,85,85	0
57	MG	BA	3327	1/1	0.82	0.31	67,67,67,67	0
57	MG	CA	1737	1/1	0.82	0.25	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1760	1/1	0.82	0.30	90,90,90,90	0
57	MG	CA	1629	1/1	0.82	0.15	59,59,59,59	0
57	MG	DB	208	1/1	0.82	0.42	76,76,76,76	1
57	MG	AA	1788	1/1	0.82	0.24	73,73,73,73	0
57	MG	D7	101	1/1	0.82	0.27	73,73,73,73	0
57	MG	BA	3108	1/1	0.82	0.11	4,4,4,4	0
57	MG	AA	1652	1/1	0.82	0.22	82,82,82,82	0
57	MG	DA	3034	1/1	0.82	0.21	52,52,52,52	0
57	MG	DA	3275	1/1	0.82	0.07	98,98,98,98	0
57	MG	DA	3162	1/1	0.83	0.23	77,77,77,77	0
57	MG	CA	1635	1/1	0.83	0.24	74,74,74,74	0
57	MG	AA	1733	1/1	0.83	0.29	141,141,141,141	0
57	MG	CA	1642	1/1	0.83	0.21	74,74,74,74	0
57	MG	CA	1676	1/1	0.83	0.18	71,71,71,71	0
57	MG	BA	3212	1/1	0.83	0.24	88,88,88,88	0
57	MG	CA	1744	1/1	0.83	0.14	63,63,63,63	0
57	MG	AA	1601	1/1	0.83	0.12	90,90,90,90	0
57	MG	BA	3345	1/1	0.83	0.18	69,69,69,69	1
57	MG	AA	1664	1/1	0.83	0.12	47,47,47,47	0
57	MG	AA	1724	1/1	0.83	0.12	68,68,68,68	1
57	MG	CA	1724	1/1	0.83	0.15	80,80,80,80	0
57	MG	BA	3417	1/1	0.83	0.15	72,72,72,72	0
57	MG	DA	3209	1/1	0.83	0.18	73,73,73,73	0
57	MG	CV	105	1/1	0.83	0.15	65,65,65,65	0
57	MG	AA	1769	1/1	0.83	0.15	80,80,80,80	0
57	MG	BA	3242	1/1	0.83	0.18	60,60,60,60	0
57	MG	BA	3247	1/1	0.83	0.20	49,49,49,49	0
57	MG	DA	3352	1/1	0.83	0.24	20,20,20,20	1
57	MG	AA	1651	1/1	0.83	0.15	70,70,70,70	0
57	MG	DA	3223	1/1	0.83	0.27	46,46,46,46	1
57	MG	CA	1731	1/1	0.83	0.22	85,85,85,85	0
57	MG	AA	1632	1/1	0.83	0.31	34,34,34,34	1
57	MG	CA	1768	1/1	0.83	0.27	72,72,72,72	0
57	MG	DC	301	1/1	0.83	0.07	91,91,91,91	1
57	MG	DA	3156	1/1	0.83	0.23	38,38,38,38	0
57	MG	DA	3012	1/1	0.83	0.13	45,45,45,45	0
57	MG	DA	3158	1/1	0.83	0.22	48,48,48,48	0
57	MG	BA	3351	1/1	0.84	0.19	135,135,135,135	0
57	MG	CA	1700	1/1	0.84	0.12	101,101,101,101	0
57	MG	DA	3224	1/1	0.84	0.14	85,85,85,85	0
57	MG	DA	3225	1/1	0.84	0.33	71,71,71,71	0
57	MG	DA	3395	1/1	0.84	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3398	1/1	0.84	0.15	84,84,84,84	0
57	MG	BA	3143	1/1	0.84	0.16	49,49,49,49	1
57	MG	DA	3280	1/1	0.84	0.17	109,109,109,109	0
57	MG	BA	3235	1/1	0.84	0.34	156,156,156,156	0
57	MG	DA	3341	1/1	0.84	0.17	54,54,54,54	0
57	MG	CA	1711	1/1	0.84	0.11	74,74,74,74	0
57	MG	DA	3410	1/1	0.84	0.17	87,87,87,87	1
57	MG	DA	3145	1/1	0.84	0.34	90,90,90,90	0
57	MG	DA	3244	1/1	0.84	0.20	62,62,62,62	0
57	MG	DA	3245	1/1	0.84	0.16	69,69,69,69	0
57	MG	BA	3336	1/1	0.84	0.11	105,105,105,105	1
57	MG	DA	3292	1/1	0.84	0.23	51,51,51,51	1
57	MG	CA	1719	1/1	0.84	0.20	93,93,93,93	0
57	MG	AA	1702	1/1	0.84	0.29	126,126,126,126	0
57	MG	DB	206	1/1	0.84	0.11	75,75,75,75	0
57	MG	DA	3358	1/1	0.84	0.32	94,94,94,94	0
57	MG	DA	3249	1/1	0.84	0.22	60,60,60,60	0
57	MG	AA	1667	1/1	0.84	0.21	72,72,72,72	0
57	MG	CA	1613	1/1	0.84	0.34	51,51,51,51	0
57	MG	AA	1634	1/1	0.84	0.28	73,73,73,73	0
57	MG	BA	3288	1/1	0.84	0.44	59,59,59,59	0
57	MG	DA	3215	1/1	0.84	0.11	68,68,68,68	1
57	MG	AA	1638	1/1	0.84	0.21	36,36,36,36	0
57	MG	DA	3169	1/1	0.84	0.34	43,43,43,43	1
57	MG	DX	103	1/1	0.84	0.18	102,102,102,102	0
57	MG	AA	1754	1/1	0.85	0.08	64,64,64,64	0
57	MG	DA	3387	1/1	0.85	0.23	66,66,66,66	0
57	MG	BA	3374	1/1	0.85	0.09	92,92,92,92	0
57	MG	BA	3180	1/1	0.85	0.23	50,50,50,50	0
57	MG	DA	3393	1/1	0.85	0.11	109,109,109,109	1
57	MG	BB	213	1/1	0.85	0.15	87,87,87,87	0
57	MG	DA	3260	1/1	0.85	0.29	81,81,81,81	0
57	MG	CA	1644	1/1	0.85	0.13	102,102,102,102	0
57	MG	AA	1726	1/1	0.85	0.31	71,71,71,71	0
57	MG	DA	3212	1/1	0.85	0.14	91,91,91,91	0
57	MG	AA	1774	1/1	0.85	0.20	88,88,88,88	0
57	MG	DA	3214	1/1	0.85	0.22	129,129,129,129	0
57	MG	AA	1710	1/1	0.85	0.19	71,71,71,71	0
57	MG	BA	3402	1/1	0.85	0.16	63,63,63,63	0
57	MG	BA	3404	1/1	0.85	0.18	56,56,56,56	0
57	MG	AA	1728	1/1	0.85	0.25	67,67,67,67	0
57	MG	CA	1660	1/1	0.85	0.36	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3407	1/1	0.85	0.20	52,52,52,52	0
57	MG	BA	3276	1/1	0.85	0.23	49,49,49,49	0
57	MG	AA	1610	1/1	0.85	0.27	49,49,49,49	0
57	MG	DA	3164	1/1	0.85	0.07	84,84,84,84	0
57	MG	BA	3283	1/1	0.85	0.11	33,33,33,33	0
57	MG	AA	1625	1/1	0.85	0.11	65,65,65,65	0
57	MG	CA	1782	1/1	0.85	0.13	77,77,77,77	0
57	MG	DB	210	1/1	0.85	0.31	74,74,74,74	0
57	MG	CA	1669	1/1	0.85	0.27	81,81,81,81	0
57	MG	DA	3179	1/1	0.85	0.27	80,80,80,80	0
57	MG	DA	3088	1/1	0.85	0.20	37,37,37,37	0
57	MG	DN	201	1/1	0.85	0.33	129,129,129,129	0
57	MG	DA	3102	1/1	0.85	0.15	129,129,129,129	1
57	MG	CA	1785	1/1	0.85	0.13	95,95,95,95	0
57	MG	BA	3125	1/1	0.85	0.24	62,62,62,62	0
57	MG	BA	3422	1/1	0.85	0.17	120,120,120,120	0
57	MG	BA	3144	1/1	0.86	0.16	58,58,58,58	0
57	MG	DA	3262	1/1	0.86	0.24	73,73,73,73	0
57	MG	AA	1787	1/1	0.86	0.17	41,41,41,41	1
57	MG	DA	3153	1/1	0.86	0.16	60,60,60,60	1
57	MG	DA	3398	1/1	0.86	0.15	86,86,86,86	0
57	MG	CA	1774	1/1	0.86	0.26	121,121,121,121	0
57	MG	BA	3091	1/1	0.86	0.24	41,41,41,41	0
57	MG	BA	3220	1/1	0.86	0.43	95,95,95,95	0
57	MG	AA	1722	1/1	0.86	0.16	75,75,75,75	0
57	MG	DA	3161	1/1	0.86	0.14	65,65,65,65	0
57	MG	DA	3278	1/1	0.86	0.13	54,54,54,54	0
57	MG	BB	201	1/1	0.86	0.21	87,87,87,87	0
57	MG	AA	1619	1/1	0.86	0.27	65,65,65,65	0
57	MG	BA	3317	1/1	0.86	0.11	167,167,167,167	0
57	MG	AA	1716	1/1	0.86	0.08	86,86,86,86	0
57	MG	BA	3117	1/1	0.86	0.39	59,59,59,59	0
57	MG	DA	3177	1/1	0.86	0.22	77,77,77,77	0
57	MG	DA	3286	1/1	0.86	0.32	75,75,75,75	0
57	MG	CA	1792	1/1	0.86	0.16	95,95,95,95	0
57	MG	AA	1759	1/1	0.86	0.24	96,96,96,96	0
57	MG	BA	3394	1/1	0.86	0.09	81,81,81,81	1
57	MG	CL	201	1/1	0.86	0.16	91,91,91,91	0
57	MG	BA	3244	1/1	0.86	0.12	88,88,88,88	0
57	MG	BA	3127	1/1	0.86	0.24	44,44,44,44	1
57	MG	BA	3131	1/1	0.86	0.14	31,31,31,31	0
57	MG	BA	3289	1/1	0.86	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1763	1/1	0.86	0.11	98,98,98,98	0
57	MG	BA	3014	1/1	0.86	0.17	61,61,61,61	0
57	MG	DA	3199	1/1	0.86	0.46	101,101,101,101	0
57	MG	CA	1614	1/1	0.86	0.41	89,89,89,89	0
57	MG	AA	1735	1/1	0.86	0.23	108,108,108,108	0
57	MG	AA	1771	1/1	0.87	0.31	40,40,40,40	0
57	MG	BA	3032	1/1	0.87	0.13	45,45,45,45	0
57	MG	CA	1641	1/1	0.87	0.21	64,64,64,64	0
57	MG	BA	3041	1/1	0.87	0.23	96,96,96,96	0
57	MG	AA	1699	1/1	0.87	0.07	78,78,78,78	0
57	MG	AA	1775	1/1	0.87	0.13	92,92,92,92	0
57	MG	DA	3355	1/1	0.87	0.33	95,95,95,95	0
57	MG	DA	3259	1/1	0.87	0.22	56,56,56,56	0
57	MG	CX	103	1/1	0.87	0.14	108,108,108,108	0
57	MG	AA	1776	1/1	0.87	0.36	103,103,103,103	0
57	MG	DA	3173	1/1	0.87	0.08	50,50,50,50	0
57	MG	DA	3176	1/1	0.87	0.27	69,69,69,69	0
57	MG	BA	3163	1/1	0.87	0.08	42,42,42,42	0
57	MG	BA	3245	1/1	0.87	0.18	42,42,42,42	0
57	MG	BA	3368	1/1	0.87	0.12	61,61,61,61	0
57	MG	BB	212	1/1	0.87	0.07	31,31,31,31	1
57	MG	CA	1708	1/1	0.87	0.08	89,89,89,89	0
57	MG	BA	3246	1/1	0.87	0.18	74,74,74,74	0
57	MG	BU	201	1/1	0.87	0.37	166,166,166,166	1
57	MG	DA	3388	1/1	0.87	0.12	68,68,68,68	0
57	MG	CA	1765	1/1	0.87	0.13	60,60,60,60	0
57	MG	DA	3056	1/1	0.87	0.22	49,49,49,49	0
57	MG	CA	1713	1/1	0.87	0.11	73,73,73,73	0
57	MG	DA	3069	1/1	0.87	0.16	75,75,75,75	0
57	MG	AA	1700	1/1	0.87	0.31	79,79,79,79	0
57	MG	DA	3084	1/1	0.87	0.21	44,44,44,44	0
57	MG	DA	3207	1/1	0.87	0.12	67,67,67,67	0
57	MG	CA	1717	1/1	0.87	0.09	82,82,82,82	0
57	MG	AA	1673	1/1	0.87	0.48	76,76,76,76	1
57	MG	DA	3090	1/1	0.87	0.43	77,77,77,77	0
57	MG	DA	3407	1/1	0.87	0.10	45,45,45,45	0
57	MG	CA	1664	1/1	0.87	0.24	53,53,53,53	0
57	MG	CA	1773	1/1	0.87	0.25	55,55,55,55	0
57	MG	BA	3375	1/1	0.87	0.19	21,21,21,21	1
57	MG	DA	3109	1/1	0.87	0.18	29,29,29,29	0
57	MG	AA	1653	1/1	0.87	0.38	82,82,82,82	0
57	MG	AA	1605	1/1	0.87	0.14	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1778	1/1	0.87	0.13	66,66,66,66	0
57	MG	BA	3390	1/1	0.87	0.13	37,37,37,37	0
57	MG	BA	3187	1/1	0.87	0.35	108,108,108,108	0
57	MG	AA	1695	1/1	0.87	0.12	52,52,52,52	0
57	MG	CA	1675	1/1	0.87	0.11	92,92,92,92	0
57	MG	BA	3257	1/1	0.87	0.38	61,61,61,61	0
57	MG	BA	3262	1/1	0.87	0.06	100,100,100,100	0
57	MG	DA	3230	1/1	0.87	0.41	71,71,71,71	0
57	MG	DA	3328	1/1	0.87	0.12	50,50,50,50	0
57	MG	DA	3148	1/1	0.87	0.10	46,46,46,46	0
57	MG	AA	1766	1/1	0.87	0.06	67,67,67,67	0
57	MG	DA	3339	1/1	0.87	0.23	57,57,57,57	1
57	MG	AA	1792	1/1	0.87	0.32	58,58,58,58	0
57	MG	AA	1749	1/1	0.87	0.21	100,100,100,100	1
57	MG	CA	1798	1/1	0.87	0.17	55,55,55,55	0
57	MG	AA	1718	1/1	0.87	0.22	72,72,72,72	0
57	MG	CA	1671	1/1	0.88	0.21	58,58,58,58	0
57	MG	CA	1632	1/1	0.88	0.48	54,54,54,54	1
57	MG	DA	3240	1/1	0.88	0.16	56,56,56,56	0
57	MG	BA	3340	1/1	0.88	0.27	90,90,90,90	1
57	MG	BA	3341	1/1	0.88	0.13	40,40,40,40	0
57	MG	DA	3101	1/1	0.88	0.17	67,67,67,67	0
57	MG	CA	1799	1/1	0.88	0.12	75,75,75,75	0
57	MG	DA	3313	1/1	0.88	0.15	80,80,80,80	0
57	MG	BA	3290	1/1	0.88	0.25	78,78,78,78	1
57	MG	AA	1797	1/1	0.88	0.27	53,53,53,53	0
57	MG	BA	3067	1/1	0.88	0.28	53,53,53,53	0
57	MG	BA	3230	1/1	0.88	0.25	97,97,97,97	0
57	MG	BA	3182	1/1	0.88	0.20	62,62,62,62	0
57	MG	AA	1703	1/1	0.88	0.11	38,38,38,38	0
57	MG	AD	301	1/1	0.88	0.11	155,155,155,155	0
57	MG	DA	3255	1/1	0.88	0.07	61,61,61,61	0
57	MG	AA	1643	1/1	0.88	0.21	84,84,84,84	0
57	MG	AA	1646	1/1	0.88	0.34	82,82,82,82	0
57	MG	DA	3130	1/1	0.88	0.22	41,41,41,41	0
57	MG	DA	3335	1/1	0.88	0.14	80,80,80,80	0
57	MG	BA	3419	1/1	0.88	0.47	90,90,90,90	1
57	MG	DA	3138	1/1	0.88	0.09	68,68,68,68	0
57	MG	DA	3416	1/1	0.88	0.25	81,81,81,81	0
57	MG	DA	3418	1/1	0.88	0.09	47,47,47,47	1
57	MG	CA	1658	1/1	0.88	0.06	78,78,78,78	0
57	MG	CA	1693	1/1	0.88	0.05	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3146	1/1	0.88	0.13	55,55,55,55	0
57	MG	AA	1678	1/1	0.88	0.07	166,166,166,166	0
57	MG	DA	3020	1/1	0.88	0.20	59,59,59,59	0
57	MG	CA	1619	1/1	0.88	0.25	80,80,80,80	0
57	MG	DA	3350	1/1	0.88	0.08	89,89,89,89	1
57	MG	CA	1697	1/1	0.88	0.06	72,72,72,72	0
57	MG	DA	3218	1/1	0.88	0.14	94,94,94,94	0
57	MG	BA	3208	1/1	0.88	0.28	61,61,61,61	0
57	MG	DA	3050	1/1	0.88	0.26	69,69,69,69	1
57	MG	AA	1612	1/1	0.88	0.18	67,67,67,67	0
57	MG	BA	3215	1/1	0.88	0.16	33,33,33,33	0
57	MG	DA	3066	1/1	0.88	0.21	43,43,43,43	0
57	MG	CA	1627	1/1	0.88	0.18	78,78,78,78	0
57	MG	AA	1623	1/1	0.88	0.20	70,70,70,70	0
57	MG	DA	3288	1/1	0.88	0.18	37,37,37,37	0
57	MG	AA	1712	1/1	0.88	0.15	61,61,61,61	0
57	MG	DA	3343	1/1	0.89	0.32	71,71,71,71	0
57	MG	DA	3006	1/1	0.89	0.24	23,23,23,23	0
57	MG	BA	3347	1/1	0.89	0.17	42,42,42,42	0
57	MG	DA	3346	1/1	0.89	0.17	54,54,54,54	0
57	MG	DA	3159	1/1	0.89	0.15	70,70,70,70	0
57	MG	BA	3284	1/1	0.89	0.29	53,53,53,53	0
57	MG	DA	3254	1/1	0.89	0.12	99,99,99,99	0
57	MG	DA	3016	1/1	0.89	0.18	51,51,51,51	0
57	MG	AA	1768	1/1	0.89	0.23	71,71,71,71	0
57	MG	DA	3028	1/1	0.89	0.20	47,47,47,47	0
57	MG	DA	3033	1/1	0.89	0.19	70,70,70,70	0
57	MG	CA	1645	1/1	0.89	0.37	66,66,66,66	0
57	MG	DA	3039	1/1	0.89	0.08	70,70,70,70	0
57	MG	DA	3041	1/1	0.89	0.15	46,46,46,46	0
57	MG	BA	3037	1/1	0.89	0.13	23,23,23,23	0
57	MG	DA	3267	1/1	0.89	0.17	71,71,71,71	0
57	MG	DA	3045	1/1	0.89	0.18	35,35,35,35	0
57	MG	AA	1707	1/1	0.89	0.13	116,116,116,116	0
57	MG	AA	1745	1/1	0.89	0.23	62,62,62,62	0
57	MG	BA	3355	1/1	0.89	0.08	92,92,92,92	0
57	MG	DA	3277	1/1	0.89	0.24	63,63,63,63	0
57	MG	BB	207	1/1	0.89	0.11	29,29,29,29	1
57	MG	BA	3199	1/1	0.89	0.48	116,116,116,116	0
57	MG	DA	3067	1/1	0.89	0.22	46,46,46,46	0
57	MG	AA	1615	1/1	0.89	0.23	65,65,65,65	0
57	MG	DA	3391	1/1	0.89	0.12	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3369	1/1	0.89	0.12	53,53,53,53	1
57	MG	BX	102	1/1	0.89	0.21	104,104,104,104	0
57	MG	BA	3207	1/1	0.89	0.19	45,45,45,45	0
57	MG	DA	3086	1/1	0.89	0.17	56,56,56,56	0
57	MG	AA	1676	1/1	0.89	0.10	48,48,48,48	0
57	MG	BA	3210	1/1	0.89	0.13	84,84,84,84	0
57	MG	BA	3252	1/1	0.89	0.13	79,79,79,79	0
57	MG	BA	3380	1/1	0.89	0.17	54,54,54,54	0
57	MG	BA	3082	1/1	0.89	0.17	37,37,37,37	0
57	MG	DA	3405	1/1	0.89	0.15	53,53,53,53	1
57	MG	AA	1659	1/1	0.89	0.22	42,42,42,42	0
57	MG	BA	3260	1/1	0.89	0.17	30,30,30,30	0
57	MG	CA	1786	1/1	0.89	0.13	71,71,71,71	1
57	MG	DA	3411	1/1	0.89	0.14	46,46,46,46	0
57	MG	DA	3305	1/1	0.89	0.50	100,100,100,100	1
57	MG	AA	1751	1/1	0.89	0.21	72,72,72,72	1
57	MG	DA	3415	1/1	0.89	0.27	96,96,96,96	0
57	MG	DA	3116	1/1	0.89	0.26	50,50,50,50	0
57	MG	DA	3221	1/1	0.89	0.30	50,50,50,50	0
57	MG	CA	1618	1/1	0.89	0.23	53,53,53,53	0
57	MG	BA	3323	1/1	0.89	0.15	86,86,86,86	1
57	MG	CA	1677	1/1	0.89	0.10	48,48,48,48	0
57	MG	CA	1620	1/1	0.89	0.16	59,59,59,59	0
57	MG	B1	101	1/1	0.89	0.13	41,41,41,41	1
57	MG	DA	3320	1/1	0.89	0.15	34,34,34,34	1
57	MG	BA	3331	1/1	0.89	0.14	65,65,65,65	1
57	MG	BA	3006	1/1	0.89	0.25	66,66,66,66	0
57	MG	BA	3223	1/1	0.89	0.23	64,64,64,64	0
57	MG	CA	1740	1/1	0.89	0.11	61,61,61,61	1
57	MG	BA	3109	1/1	0.89	0.14	39,39,39,39	0
57	MG	CW	104	1/1	0.89	0.07	130,130,130,130	1
57	MG	CA	1686	1/1	0.89	0.21	43,43,43,43	0
57	MG	BA	3409	1/1	0.89	0.21	20,20,20,20	0
57	MG	AA	1698	1/1	0.89	0.09	42,42,42,42	0
57	MG	BA	3231	1/1	0.89	0.23	38,38,38,38	0
57	MG	BA	3120	1/1	0.89	0.24	90,90,90,90	0
57	MG	BA	3015	1/1	0.89	0.19	33,33,33,33	0
57	MG	DA	3362	1/1	0.90	0.21	112,112,112,112	0
57	MG	BA	3326	1/1	0.90	0.16	46,46,46,46	1
57	MG	BA	3379	1/1	0.90	0.09	36,36,36,36	0
57	MG	D5	102	1/1	0.90	0.16	39,39,39,39	1
57	MG	CA	1603	1/1	0.90	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1694	1/1	0.90	0.26	84,84,84,84	0
57	MG	DA	3375	1/1	0.90	0.13	83,83,83,83	0
57	MG	DA	3004	1/1	0.90	0.28	86,86,86,86	0
57	MG	DA	3378	1/1	0.90	0.23	72,72,72,72	0
57	MG	BA	3329	1/1	0.90	0.14	126,126,126,126	0
57	MG	CA	1764	1/1	0.90	0.22	68,68,68,68	1
57	MG	BA	3184	1/1	0.90	0.20	38,38,38,38	0
57	MG	DA	3291	1/1	0.90	0.18	58,58,58,58	0
57	MG	DA	3015	1/1	0.90	0.27	79,79,79,79	0
57	MG	AA	1636	1/1	0.90	0.26	74,74,74,74	0
57	MG	AA	1611	1/1	0.90	0.15	63,63,63,63	0
57	MG	DA	3297	1/1	0.90	0.17	71,71,71,71	0
57	MG	BA	3281	1/1	0.90	0.16	53,53,53,53	0
57	MG	AX	102	1/1	0.90	0.14	83,83,83,83	0
57	MG	BA	3401	1/1	0.90	0.29	81,81,81,81	0
57	MG	DA	3308	1/1	0.90	0.11	53,53,53,53	0
57	MG	AA	1793	1/1	0.90	0.16	91,91,91,91	0
57	MG	BA	3003	1/1	0.90	0.39	85,85,85,85	0
57	MG	DA	3239	1/1	0.90	0.24	79,79,79,79	0
57	MG	CA	1672	1/1	0.90	0.16	59,59,59,59	0
57	MG	BA	3152	1/1	0.90	0.21	93,93,93,93	0
57	MG	BA	3346	1/1	0.90	0.20	67,67,67,67	0
57	MG	DA	3406	1/1	0.90	0.07	51,51,51,51	0
57	MG	AA	1627	1/1	0.90	0.12	54,54,54,54	0
57	MG	BA	3157	1/1	0.90	0.10	74,74,74,74	0
57	MG	BA	3105	1/1	0.90	0.21	50,50,50,50	0
57	MG	AA	1668	1/1	0.90	0.19	51,51,51,51	0
57	MG	BA	3161	1/1	0.90	0.25	86,86,86,86	0
57	MG	AW	101	1/1	0.90	0.06	157,157,157,157	0
57	MG	DA	3414	1/1	0.90	0.23	84,84,84,84	0
57	MG	AA	1669	1/1	0.90	0.16	57,57,57,57	0
57	MG	CA	1789	1/1	0.90	0.20	64,64,64,64	1
57	MG	BA	3356	1/1	0.90	0.09	41,41,41,41	0
57	MG	BA	3366	1/1	0.90	0.33	112,112,112,112	0
57	MG	AA	1721	1/1	0.90	0.29	90,90,90,90	0
57	MG	DA	3187	1/1	0.90	0.16	55,55,55,55	0
57	MG	BA	3123	1/1	0.90	0.30	29,29,29,29	0
57	MG	DA	3189	1/1	0.90	0.20	69,69,69,69	0
57	MG	DA	3190	1/1	0.90	0.19	67,67,67,67	0
57	MG	DA	3191	1/1	0.90	0.17	41,41,41,41	0
57	MG	AA	1617	1/1	0.90	0.25	51,51,51,51	0
57	MG	DA	3265	1/1	0.90	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3225	1/1	0.90	0.57	128,128,128,128	0
57	MG	CN	101	1/1	0.90	0.09	57,57,57,57	0
57	MG	CA	1646	1/1	0.90	0.14	81,81,81,81	0
57	MG	BA	3372	1/1	0.90	0.27	57,57,57,57	1
57	MG	BA	3226	1/1	0.90	0.14	58,58,58,58	0
57	MG	CA	1695	1/1	0.90	0.22	54,54,54,54	0
57	MG	CA	1753	1/1	0.90	0.76	130,130,130,130	1
57	MG	BA	3228	1/1	0.90	0.30	51,51,51,51	0
57	MG	CA	1654	1/1	0.90	0.19	69,69,69,69	0
58	PAR	CA	1800	42/42	0.90	0.16	86,91,109,113	0
57	MG	AA	1738	1/1	0.91	0.13	55,55,55,55	1
57	MG	CA	1703	1/1	0.91	0.08	87,87,87,87	0
57	MG	BA	3149	1/1	0.91	0.10	13,13,13,13	1
57	MG	BA	3376	1/1	0.91	0.23	81,81,81,81	0
57	MG	DA	3036	1/1	0.91	0.33	32,32,32,32	0
57	MG	CA	1791	1/1	0.91	0.09	85,85,85,85	1
57	MG	BA	3007	1/1	0.91	0.19	22,22,22,22	0
57	MG	BB	208	1/1	0.91	0.38	61,61,61,61	1
57	MG	BA	3062	1/1	0.91	0.34	31,31,31,31	0
57	MG	CA	1797	1/1	0.91	0.12	120,120,120,120	0
57	MG	BA	3118	1/1	0.91	0.09	68,68,68,68	0
57	MG	DA	3336	1/1	0.91	0.05	77,77,77,77	1
57	MG	BA	3193	1/1	0.91	0.06	40,40,40,40	0
57	MG	BA	3291	1/1	0.91	0.19	42,42,42,42	0
57	MG	DA	3057	1/1	0.91	0.20	31,31,31,31	0
57	MG	DA	3058	1/1	0.91	0.29	88,88,88,88	0
57	MG	DA	3059	1/1	0.91	0.26	46,46,46,46	0
57	MG	BA	3253	1/1	0.91	0.28	87,87,87,87	0
57	MG	BA	3119	1/1	0.91	0.15	35,35,35,35	0
57	MG	BA	3299	1/1	0.91	0.17	46,46,46,46	1
57	MG	AA	1679	1/1	0.91	0.30	56,56,56,56	0
57	MG	BA	3197	1/1	0.91	0.18	46,46,46,46	0
57	MG	AA	1758	1/1	0.91	0.06	97,97,97,97	0
57	MG	DA	3170	1/1	0.91	0.10	60,60,60,60	0
57	MG	BA	3021	1/1	0.91	0.19	30,30,30,30	0
57	MG	BA	3201	1/1	0.91	0.10	35,35,35,35	0
57	MG	DA	3231	1/1	0.91	0.29	31,31,31,31	0
57	MG	DA	3290	1/1	0.91	0.40	73,73,73,73	0
57	MG	DA	3175	1/1	0.91	0.09	63,63,63,63	0
57	MG	BA	3266	1/1	0.91	0.12	50,50,50,50	0
57	MG	BA	3360	1/1	0.91	0.36	140,140,140,140	0
57	MG	B0	101	1/1	0.91	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3271	1/1	0.91	0.12	43,43,43,43	0
57	MG	DA	3104	1/1	0.91	0.19	37,37,37,37	0
57	MG	AA	1732	1/1	0.91	0.34	61,61,61,61	0
57	MG	DB	212	1/1	0.91	0.05	99,99,99,99	1
57	MG	DA	3304	1/1	0.91	0.16	49,49,49,49	0
57	MG	BA	3243	1/1	0.91	0.26	65,65,65,65	0
57	MG	AA	1729	1/1	0.91	0.24	69,69,69,69	0
57	MG	BA	3211	1/1	0.91	0.16	40,40,40,40	0
57	MG	BA	3107	1/1	0.91	0.26	44,44,44,44	0
57	MG	DX	101	1/1	0.91	0.16	45,45,45,45	0
57	MG	DA	3013	1/1	0.91	0.24	31,31,31,31	0
57	MG	CA	1742	1/1	0.91	0.17	70,70,70,70	0
57	MG	CA	1743	1/1	0.91	0.22	65,65,65,65	0
57	MG	DA	3163	1/1	0.92	0.23	52,52,52,52	0
57	MG	BA	3277	1/1	0.92	0.29	35,35,35,35	1
57	MG	DA	3299	1/1	0.92	0.23	93,93,93,93	0
57	MG	DA	3074	1/1	0.92	0.18	26,26,26,26	0
57	MG	DA	3232	1/1	0.92	0.28	93,93,93,93	0
57	MG	DA	3168	1/1	0.92	0.12	36,36,36,36	0
57	MG	DA	3080	1/1	0.92	0.12	63,63,63,63	0
57	MG	DA	3081	1/1	0.92	0.13	38,38,38,38	0
57	MG	AA	1753	1/1	0.92	0.04	103,103,103,103	0
57	MG	BA	3035	1/1	0.92	0.25	2,2,2,2	0
57	MG	DA	3174	1/1	0.92	0.13	53,53,53,53	0
57	MG	BA	3189	1/1	0.92	0.13	8,8,8,8	0
57	MG	B2	602	1/1	0.92	0.13	55,55,55,55	0
57	MG	CA	1730	1/1	0.92	0.18	43,43,43,43	0
57	MG	DA	3092	1/1	0.92	0.23	46,46,46,46	0
57	MG	DA	3099	1/1	0.92	0.14	40,40,40,40	0
57	MG	DA	3001	1/1	0.92	0.06	42,42,42,42	0
57	MG	AA	1645	1/1	0.92	0.17	41,41,41,41	0
57	MG	DA	3322	1/1	0.92	0.18	62,62,62,62	0
57	MG	DA	3186	1/1	0.92	0.16	48,48,48,48	0
57	MG	CA	1616	1/1	0.92	0.25	43,43,43,43	0
57	MG	BA	3320	1/1	0.92	0.51	141,141,141,141	0
57	MG	AA	1670	1/1	0.92	0.18	49,49,49,49	0
57	MG	BA	3381	1/1	0.92	0.26	29,29,29,29	0
57	MG	BA	3382	1/1	0.92	0.19	31,31,31,31	0
57	MG	DA	3112	1/1	0.92	0.15	39,39,39,39	0
57	MG	AA	1675	1/1	0.92	0.22	63,63,63,63	0
57	MG	BA	3384	1/1	0.92	0.25	53,53,53,53	0
57	MG	DA	3019	1/1	0.92	0.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1624	1/1	0.92	0.14	55,55,55,55	0
57	MG	BA	3174	1/1	0.92	0.26	55,55,55,55	0
57	MG	CA	1667	1/1	0.92	0.18	55,55,55,55	0
57	MG	AA	1750	1/1	0.92	0.08	62,62,62,62	1
57	MG	DA	3133	1/1	0.92	0.17	35,35,35,35	0
57	MG	AA	1790	1/1	0.92	0.12	63,63,63,63	0
57	MG	CA	1748	1/1	0.92	0.17	63,63,63,63	0
57	MG	CA	1749	1/1	0.92	0.09	98,98,98,98	0
57	MG	BB	210	1/1	0.92	0.20	27,27,27,27	0
57	MG	CA	1794	1/1	0.92	0.38	81,81,81,81	0
57	MG	CA	1631	1/1	0.92	0.19	65,65,65,65	0
57	MG	DA	3283	1/1	0.92	0.08	77,77,77,77	0
57	MG	BA	3332	1/1	0.92	0.21	29,29,29,29	0
57	MG	BA	3069	1/1	0.92	0.24	63,63,63,63	0
57	MG	BN	201	1/1	0.92	0.12	64,64,64,64	0
57	MG	BA	3080	1/1	0.92	0.16	26,26,26,26	0
57	MG	CA	1758	1/1	0.92	0.14	64,64,64,64	1
57	MG	BA	3275	1/1	0.92	0.33	98,98,98,98	0
57	MG	AA	1647	1/1	0.92	0.08	74,74,74,74	0
57	MG	BA	3370	1/1	0.92	0.18	113,113,113,113	0
57	MG	CA	1681	1/1	0.92	0.22	49,49,49,49	0
57	MG	BA	3406	1/1	0.92	0.17	38,38,38,38	1
57	MG	DA	3331	1/1	0.93	0.27	155,155,155,155	1
57	MG	DA	3334	1/1	0.93	0.11	72,72,72,72	0
57	MG	AA	1639	1/1	0.93	0.27	99,99,99,99	0
57	MG	BA	3039	1/1	0.93	0.16	14,14,14,14	0
57	MG	DA	3337	1/1	0.93	0.06	76,76,76,76	0
57	MG	BA	3188	1/1	0.93	0.12	64,64,64,64	0
57	MG	DA	3149	1/1	0.93	0.21	57,57,57,57	0
57	MG	BB	203	1/1	0.93	0.14	14,14,14,14	1
57	MG	AA	1685	1/1	0.93	0.14	42,42,42,42	0
57	MG	CA	1706	1/1	0.93	0.23	80,80,80,80	0
57	MG	BA	3265	1/1	0.93	0.09	30,30,30,30	0
57	MG	CA	1653	1/1	0.93	0.09	83,83,83,83	0
57	MG	BA	3227	1/1	0.93	0.15	74,74,74,74	0
57	MG	DA	3040	1/1	0.93	0.14	25,25,25,25	0
57	MG	CA	1772	1/1	0.93	0.07	77,77,77,77	0
57	MG	DA	3160	1/1	0.93	0.18	67,67,67,67	0
57	MG	CA	1712	1/1	0.93	0.10	81,81,81,81	0
57	MG	BA	3190	1/1	0.93	0.20	51,51,51,51	0
57	MG	DA	3047	1/1	0.93	0.10	28,28,28,28	0
57	MG	BA	3322	1/1	0.93	0.30	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3049	1/1	0.93	0.35	71,71,71,71	0
57	MG	DA	3356	1/1	0.93	0.17	57,57,57,57	0
57	MG	B5	102	1/1	0.93	0.20	58,58,58,58	1
57	MG	DA	3261	1/1	0.93	0.20	95,95,95,95	0
57	MG	DA	3365	1/1	0.93	0.06	19,19,19,19	0
57	MG	CA	1718	1/1	0.93	0.07	67,67,67,67	0
57	MG	DA	3368	1/1	0.93	0.11	45,45,45,45	1
57	MG	BA	3324	1/1	0.93	0.12	39,39,39,39	1
57	MG	BA	3272	1/1	0.93	0.12	46,46,46,46	0
57	MG	BA	3115	1/1	0.93	0.14	27,27,27,27	0
57	MG	BX	101	1/1	0.93	0.16	58,58,58,58	0
57	MG	DA	3374	1/1	0.93	0.14	37,37,37,37	1
57	MG	BA	3233	1/1	0.93	0.23	24,24,24,24	0
57	MG	BA	3234	1/1	0.93	0.16	56,56,56,56	0
57	MG	DA	3271	1/1	0.93	0.23	47,47,47,47	0
57	MG	AA	1680	1/1	0.93	0.26	53,53,53,53	0
57	MG	DA	3273	1/1	0.93	0.10	59,59,59,59	0
57	MG	AA	1784	1/1	0.93	0.09	81,81,81,81	1
57	MG	DA	3070	1/1	0.93	0.22	94,94,94,94	0
57	MG	BA	3066	1/1	0.93	0.18	26,26,26,26	0
57	MG	BA	3389	1/1	0.93	0.22	62,62,62,62	0
57	MG	DA	3184	1/1	0.93	0.14	36,36,36,36	0
57	MG	BA	3280	1/1	0.93	0.10	28,28,28,28	0
57	MG	AA	1616	1/1	0.93	0.22	70,70,70,70	0
57	MG	AA	1608	1/1	0.93	0.18	46,46,46,46	0
57	MG	CA	1796	1/1	0.93	0.11	119,119,119,119	0
57	MG	BA	3395	1/1	0.93	0.13	113,113,113,113	0
57	MG	AA	1772	1/1	0.93	0.15	85,85,85,85	0
57	MG	BA	3399	1/1	0.93	0.24	64,64,64,64	0
57	MG	BA	3400	1/1	0.93	0.09	47,47,47,47	0
57	MG	CA	1738	1/1	0.93	0.07	62,62,62,62	0
57	MG	BA	3164	1/1	0.93	0.08	56,56,56,56	0
57	MG	BA	3126	1/1	0.93	0.21	39,39,39,39	0
57	MG	BA	3403	1/1	0.93	0.20	65,65,65,65	0
57	MG	DA	3105	1/1	0.93	0.20	54,54,54,54	0
57	MG	DA	3205	1/1	0.93	0.08	37,37,37,37	0
57	MG	DA	3294	1/1	0.93	0.07	54,54,54,54	0
57	MG	BA	3176	1/1	0.93	0.26	97,97,97,97	0
57	MG	BA	3019	1/1	0.93	0.18	28,28,28,28	0
57	MG	DA	3298	1/1	0.93	0.15	56,56,56,56	0
57	MG	BA	3213	1/1	0.93	0.06	93,93,93,93	1
57	MG	DA	3211	1/1	0.93	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3214	1/1	0.93	0.38	83,83,83,83	0
57	MG	BA	3128	1/1	0.93	0.14	27,27,27,27	0
57	MG	DA	3113	1/1	0.93	0.11	27,27,27,27	0
57	MG	DA	3307	1/1	0.93	0.14	51,51,51,51	0
57	MG	BA	3413	1/1	0.93	0.21	33,33,33,33	0
57	MG	DB	201	1/1	0.93	0.07	74,74,74,74	0
57	MG	DA	3216	1/1	0.93	0.37	74,74,74,74	0
57	MG	DA	3118	1/1	0.93	0.28	62,62,62,62	0
57	MG	AA	1665	1/1	0.93	0.24	53,53,53,53	0
57	MG	BA	3305	1/1	0.93	0.50	101,101,101,101	0
57	MG	DA	3220	1/1	0.93	0.21	26,26,26,26	0
57	MG	BA	3308	1/1	0.93	0.09	114,114,114,114	1
57	MG	DA	3124	1/1	0.93	0.25	28,28,28,28	0
57	MG	CA	1692	1/1	0.93	0.16	59,59,59,59	0
57	MG	DA	3003	1/1	0.93	0.14	91,91,91,91	0
57	MG	CA	1637	1/1	0.93	0.12	83,83,83,83	0
57	MG	DA	3132	1/1	0.93	0.09	41,41,41,41	0
57	MG	DD	302	1/1	0.93	0.23	46,46,46,46	0
57	MG	DA	3323	1/1	0.93	0.34	53,53,53,53	1
57	MG	BA	3418	1/1	0.93	0.09	59,59,59,59	0
57	MG	DA	3135	1/1	0.93	0.07	39,39,39,39	0
57	MG	DA	3326	1/1	0.93	0.26	78,78,78,78	1
57	MG	AA	1755	1/1	0.93	0.11	84,84,84,84	0
57	MG	BA	3365	1/1	0.93	0.07	1,1,1,1	0
57	MG	AA	1765	1/1	0.93	0.06	94,94,94,94	0
57	MG	AA	1764	1/1	0.94	0.09	64,64,64,64	0
57	MG	BA	3328	1/1	0.94	0.15	168,168,168,168	0
57	MG	BA	3219	1/1	0.94	0.21	30,30,30,30	0
57	MG	BA	3010	1/1	0.94	0.21	41,41,41,41	0
57	MG	BA	3012	1/1	0.94	0.18	16,16,16,16	0
57	MG	BA	3334	1/1	0.94	0.12	79,79,79,79	0
57	MG	DA	3053	1/1	0.94	0.10	26,26,26,26	0
57	MG	DA	3347	1/1	0.94	0.06	53,53,53,53	0
57	MG	BA	3396	1/1	0.94	0.15	11,11,11,11	0
57	MG	DA	3258	1/1	0.94	0.17	37,37,37,37	0
57	MG	CA	1615	1/1	0.94	0.27	70,70,70,70	0
57	MG	BA	3222	1/1	0.94	0.09	84,84,84,84	0
57	MG	AA	1736	1/1	0.94	0.11	87,87,87,87	0
57	MG	DA	3060	1/1	0.94	0.14	30,30,30,30	0
57	MG	BA	3338	1/1	0.94	0.20	52,52,52,52	0
57	MG	AA	1711	1/1	0.94	0.10	73,73,73,73	0
57	MG	DA	3357	1/1	0.94	0.19	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1618	1/1	0.94	0.23	38,38,38,38	0
57	MG	DA	3360	1/1	0.94	0.08	83,83,83,83	0
57	MG	DA	3361	1/1	0.94	0.14	64,64,64,64	0
57	MG	AW	103	1/1	0.94	0.06	106,106,106,106	0
57	MG	BA	3023	1/1	0.94	0.14	23,23,23,23	0
57	MG	DA	3366	1/1	0.94	0.10	29,29,29,29	1
57	MG	AA	1752	1/1	0.94	0.24	120,120,120,120	1
57	MG	CA	1741	1/1	0.94	0.10	53,53,53,53	0
57	MG	BA	3181	1/1	0.94	0.25	49,49,49,49	0
57	MG	DA	3180	1/1	0.94	0.15	35,35,35,35	0
57	MG	DA	3274	1/1	0.94	0.08	60,60,60,60	0
57	MG	AA	1624	1/1	0.94	0.18	52,52,52,52	0
57	MG	DA	3083	1/1	0.94	0.13	33,33,33,33	0
57	MG	AA	1649	1/1	0.94	0.09	56,56,56,56	1
57	MG	BA	3038	1/1	0.94	0.11	41,41,41,41	0
57	MG	AA	1658	1/1	0.94	0.11	25,25,25,25	0
57	MG	BA	3236	1/1	0.94	0.08	44,44,44,44	0
57	MG	DA	3380	1/1	0.94	0.27	52,52,52,52	0
57	MG	CA	1634	1/1	0.94	0.28	53,53,53,53	0
57	MG	BA	3237	1/1	0.94	0.20	74,74,74,74	0
57	MG	CX	101	1/1	0.94	0.21	123,123,123,123	0
57	MG	AA	1730	1/1	0.94	0.12	107,107,107,107	0
57	MG	DA	3193	1/1	0.94	0.11	48,48,48,48	0
57	MG	DA	3194	1/1	0.94	0.06	59,59,59,59	0
57	MG	D1	101	1/1	0.94	0.11	29,29,29,29	1
57	MG	BA	3045	1/1	0.94	0.17	1,1,1,1	0
57	MG	AA	1630	1/1	0.94	0.10	55,55,55,55	0
57	MG	DA	3394	1/1	0.94	0.07	103,103,103,103	0
57	MG	BA	3052	1/1	0.94	0.19	13,13,13,13	0
57	MG	D7	102	1/1	0.94	0.13	62,62,62,62	1
57	MG	DA	3201	1/1	0.94	0.35	88,88,88,88	0
57	MG	BA	3298	1/1	0.94	0.18	69,69,69,69	0
57	MG	AA	1644	1/1	0.94	0.16	110,110,110,110	0
57	MG	AA	1663	1/1	0.94	0.22	47,47,47,47	0
57	MG	DA	3403	1/1	0.94	0.13	55,55,55,55	0
57	MG	BA	3064	1/1	0.94	0.17	20,20,20,20	0
57	MG	DA	3114	1/1	0.94	0.11	29,29,29,29	0
57	MG	B2	601	1/1	0.94	0.09	55,55,55,55	1
57	MG	DA	3008	1/1	0.94	0.16	36,36,36,36	0
57	MG	BA	3148	1/1	0.94	0.27	57,57,57,57	0
57	MG	AA	1631	1/1	0.94	0.23	54,54,54,54	0
57	MG	CA	1651	1/1	0.94	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3306	1/1	0.94	0.07	51,51,51,51	0
57	MG	AA	1747	1/1	0.94	0.08	135,135,135,135	0
57	MG	DA	3126	1/1	0.94	0.15	59,59,59,59	0
57	MG	DA	3310	1/1	0.94	0.06	54,54,54,54	1
57	MG	BA	3151	1/1	0.94	0.14	45,45,45,45	1
57	MG	DA	3018	1/1	0.94	0.18	31,31,31,31	0
57	MG	DA	3129	1/1	0.94	0.12	22,22,22,22	0
57	MG	BA	3209	1/1	0.94	0.18	14,14,14,14	0
57	MG	BA	3071	1/1	0.94	0.20	52,52,52,52	0
57	MG	DA	3023	1/1	0.94	0.17	20,20,20,20	0
57	MG	DA	3134	1/1	0.94	0.10	57,57,57,57	0
57	MG	DA	3026	1/1	0.94	0.13	19,19,19,19	0
57	MG	DA	3027	1/1	0.94	0.25	37,37,37,37	0
57	MG	BA	3154	1/1	0.94	0.20	13,13,13,13	0
57	MG	DA	3029	1/1	0.94	0.25	40,40,40,40	0
57	MG	DA	3141	1/1	0.94	0.24	67,67,67,67	0
57	MG	DA	3032	1/1	0.94	0.36	66,66,66,66	0
57	MG	BA	3258	1/1	0.94	0.12	32,32,32,32	0
57	MG	DA	3147	1/1	0.94	0.09	59,59,59,59	0
57	MG	DA	3236	1/1	0.94	0.10	47,47,47,47	0
57	MG	DA	3238	1/1	0.94	0.12	56,56,56,56	0
57	MG	AN	101	1/1	0.94	0.10	50,50,50,50	0
57	MG	DA	3035	1/1	0.94	0.04	55,55,55,55	0
57	MG	AA	1620	1/1	0.94	0.06	54,54,54,54	0
57	MG	BA	3088	1/1	0.94	0.10	21,21,21,21	0
57	MG	DV	201	1/1	0.94	0.05	70,70,70,70	0
57	MG	BA	3089	1/1	0.94	0.24	43,43,43,43	0
57	MG	CA	1605	1/1	0.94	0.13	47,47,47,47	0
57	MG	DA	3155	1/1	0.94	0.19	21,21,21,21	1
58	PAR	AA	1799	42/42	0.94	0.12	60,65,83,87	0
57	MG	CA	1723	1/1	0.94	0.20	86,86,86,86	0
57	MG	AA	1785	1/1	0.95	0.29	105,105,105,105	0
57	MG	BA	3202	1/1	0.95	0.26	16,16,16,16	0
57	MG	BA	3333	1/1	0.95	0.10	40,40,40,40	0
57	MG	BA	3282	1/1	0.95	0.22	23,23,23,23	0
57	MG	CA	1659	1/1	0.95	0.20	42,42,42,42	0
57	MG	BA	3335	1/1	0.95	0.09	62,62,62,62	0
57	MG	BA	3204	1/1	0.95	0.14	33,33,33,33	0
57	MG	DA	3021	1/1	0.95	0.08	35,35,35,35	0
57	MG	DA	3022	1/1	0.95	0.16	34,34,34,34	0
57	MG	CA	1604	1/1	0.95	0.05	63,63,63,63	0
57	MG	DA	3024	1/1	0.95	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3125	1/1	0.95	0.10	53,53,53,53	0
57	MG	DA	3025	1/1	0.95	0.19	13,13,13,13	0
57	MG	AA	1693	1/1	0.95	0.06	54,54,54,54	0
57	MG	BA	3392	1/1	0.95	0.14	139,139,139,139	0
57	MG	AA	1604	1/1	0.95	0.06	55,55,55,55	0
57	MG	BA	3079	1/1	0.95	0.11	31,31,31,31	0
57	MG	AA	1660	1/1	0.95	0.23	43,43,43,43	0
57	MG	AA	1697	1/1	0.95	0.08	78,78,78,78	0
57	MG	BA	3087	1/1	0.95	0.16	10,10,10,10	0
57	MG	BA	3343	1/1	0.95	0.09	37,37,37,37	0
57	MG	BA	3344	1/1	0.95	0.14	57,57,57,57	0
57	MG	BA	3292	1/1	0.95	0.06	23,23,23,23	0
57	MG	BA	3294	1/1	0.95	0.20	33,33,33,33	0
57	MG	DA	3303	1/1	0.95	0.21	30,30,30,30	0
57	MG	DA	3140	1/1	0.95	0.28	90,90,90,90	0
57	MG	CA	1790	1/1	0.95	0.10	48,48,48,48	0
57	MG	BA	3175	1/1	0.95	0.18	46,46,46,46	0
57	MG	BA	3348	1/1	0.95	0.12	79,79,79,79	0
57	MG	AA	1791	1/1	0.95	0.12	26,26,26,26	1
57	MG	BA	3048	1/1	0.95	0.27	33,33,33,33	0
57	MG	BA	3178	1/1	0.95	0.14	24,24,24,24	0
57	MG	DA	3150	1/1	0.95	0.08	65,65,65,65	1
57	MG	BA	3300	1/1	0.95	0.18	3,3,3,3	0
57	MG	BA	3217	1/1	0.95	0.08	78,78,78,78	0
57	MG	BA	3414	1/1	0.95	0.08	60,60,60,60	0
57	MG	BA	3050	1/1	0.95	0.17	30,30,30,30	0
57	MG	DA	3233	1/1	0.95	0.21	36,36,36,36	0
57	MG	CE	201	1/1	0.95	0.05	90,90,90,90	0
57	MG	BA	3132	1/1	0.95	0.12	14,14,14,14	0
57	MG	BA	3133	1/1	0.95	0.06	19,19,19,19	0
57	MG	BA	3135	1/1	0.95	0.27	36,36,36,36	0
57	MG	AA	1654	1/1	0.95	0.05	52,52,52,52	1
57	MG	BA	3055	1/1	0.95	0.13	18,18,18,18	0
57	MG	CA	1747	1/1	0.95	0.21	62,62,62,62	0
57	MG	BA	3104	1/1	0.95	0.12	20,20,20,20	0
57	MG	BA	3056	1/1	0.95	0.17	17,17,17,17	0
57	MG	AA	1637	1/1	0.95	0.12	58,58,58,58	0
57	MG	DA	3165	1/1	0.95	0.06	78,78,78,78	0
57	MG	CA	1751	1/1	0.95	0.11	66,66,66,66	1
57	MG	BA	3028	1/1	0.95	0.16	12,12,12,12	0
57	MG	BA	3004	1/1	0.95	0.17	42,42,42,42	0
57	MG	BA	3194	1/1	0.95	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	D5	101	1/1	0.95	0.16	51,51,51,51	0
57	MG	DB	204	1/1	0.95	0.07	90,90,90,90	0
57	MG	CA	1755	1/1	0.95	0.03	107,107,107,107	0
57	MG	BA	3110	1/1	0.95	0.07	44,44,44,44	0
57	MG	BA	3153	1/1	0.95	0.20	20,20,20,20	1
57	MG	DA	3089	1/1	0.95	0.12	26,26,26,26	0
57	MG	BA	3111	1/1	0.95	0.18	23,23,23,23	0
57	MG	DA	3091	1/1	0.95	0.10	39,39,39,39	0
57	MG	CA	1702	1/1	0.95	0.14	66,66,66,66	0
57	MG	DA	3095	1/1	0.95	0.05	37,37,37,37	0
57	MG	DA	3181	1/1	0.95	0.18	100,100,100,100	0
57	MG	DD	301	1/1	0.95	0.17	38,38,38,38	0
57	MG	DA	3098	1/1	0.95	0.30	38,38,38,38	0
57	MG	BA	3378	1/1	0.95	0.14	8,8,8,8	0
57	MG	BB	211	1/1	0.95	0.12	119,119,119,119	0
57	MG	DA	3185	1/1	0.95	0.14	33,33,33,33	0
57	MG	BA	3112	1/1	0.95	0.14	15,15,15,15	0
57	MG	DA	3103	1/1	0.95	0.21	34,34,34,34	0
57	MG	DA	3007	1/1	0.95	0.30	59,59,59,59	0
57	MG	AA	1773	1/1	0.95	0.12	72,72,72,72	0
57	MG	DA	3009	1/1	0.95	0.06	45,45,45,45	0
57	MG	BB	214	1/1	0.95	0.16	75,75,75,75	1
57	MG	BA	3102	1/1	0.96	0.16	13,13,13,13	0
57	MG	DA	3073	1/1	0.96	0.07	36,36,36,36	0
57	MG	DA	3171	1/1	0.96	0.12	43,43,43,43	0
57	MG	AA	1606	1/1	0.96	0.08	34,34,34,34	0
57	MG	DA	3076	1/1	0.96	0.11	45,45,45,45	0
57	MG	CW	101	1/1	0.96	0.09	144,144,144,144	0
57	MG	AA	1767	1/1	0.96	0.12	44,44,44,44	0
57	MG	BA	3009	1/1	0.96	0.17	17,17,17,17	0
57	MG	CW	105	1/1	0.96	0.07	70,70,70,70	1
57	MG	AA	1674	1/1	0.96	0.10	42,42,42,42	0
57	MG	BA	3295	1/1	0.96	0.20	64,64,64,64	0
57	MG	CA	1679	1/1	0.96	0.04	86,86,86,86	0
57	MG	BA	3146	1/1	0.96	0.15	57,57,57,57	0
57	MG	BA	3255	1/1	0.96	0.13	37,37,37,37	0
57	MG	BA	3256	1/1	0.96	0.16	11,11,11,11	0
57	MG	BA	3183	1/1	0.96	0.16	20,20,20,20	0
57	MG	CA	1621	1/1	0.96	0.09	58,58,58,58	0
57	MG	BA	3040	1/1	0.96	0.12	20,20,20,20	0
57	MG	BA	3304	1/1	0.96	0.09	81,81,81,81	0
57	MG	DA	3371	1/1	0.96	0.09	61,61,61,61	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3100	1/1	0.96	0.06	63,63,63,63	0
57	MG	AA	1662	1/1	0.96	0.05	95,95,95,95	0
57	MG	BA	3412	1/1	0.96	0.12	30,30,30,30	0
57	MG	CA	1689	1/1	0.96	0.07	40,40,40,40	0
57	MG	BA	3261	1/1	0.96	0.21	23,23,23,23	0
57	MG	DA	3377	1/1	0.96	0.15	24,24,24,24	0
57	MG	DA	3005	1/1	0.96	0.18	52,52,52,52	0
57	MG	CA	1628	1/1	0.96	0.08	81,81,81,81	0
57	MG	BA	3075	1/1	0.96	0.15	31,31,31,31	0
57	MG	DA	3381	1/1	0.96	0.08	45,45,45,45	0
57	MG	DA	3382	1/1	0.96	0.03	74,74,74,74	0
57	MG	BA	3078	1/1	0.96	0.09	13,13,13,13	0
57	MG	BA	3114	1/1	0.96	0.15	3,3,3,3	0
57	MG	DA	3385	1/1	0.96	0.11	79,79,79,79	0
57	MG	BA	3361	1/1	0.96	0.05	28,28,28,28	0
57	MG	CA	1760	1/1	0.96	0.04	145,145,145,145	0
57	MG	DA	3200	1/1	0.96	0.10	59,59,59,59	0
57	MG	BA	3362	1/1	0.96	0.15	85,85,85,85	0
57	MG	AA	1719	1/1	0.96	0.10	52,52,52,52	0
57	MG	DA	3204	1/1	0.96	0.30	39,39,39,39	0
57	MG	AA	1789	1/1	0.96	0.17	81,81,81,81	1
57	MG	CA	1699	1/1	0.96	0.05	50,50,50,50	0
57	MG	CA	1638	1/1	0.96	0.19	42,42,42,42	0
57	MG	DA	3396	1/1	0.96	0.15	145,145,145,145	0
57	MG	CA	1639	1/1	0.96	0.10	62,62,62,62	0
57	MG	BA	3267	1/1	0.96	0.13	56,56,56,56	0
57	MG	BA	3315	1/1	0.96	0.04	83,83,83,83	0
57	MG	CA	1769	1/1	0.96	0.07	27,27,27,27	0
57	MG	DA	3401	1/1	0.96	0.07	57,57,57,57	0
57	MG	CA	1704	1/1	0.96	0.13	114,114,114,114	0
57	MG	AA	1778	1/1	0.96	0.41	65,65,65,65	1
57	MG	BA	3156	1/1	0.96	0.06	20,20,20,20	0
57	MG	CA	1707	1/1	0.96	0.09	119,119,119,119	0
57	MG	DA	3131	1/1	0.96	0.08	23,23,23,23	0
57	MG	BA	3319	1/1	0.96	0.15	3,3,3,3	1
57	MG	AA	1696	1/1	0.96	0.04	47,47,47,47	0
57	MG	DA	3409	1/1	0.96	0.11	121,121,121,121	0
57	MG	CA	1776	1/1	0.96	0.05	46,46,46,46	0
57	MG	BB	205	1/1	0.96	0.12	25,25,25,25	0
57	MG	BA	3022	1/1	0.96	0.20	20,20,20,20	0
57	MG	BA	3121	1/1	0.96	0.14	40,40,40,40	0
57	MG	CA	1715	1/1	0.96	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3038	1/1	0.96	0.08	49,49,49,49	0
57	MG	BA	3001	1/1	0.96	0.06	33,33,33,33	0
57	MG	AI	201	1/1	0.96	0.12	109,109,109,109	0
57	MG	BA	3092	1/1	0.96	0.12	28,28,28,28	0
57	MG	BA	3278	1/1	0.96	0.12	127,127,127,127	0
57	MG	BA	3094	1/1	0.96	0.08	24,24,24,24	0
57	MG	BA	3330	1/1	0.96	0.15	85,85,85,85	1
57	MG	BD	301	1/1	0.96	0.14	16,16,16,16	0
57	MG	DA	3235	1/1	0.96	0.17	30,30,30,30	0
57	MG	BF	301	1/1	0.96	0.07	41,41,41,41	0
57	MG	DB	205	1/1	0.96	0.04	55,55,55,55	0
57	MG	DA	3237	1/1	0.96	0.10	156,156,156,156	0
57	MG	BA	3205	1/1	0.96	0.14	17,17,17,17	0
57	MG	BA	3167	1/1	0.96	0.32	32,32,32,32	1
57	MG	DA	3330	1/1	0.96	0.07	51,51,51,51	1
57	MG	BA	3169	1/1	0.96	0.13	18,18,18,18	0
57	MG	DA	3333	1/1	0.96	0.12	108,108,108,108	0
57	MG	DA	3241	1/1	0.96	0.15	32,32,32,32	0
57	MG	DA	3054	1/1	0.96	0.17	90,90,90,90	0
57	MG	BA	3385	1/1	0.96	0.05	87,87,87,87	0
57	MG	BA	3170	1/1	0.96	0.09	61,61,61,61	0
57	MG	BA	3388	1/1	0.96	0.15	12,12,12,12	0
57	MG	DF	302	1/1	0.96	0.20	91,91,91,91	0
57	MG	BA	3095	1/1	0.96	0.19	27,27,27,27	0
57	MG	AA	1633	1/1	0.96	0.08	40,40,40,40	0
57	MG	DA	3064	1/1	0.96	0.06	32,32,32,32	0
57	MG	BA	3286	1/1	0.96	0.17	16,16,16,16	0
57	MG	CI	201	1/1	0.96	0.06	75,75,75,75	0
57	MG	CA	1607	1/1	0.96	0.13	30,30,30,30	0
57	MG	BA	3287	1/1	0.96	0.21	31,31,31,31	0
57	MG	BA	3059	1/1	0.96	0.13	9,9,9,9	0
57	MG	DA	3071	1/1	0.96	0.24	23,23,23,23	0
57	MG	BA	3068	1/1	0.97	0.06	38,38,38,38	0
57	MG	BA	3011	1/1	0.97	0.10	32,32,32,32	0
57	MG	DA	3203	1/1	0.97	0.06	56,56,56,56	0
57	MG	B5	101	1/1	0.97	0.11	42,42,42,42	0
57	MG	DA	3043	1/1	0.97	0.09	51,51,51,51	0
57	MG	DA	3206	1/1	0.97	0.06	33,33,33,33	0
57	MG	BA	3113	1/1	0.97	0.12	3,3,3,3	0
57	MG	BA	3074	1/1	0.97	0.08	24,24,24,24	0
57	MG	BA	3350	1/1	0.97	0.11	81,81,81,81	1
57	MG	AA	1779	1/1	0.97	0.06	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B7	101	1/1	0.97	0.11	45,45,45,45	1
57	MG	BA	3206	1/1	0.97	0.09	22,22,22,22	0
57	MG	BA	3301	1/1	0.97	0.25	57,57,57,57	0
57	MG	DA	3295	1/1	0.97	0.07	78,78,78,78	0
57	MG	BA	3016	1/1	0.97	0.28	28,28,28,28	0
57	MG	BA	3044	1/1	0.97	0.11	1,1,1,1	0
57	MG	BA	3017	1/1	0.97	0.08	9,9,9,9	0
57	MG	DA	3142	1/1	0.97	0.33	65,65,65,65	0
57	MG	DA	3143	1/1	0.97	0.23	18,18,18,18	0
57	MG	DA	3144	1/1	0.97	0.07	63,63,63,63	1
57	MG	DA	3302	1/1	0.97	0.04	43,43,43,43	1
57	MG	BA	3083	1/1	0.97	0.19	30,30,30,30	0
57	MG	BA	3165	1/1	0.97	0.07	38,38,38,38	0
57	MG	BA	3363	1/1	0.97	0.10	73,73,73,73	0
57	MG	DA	3061	1/1	0.97	0.13	30,30,30,30	0
57	MG	DA	3063	1/1	0.97	0.17	32,32,32,32	0
57	MG	BA	3166	1/1	0.97	0.07	31,31,31,31	0
57	MG	BA	3018	1/1	0.97	0.17	9,9,9,9	0
57	MG	BA	3168	1/1	0.97	0.13	87,87,87,87	0
57	MG	AA	1628	1/1	0.97	0.06	37,37,37,37	0
57	MG	CA	1636	1/1	0.97	0.16	50,50,50,50	0
57	MG	AA	1782	1/1	0.97	0.15	96,96,96,96	1
57	MG	D2	603	1/1	0.97	0.09	95,95,95,95	0
57	MG	BA	3316	1/1	0.97	0.08	55,55,55,55	1
57	MG	BA	3171	1/1	0.97	0.06	31,31,31,31	0
57	MG	BA	3172	1/1	0.97	0.05	52,52,52,52	0
57	MG	BA	3268	1/1	0.97	0.11	34,34,34,34	0
57	MG	DA	3078	1/1	0.97	0.10	20,20,20,20	0
57	MG	BA	3269	1/1	0.97	0.18	38,38,38,38	0
57	MG	BA	3090	1/1	0.97	0.12	29,29,29,29	0
57	MG	AA	1756	1/1	0.97	0.12	47,47,47,47	1
57	MG	BA	3377	1/1	0.97	0.16	126,126,126,126	0
57	MG	DA	3085	1/1	0.97	0.05	32,32,32,32	0
57	MG	DA	3167	1/1	0.97	0.10	37,37,37,37	0
57	MG	BA	3129	1/1	0.97	0.15	10,10,10,10	0
57	MG	BA	3053	1/1	0.97	0.16	64,64,64,64	0
57	MG	BA	3093	1/1	0.97	0.06	7,7,7,7	0
57	MG	AL	201	1/1	0.97	0.08	81,81,81,81	0
57	MG	BD	302	1/1	0.97	0.12	22,22,22,22	0
57	MG	CA	1652	1/1	0.97	0.11	52,52,52,52	0
57	MG	BE	301	1/1	0.97	0.10	30,30,30,30	0
57	MG	BA	3134	1/1	0.97	0.05	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3026	1/1	0.97	0.15	8,8,8,8	0
57	MG	BA	3136	1/1	0.97	0.17	16,16,16,16	0
57	MG	BV	201	1/1	0.97	0.11	64,64,64,64	0
57	MG	DA	3257	1/1	0.97	0.04	52,52,52,52	0
57	MG	BA	3027	1/1	0.97	0.10	30,30,30,30	0
57	MG	AA	1642	1/1	0.97	0.14	45,45,45,45	0
57	MG	CA	1601	1/1	0.97	0.06	140,140,140,140	0
57	MG	BA	3185	1/1	0.97	0.09	1,1,1,1	0
57	MG	BA	3060	1/1	0.97	0.16	1,1,1,1	0
57	MG	CA	1663	1/1	0.97	0.04	53,53,53,53	0
57	MG	BA	3145	1/1	0.97	0.09	27,27,27,27	0
57	MG	DA	3348	1/1	0.97	0.05	64,64,64,64	0
57	MG	BA	3103	1/1	0.97	0.10	31,31,31,31	0
57	MG	BA	3147	1/1	0.97	0.11	26,26,26,26	0
57	MG	BA	3031	1/1	0.97	0.23	44,44,44,44	0
57	MG	CA	1787	1/1	0.97	0.05	66,66,66,66	0
57	MG	DA	3030	1/1	0.97	0.10	47,47,47,47	0
57	MG	DE	301	1/1	0.97	0.10	39,39,39,39	0
57	MG	DA	3115	1/1	0.97	0.10	22,22,22,22	0
57	MG	DA	3031	1/1	0.97	0.12	41,41,41,41	0
57	MG	BA	3192	1/1	0.97	0.04	21,21,21,21	0
57	MG	BA	3063	1/1	0.97	0.12	1,1,1,1	0
57	MG	DA	3120	1/1	0.97	0.07	39,39,39,39	0
57	MG	CA	1670	1/1	0.97	0.05	69,69,69,69	0
57	MG	AA	1688	1/1	0.97	0.13	35,35,35,35	0
57	MG	AV	102	1/1	0.97	0.04	93,93,93,93	1
57	MG	CA	1732	1/1	0.97	0.06	82,82,82,82	0
57	MG	BA	3036	1/1	0.97	0.10	29,29,29,29	0
57	MG	DA	3014	1/1	0.98	0.08	31,31,31,31	0
57	MG	DA	3268	1/1	0.98	0.09	41,41,41,41	0
57	MG	DA	3269	1/1	0.98	0.10	47,47,47,47	0
57	MG	CA	1710	1/1	0.98	0.03	54,54,54,54	0
57	MG	BA	3198	1/1	0.98	0.11	51,51,51,51	0
57	MG	DA	3017	1/1	0.98	0.23	31,31,31,31	0
57	MG	BA	3124	1/1	0.98	0.07	46,46,46,46	0
57	MG	BA	3386	1/1	0.98	0.06	76,76,76,76	0
57	MG	CA	1714	1/1	0.98	0.03	62,62,62,62	0
57	MG	BA	3061	1/1	0.98	0.15	10,10,10,10	0
57	MG	BO	201	1/1	0.98	0.07	29,29,29,29	0
57	MG	DA	3107	1/1	0.98	0.04	32,32,32,32	0
57	MG	AA	1780	1/1	0.98	0.15	115,115,115,115	0
57	MG	BA	3005	1/1	0.98	0.21	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3110	1/1	0.98	0.10	41,41,41,41	0
57	MG	BA	3203	1/1	0.98	0.06	30,30,30,30	0
57	MG	CA	1781	1/1	0.98	0.06	58,58,58,58	0
57	MG	BA	3391	1/1	0.98	0.05	37,37,37,37	0
57	MG	AA	1709	1/1	0.98	0.04	49,49,49,49	0
57	MG	CA	1784	1/1	0.98	0.06	68,68,68,68	1
57	MG	BA	3098	1/1	0.98	0.08	6,6,6,6	0
57	MG	BA	3293	1/1	0.98	0.05	87,87,87,87	0
57	MG	BA	3099	1/1	0.98	0.05	37,37,37,37	0
57	MG	BA	3065	1/1	0.98	0.09	1,1,1,1	0
57	MG	BA	3397	1/1	0.98	0.14	73,73,73,73	0
57	MG	BA	3020	1/1	0.98	0.10	28,28,28,28	0
57	MG	CA	1608	1/1	0.98	0.06	39,39,39,39	0
57	MG	DA	3037	1/1	0.98	0.10	45,45,45,45	0
57	MG	DA	3208	1/1	0.98	0.04	32,32,32,32	0
57	MG	AE	201	1/1	0.98	0.07	101,101,101,101	0
57	MG	BA	3042	1/1	0.98	0.12	36,36,36,36	0
57	MG	BA	3008	1/1	0.98	0.11	3,3,3,3	0
57	MG	BA	3173	1/1	0.98	0.04	33,33,33,33	0
57	MG	BA	3137	1/1	0.98	0.04	33,33,33,33	0
57	MG	BA	3302	1/1	0.98	0.07	26,26,26,26	0
57	MG	AA	1725	1/1	0.98	0.07	104,104,104,104	0
57	MG	DA	3046	1/1	0.98	0.22	30,30,30,30	0
57	MG	BA	3139	1/1	0.98	0.13	85,85,85,85	0
57	MG	BA	3140	1/1	0.98	0.27	66,66,66,66	0
57	MG	BA	3408	1/1	0.98	0.13	43,43,43,43	0
57	MG	DA	3137	1/1	0.98	0.07	21,21,21,21	0
57	MG	BA	3141	1/1	0.98	0.26	56,56,56,56	0
57	MG	BA	3410	1/1	0.98	0.16	120,120,120,120	0
57	MG	DA	3052	1/1	0.98	0.08	30,30,30,30	0
57	MG	CV	101	1/1	0.98	0.08	20,20,20,20	0
57	MG	CV	102	1/1	0.98	0.07	46,46,46,46	1
57	MG	BA	3411	1/1	0.98	0.08	51,51,51,51	1
57	MG	BA	3218	1/1	0.98	0.10	6,6,6,6	0
57	MG	DA	3316	1/1	0.98	0.04	88,88,88,88	0
57	MG	BA	3358	1/1	0.98	0.08	24,24,24,24	0
57	MG	BA	3106	1/1	0.98	0.06	20,20,20,20	0
57	MG	BA	3073	1/1	0.98	0.06	5,5,5,5	0
57	MG	CW	103	1/1	0.98	0.03	87,87,87,87	0
57	MG	DA	3062	1/1	0.98	0.17	33,33,33,33	0
57	MG	CA	1626	1/1	0.98	0.12	34,34,34,34	0
57	MG	BA	3046	1/1	0.98	0.09	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3065	1/1	0.98	0.07	17,17,17,17	0
57	MG	BA	3025	1/1	0.98	0.21	9,9,9,9	0
57	MG	AA	1609	1/1	0.98	0.06	36,36,36,36	0
57	MG	AA	1626	1/1	0.98	0.05	37,37,37,37	0
57	MG	AA	1691	1/1	0.98	0.06	27,27,27,27	0
57	MG	BA	3013	1/1	0.98	0.09	7,7,7,7	0
57	MG	DA	3242	1/1	0.98	0.05	18,18,18,18	0
57	MG	D2	601	1/1	0.98	0.09	35,35,35,35	1
57	MG	DA	3332	1/1	0.98	0.27	33,33,33,33	0
57	MG	CA	1633	1/1	0.98	0.04	42,42,42,42	0
57	MG	AA	1713	1/1	0.98	0.06	53,53,53,53	0
57	MG	BA	3085	1/1	0.98	0.07	21,21,21,21	0
57	MG	DA	3075	1/1	0.98	0.08	37,37,37,37	0
57	MG	BA	3321	1/1	0.98	0.09	80,80,80,80	0
57	MG	DA	3077	1/1	0.98	0.08	29,29,29,29	0
57	MG	BA	3229	1/1	0.98	0.24	20,20,20,20	0
57	MG	DA	3079	1/1	0.98	0.06	37,37,37,37	0
57	MG	BA	3086	1/1	0.98	0.13	32,32,32,32	0
57	MG	BA	3033	1/1	0.98	0.19	33,33,33,33	0
57	MG	BA	3325	1/1	0.98	0.10	88,88,88,88	1
57	MG	BA	3034	1/1	0.98	0.09	40,40,40,40	0
57	MG	BA	3058	1/1	0.98	0.22	19,19,19,19	0
57	MG	DF	301	1/1	0.98	0.04	56,56,56,56	0
57	MG	BB	209	1/1	0.98	0.38	1,1,1,1	1
57	MG	AA	1692	1/1	0.98	0.04	72,72,72,72	0
57	MG	BA	3122	1/1	0.98	0.12	94,94,94,94	0
57	MG	BA	3159	1/1	0.98	0.07	37,37,37,37	0
57	MG	BA	3238	1/1	0.98	0.15	51,51,51,51	0
57	MG	BA	3239	1/1	0.98	0.10	20,20,20,20	0
57	MG	AA	1614	1/1	0.98	0.20	14,14,14,14	0
57	MG	DA	3093	1/1	0.98	0.12	36,36,36,36	0
57	MG	CA	1650	1/1	0.98	0.07	89,89,89,89	1
57	MG	DA	3096	1/1	0.98	0.10	24,24,24,24	0
59	ZN	D9	101	1/1	0.98	0.08	136,136,136,136	0
57	MG	AA	1687	1/1	0.99	0.04	9,9,9,9	1
57	MG	AV	101	1/1	0.99	0.09	36,36,36,36	0
57	MG	BA	3084	1/1	0.99	0.06	12,12,12,12	0
57	MG	AX	101	1/1	0.99	0.06	118,118,118,118	0
57	MG	BA	3070	1/1	0.99	0.23	2,2,2,2	0
57	MG	BA	3191	1/1	0.99	0.07	14,14,14,14	0
57	MG	DA	3010	1/1	0.99	0.14	18,18,18,18	0
57	MG	BA	3049	1/1	0.99	0.11	84,84,84,84	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1714	1/1	0.99	0.03	29,29,29,29	0
57	MG	DA	3417	1/1	0.99	0.06	37,37,37,37	0
57	MG	BA	3232	1/1	0.99	0.10	27,27,27,27	0
57	MG	DA	3044	1/1	0.99	0.08	40,40,40,40	0
57	MG	BA	3051	1/1	0.99	0.09	5,5,5,5	0
57	MG	BA	3002	1/1	0.99	0.07	139,139,139,139	0
57	MG	BA	3076	1/1	0.99	0.10	25,25,25,25	0
57	MG	BA	3142	1/1	0.99	0.25	20,20,20,20	0
57	MG	BA	3043	1/1	0.99	0.04	20,20,20,20	0
57	MG	DA	3117	1/1	0.99	0.03	16,16,16,16	0
57	MG	DA	3082	1/1	0.99	0.06	59,59,59,59	0
57	MG	BA	3303	1/1	0.99	0.08	49,49,49,49	1
57	MG	BA	3259	1/1	0.99	0.06	24,24,24,24	0
57	MG	CX	102	1/1	0.99	0.05	110,110,110,110	0
57	MG	BA	3029	1/1	0.99	0.04	40,40,40,40	0
57	MG	DA	3309	1/1	0.99	0.02	47,47,47,47	0
57	MG	DA	3123	1/1	0.99	0.07	89,89,89,89	0
57	MG	DA	3390	1/1	0.99	0.04	48,48,48,48	0
57	MG	BA	3306	1/1	0.99	0.04	18,18,18,18	0
57	MG	DA	3055	1/1	0.99	0.06	31,31,31,31	0
57	MG	BA	3357	1/1	0.99	0.14	84,84,84,84	0
57	MG	BA	3307	1/1	0.99	0.04	23,23,23,23	0
57	MG	BA	3359	1/1	0.99	0.06	86,86,86,86	1
57	MG	BA	3030	1/1	0.99	0.09	18,18,18,18	0
57	MG	BA	3240	1/1	0.99	0.03	11,11,11,11	0
57	MG	DA	3094	1/1	0.99	0.04	22,22,22,22	0
57	MG	BA	3081	1/1	0.99	0.05	7,7,7,7	0
57	MG	BA	3096	1/1	0.99	0.05	1,1,1,1	0
57	MG	DA	3359	1/1	0.99	0.04	62,62,62,62	1
57	MG	DA	3097	1/1	0.99	0.02	25,25,25,25	0
57	MG	BA	3364	1/1	0.99	0.06	35,35,35,35	0
57	MG	BA	3130	1/1	0.99	0.08	8,8,8,8	0
57	MG	DA	3363	1/1	0.99	0.04	68,68,68,68	0
57	MG	DA	3364	1/1	0.99	0.08	52,52,52,52	0
59	ZN	AD	302	1/1	0.99	0.11	55,55,55,55	0
59	ZN	AN	102	1/1	0.99	0.06	109,109,109,109	0
59	ZN	B9	101	1/1	0.99	0.04	94,94,94,94	0
59	ZN	CD	301	1/1	0.99	0.10	55,55,55,55	0
59	ZN	CN	102	1/1	0.99	0.02	120,120,120,120	0
57	MG	BA	3097	1/1	0.99	0.17	7,7,7,7	0
57	MG	DA	3234	1/1	1.00	0.04	22,22,22,22	0
57	MG	BA	3116	1/1	1.00	0.01	4,4,4,4	0

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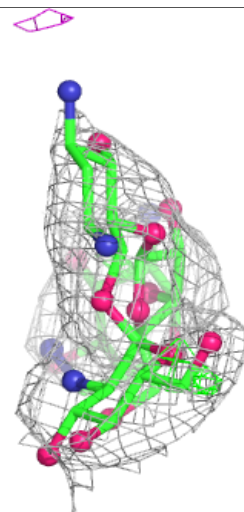
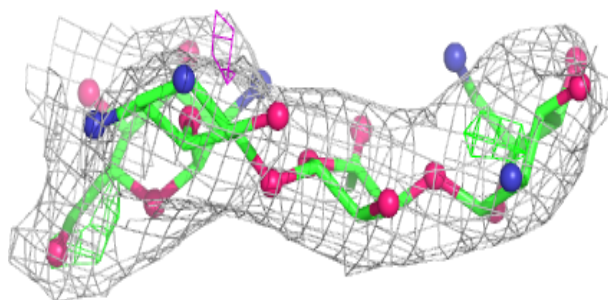
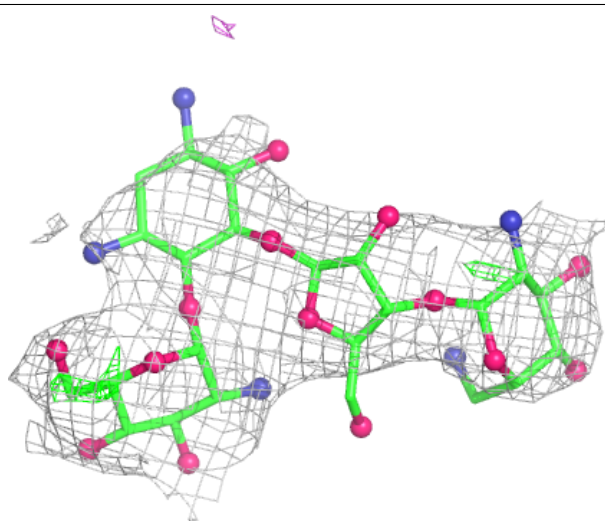
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3054	1/1	1.00	0.05	1,1,1,1	0
57	MG	BA	3077	1/1	1.00	0.01	1,1,1,1	0
57	MG	BA	3024	1/1	1.00	0.20	11,11,11,11	0
57	MG	BA	3072	1/1	1.00	0.03	3,3,3,3	0

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

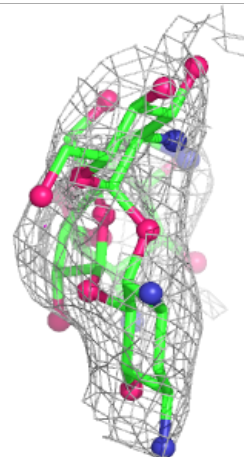
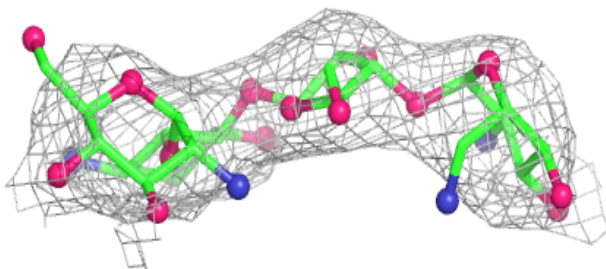
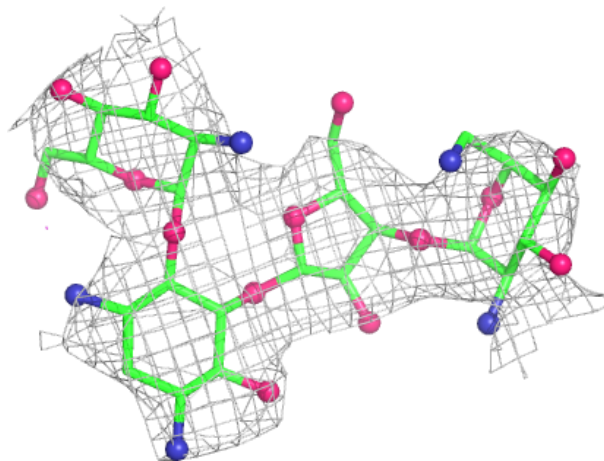
Electron density around PAR CA 1800:

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



Electron density around PAR AA 1799:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.