wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 08:51 PM EST

PDB ID	:	1VY5
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptydil-tRNA in the A site and deacylated tRNA in the P site.
Authors	:	Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on	:	2014-05-13
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

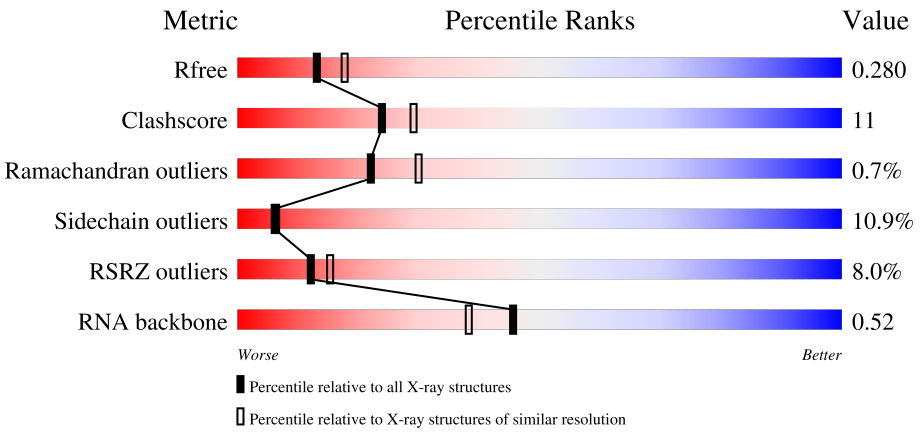
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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 <=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	1521	2%, 52%, 37%, 9%
1	CA	1521	4%, 45%, 42%, 10%
2	AB	256	12%, 42%, 41%, 6%, 10%
2	CB	256	20%, 36%, 43%, 11%, 10%

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Mol	Chain	Length	Quality of chain
3	AC	239	14% 56% 27% 14%
3	CC	239	32% 46% 35% 5% 14%
4	AD	209	13% 57% 38%
4	CD	209	8% 60% 34% 5%
5	AE	162	10% 60% 28% 9%
5	CE	162	18% 62% 25% 9%
6	AF	101	5% 71% 23% 5%
6	CF	101	5% 72% 24%
7	AG	156	6% 71% 22% 6%
7	CG	156	15% 67% 28% 5%
8	AH	138	18% 71% 26%
8	CH	138	20% 59% 38%
9	AI	128	20% 53% 40% 6%
9	CI	128	56% 50% 42% 7%
10	AJ	105	18% 51% 33% 8% 8%
10	CJ	105	33% 49% 36% 7% 9%
11	AK	129	6% 59% 28% 12%
11	CK	129	6% 70% 16% 12%
12	AL	132	4% 68% 23% 8%
12	CL	132	18% 68% 22% 8%
13	AM	126	7% 63% 29% 5%
13	CM	126	42% 55% 39%
14	AN	61	15% 66% 30%
14	CN	61	62% 51% 38% 10%
15	AO	89	7% 56% 37% 6%

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Mol	Chain	Length	Quality of chain
15	CO	89	9% 57% 35% 7%
16	AP	88	27% 68% 23% 7%
16	CP	88	8% 56% 33% 5% 7%
17	AQ	105	10% 66% 25% 6%
17	CQ	105	24% 71% 20% 6%
18	AR	88	6% 51% 24% 23%
18	CR	88	3% 52% 22% 23%
19	AS	93	3% 49% 35% 11%
19	CS	93	33% 48% 39% 11%
20	AT	106	13% 53% 32% 6% 9%
20	CT	106	14% 56% 29% 6% 9%
21	AU	27	26% 52% 26% 7% 15%
21	CU	27	56% 37% 48% 15%
22	AV	24	29% 38% 12% 46%
22	CV	24	33% 29% 12% 8% 50%
23	AW	76	33% 14% 54% 24% 5%
23	CW	76	68% 13% 41% 33% 8% 5%
24	AX	77	% 45% 34% 18%
24	CX	77	5% 34% 45% 18%
25	AY	76	28% 13% 34% 39% 11%
25	CY	76	42% 8% 45% 36% 8%
26	BA	2915	% 61% 28% 7%
26	DA	2915	2% 52% 35% 9%
27	BB	121	75% 18% 6%
27	DB	121	4% 48% 41% 10%

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Mol	Chain	Length	Quality of chain
28	BD	276	3% 74% 21%
28	DD	276	5% 72% 22% 5%
29	BE	206	3% 76% 19%
29	DE	206	2% 70% 22% 6%
30	BF	210	69% 25%
30	DF	210	3% 64% 29%
31	BG	182	5% 70% 25%
31	DG	182	22% 47% 45% 7%
32	BH	180	2% 63% 30%
32	DH	180	19% 64% 28%
33	BI	148	3% 60% 28% 10%
33	DI	148	9% 66% 27% 5%
34	BN	140	2% 79% 18%
34	DN	140	6% 71% 24%
35	BO	122	71% 27%
35	DO	122	2% 65% 34%
36	BP	150	2% 65% 29% 5%
36	DP	150	15% 68% 23% 7%
37	BQ	141	% 72% 21% 6%
37	DQ	141	18% 66% 31%
38	BR	118	68% 27% 5%
38	DR	118	2% 64% 30% 7%
39	BS	112	% 71% 24%
39	DS	112	22% 58% 34% 6%
40	BT	146	66% 21% 10%

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Mol	Chain	Length	Quality of chain
40	DT	146	3% 63% 22% 5% 10%
41	BU	118	% 77% 18%
41	DU	118	8% 62% 34%
42	BV	101	75% 23%
42	DV	101	4% 68% 23% 6%
43	BW	113	85% 12%
43	DW	113	4% 87% 11%
44	BX	96	74% 21%
44	DX	96	9% 63% 32%
45	BY	110	% 63% 30% 5%
45	DY	110	16% 65% 32%
46	BZ	206	7% 56% 24% 17%
46	DZ	206	22% 46% 35% 16%
47	B0	85	7% 76% 20%
47	D0	85	25% 68% 24% 6%
48	B1	98	7% 73% 22%
48	D1	98	13% 73% 20% 5%
49	B2	72	65% 29%
49	D2	72	7% 69% 26%
50	B3	60	73% 20% 5%
50	D3	60	12% 58% 38%
51	B4	71	7% 56% 25% 13%
51	D4	71	17% 48% 32% 15%
52	B5	60	2% 72% 22% 5%
52	D5	60	3% 72% 23%

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Mol	Chain	Length	Quality of chain
53	B6	54	2% 56% 37% 6%
53	D6	54	15% 76% 19%
54	B7	49	6% 76% 20%
54	D7	49	16% 73% 24%
55	B8	65	3% 72% 23%
55	D8	65	28% 74% 25%
56	B9	37	5% 78% 22%
56	D9	37	14% 59% 38%

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
25	5MU	CY	54	-	-	-	X
25	PSU	CY	55	-	-	-	X
57	MG	DA	3651	-	-	-	X
57	MG	DD	303	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 297141 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
			Total	C	N	O	P			
1	AA	1498	32205	14333	5970	10404	1498	0	0	0
1	CA	1503	32312	14381	5990	10438	1503	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	231	1846	1179	331	331	5	0	0	0
2	CB	231	1825	1167	326	327	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	1552	976	302	273	1	0	0	0
3	CC	206	1542	968	300	273	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	1659	1040	326	286	7	0	0	0
4	CD	208	1674	1050	333	284	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	148	1129	714	213	198	4	0	0	0
5	CE	148	1133	716	214	199	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AF	100	806	511	143	149	3	0	0	0
6	CF	100	816	516	146	151	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AG	155	1231	766	243	216	6	0	0	0
7	CG	155	1235	769	244	216	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	AH	137	1088	689	206	191	2	0	0	0
8	CH	137	1088	689	206	191	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	AI	127	983	623	193	167	0	0	0
9	CI	127	978	619	190	169	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	AJ	97	709	440	138	131	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	CJ	96	714	445	138	131	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	114	829	516	155	155	3	0	0	0
11	CK	114	833	519	156	155	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	122	930	585	185	159	1	0	0	0
12	CL	122	930	585	185	159	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	123	958	592	198	166	2	0	0	0
13	CM	122	950	586	197	165	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	728	456	144	126	2	0	0	0
15	CO	88	728	456	144	126	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	82	681	433	134	113	1	0	0	0
16	CP	82	677	430	133	113	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AQ	99	823	528	151	142	2	0	0	0
17	CQ	99	823	528	151	142	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AR	68	555	355	108	92	0	0	0
18	CR	68	555	355	108	92	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	83	652	417	120	113	2	0	0	0
19	CS	83	646	412	119	113	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AT	96	728	446	156	124	2	0	0	0
20	CT	96	727	446	155	124	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	AU	23	199	122	48	29	0	0	0
21	CU	23	199	122	48	29	0	0	0

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	13	277	125	51	88	13	0	0	0
22	CV	12	252	115	46	80	11	0	0	0

- Molecule 23 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
23	AW	74	1607	727	288	516	73	3	0	0	0
23	CW	72	1560	702	281	503	72	2	0	0	0

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
24	AX	76	1625	725	294	529	76	1	0	0	0
24	CX	76	1625	725	294	529	76	1	0	0	0

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
25	AY	74	1581	707	285	515	73	1	0	0	0
25	CY	73	1561	698	283	507	72	1	0	0	0

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	BA	2819	60729	27026	11370	19515	2818	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	DA	2800	60311	26840	11284	19388	2799	0	0	0

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	BB	120	2573	1146	476	832	119	0	0	0
27	DB	120	2573	1146	476	832	119	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BD	275	2136	1349	423	361	3	0	0	0
28	DD	275	2136	1349	423	361	3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BE	204	1559	985	298	270	6	0	0	0
29	DE	204	1559	985	298	270	6	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BF	203	1584	1009	298	275	2	0	0	1
30	DF	203	1580	1007	297	274	2	0	0	1

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BG	181	1425	914	256	251	4	0	0	0
31	DG	181	1424	911	258	251	4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BH	174	1330	845	248	236	1	0	0	0
32	DH	174	1330	845	248	236	1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BI	146	1085	693	189	202	1	0	0	0
33	DI	146	1061	680	186	194	1	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	BN	140	1117	719	207	187	4	0	0	0
34	DN	140	1117	719	207	187	4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	BP	149	1135	706	230	196	3	0	0	0
36	DP	149	1135	706	230	196	3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	BR	118	968	604	203	160	1	0	0	0
38	DR	118	968	604	203	160	1	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	BS	110	877	553	175	149	0	0	0
39	DS	110	870	549	173	148	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BT	131	1091	680	225	185	1	0	0	0
40	DT	131	1083	675	224	183	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BU	116	959	608	201	149	1	0	0	0
41	DU	116	959	608	201	149	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BV	101	771	495	140	135	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	DV	101	771	495	140	135	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BW	112	886	557	174	153	2	0	0	0
43	DW	112	886	557	174	153	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BX	95	750	488	135	126	1	0	0	0
44	DX	95	750	488	135	126	1	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BY	107	806	517	152	131	6	0	0	0
45	DY	107	806	517	152	131	6	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BZ	171	1349	862	243	242	2	0	0	0
46	DZ	174	1360	870	243	245	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	B0	83	653	404	139	109	1	0	0	0
47	D0	83	653	404	139	109	1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	B1	97	755	475	148	131	1	0	0	0
48	D1	97	755	475	148	131	1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	B2	70	588	365	118	103	2	0	0	0
49	D2	70	588	365	118	103	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	B3	59	469	298	90	81	0	0	0
50	D3	59	464	296	90	78	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	B4	69	558	352	102	99	5	0	0	0
51	D4	69	532	339	97	91	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B5	59	455	285	89	76	5	0	0	0
52	D5	59	455	285	89	76	5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	B6	53	453	281	91	77	4	0	0	0
53	D6	53	449	279	91	75	4	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	B7	48	418	257	104	55	2	0	0	0
54	D7	48	418	257	104	55	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B8	64	511	328	99	82	2	0	0	0
55	D8	64	517	331	102	82	2	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	B9	37	307	188	68	47	4	0	0	0
56	D9	37	307	188	68	47	4	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	AA	214	214	214	0	0
57	AE	3	3	3	0	0
57	AF	1	1	1	0	0
57	AK	1	1	1	0	0
57	AM	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	AN	2	2	2	0	0
57	AW	4	4	4	0	0
57	AX	15	15	15	0	0
57	AY	3	3	3	0	0
57	BA	812	812	812	0	0
57	BB	20	20	20	0	0
57	BD	9	9	9	0	0
57	BE	8	8	8	0	0
57	BF	9	9	9	0	0
57	BG	3	3	3	0	0
57	BN	6	6	6	0	0
57	BO	2	2	2	0	0
57	BP	5	5	5	0	0
57	BQ	5	5	5	0	0
57	BR	2	2	2	0	0
57	BU	8	8	8	0	0
57	BV	5	5	5	0	0
57	BW	4	4	4	0	0
57	BX	3	3	3	0	0
57	BY	1	1	1	0	0
57	BZ	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	B0	3	3	3	0	0
57	B1	1	1	1	0	0
57	B2	1	1	1	0	0
57	B3	2	2	2	0	0
57	B4	1	1	1	0	0
57	B5	1	1	1	0	0
57	B6	2	2	2	0	0
57	B7	5	5	5	0	0
57	B8	1	1	1	0	0
57	B9	1	1	1	0	0
57	CA	170	170	170	0	0
57	CD	1	1	1	0	0
57	CE	1	1	1	0	0
57	CF	1	1	1	0	0
57	CJ	1	1	1	0	0
57	CK	1	1	1	0	0
57	CT	1	1	1	0	0
57	CV	1	1	1	0	0
57	CW	1	1	1	0	0
57	CX	3	3	3	0	0
57	DA	677	677	677	0	0

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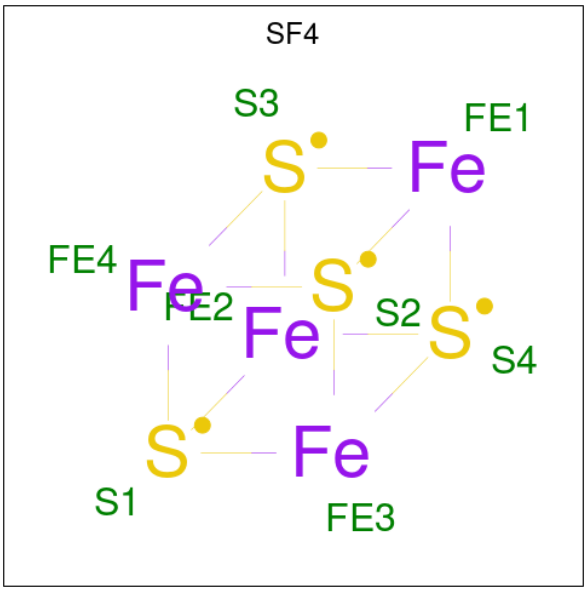
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	DB	13	13	13	0	0
57	DD	9	9	9	0	0
57	DE	4	4	4	0	0
57	DF	4	4	4	0	0
57	DG	1	1	1	0	0
57	DN	1	1	1	0	0
57	DO	1	1	1	0	0
57	DP	2	2	2	0	0
57	DQ	4	4	4	0	0
57	DR	1	1	1	0	0
57	DU	2	2	2	0	0
57	DV	3	3	3	0	0
57	DW	4	4	4	0	0
57	DX	1	1	1	0	0
57	DY	1	1	1	0	0
57	D0	1	1	1	0	0
57	D3	1	1	1	0	0
57	D8	1	1	1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AD	1	Total Fe S 8 4 4	0	0
58	CD	1	Total Fe S 8 4 4	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AN	1	Total Zn 1 1	0	0
59	BY	1	Total Zn 1 1	0	0
59	B4	1	Total Zn 1 1	0	0
59	B5	1	Total Zn 1 1	0	0
59	B6	1	Total Zn 1 1	0	0
59	B9	1	Total Zn 1 1	0	0
59	CN	1	Total Zn 1 1	0	0
59	DY	1	Total Zn 1 1	0	0
59	D4	1	Total Zn 1 1	0	0
59	D5	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	D6	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AX	1	Total K 1 1	0	0
60	CX	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	227	Total O 227 227	0	0
61	AE	2	Total O 2 2	0	0
61	AJ	1	Total O 1 1	0	0
61	AL	1	Total O 1 1	0	0
61	AM	1	Total O 1 1	0	0
61	AU	1	Total O 1 1	0	0
61	AV	3	Total O 3 3	0	0
61	AW	3	Total O 3 3	0	0
61	AX	6	Total O 6 6	0	0
61	AY	1	Total O 1 1	0	0
61	BA	1383	Total O 1383 1383	0	0
61	BB	36	Total O 36 36	0	0
61	BD	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BE	14	Total O 14 14	0	0
61	BF	8	Total O 8 8	0	0
61	BG	3	Total O 3 3	0	0
61	BI	1	Total O 1 1	0	0
61	BO	4	Total O 4 4	0	0
61	BP	16	Total O 16 16	0	0
61	BQ	4	Total O 4 4	0	0
61	BR	2	Total O 2 2	0	0
61	BT	2	Total O 2 2	0	0
61	BU	3	Total O 3 3	0	0
61	BV	2	Total O 2 2	0	0
61	BW	1	Total O 1 1	0	0
61	BX	4	Total O 4 4	0	0
61	BZ	1	Total O 1 1	0	0
61	B0	3	Total O 3 3	0	0
61	B1	1	Total O 1 1	0	0
61	B3	2	Total O 2 2	0	0
61	B5	2	Total O 2 2	0	0
61	B6	1	Total O 1 1	0	0
61	B7	2	Total O 2 2	0	0
61	B8	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	CA	185	Total O 185 185	0	0
61	CJ	2	Total O 2 2	0	0
61	CL	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CV	1	Total O 1 1	0	0
61	CW	2	Total O 2 2	0	0
61	DA	1025	Total O 1025 1025	0	0
61	DB	9	Total O 9 9	0	0
61	DD	19	Total O 19 19	0	0
61	DE	11	Total O 11 11	0	0
61	DF	3	Total O 3 3	0	0
61	DN	2	Total O 2 2	0	0
61	DO	1	Total O 1 1	0	0
61	DP	16	Total O 16 16	0	0
61	DR	1	Total O 1 1	0	0
61	DT	3	Total O 3 3	0	0
61	DU	2	Total O 2 2	0	0
61	DX	3	Total O 3 3	0	0
61	DY	2	Total O 2 2	0	0
61	D0	3	Total O 3 3	0	0
61	D1	1	Total O 1 1	0	0

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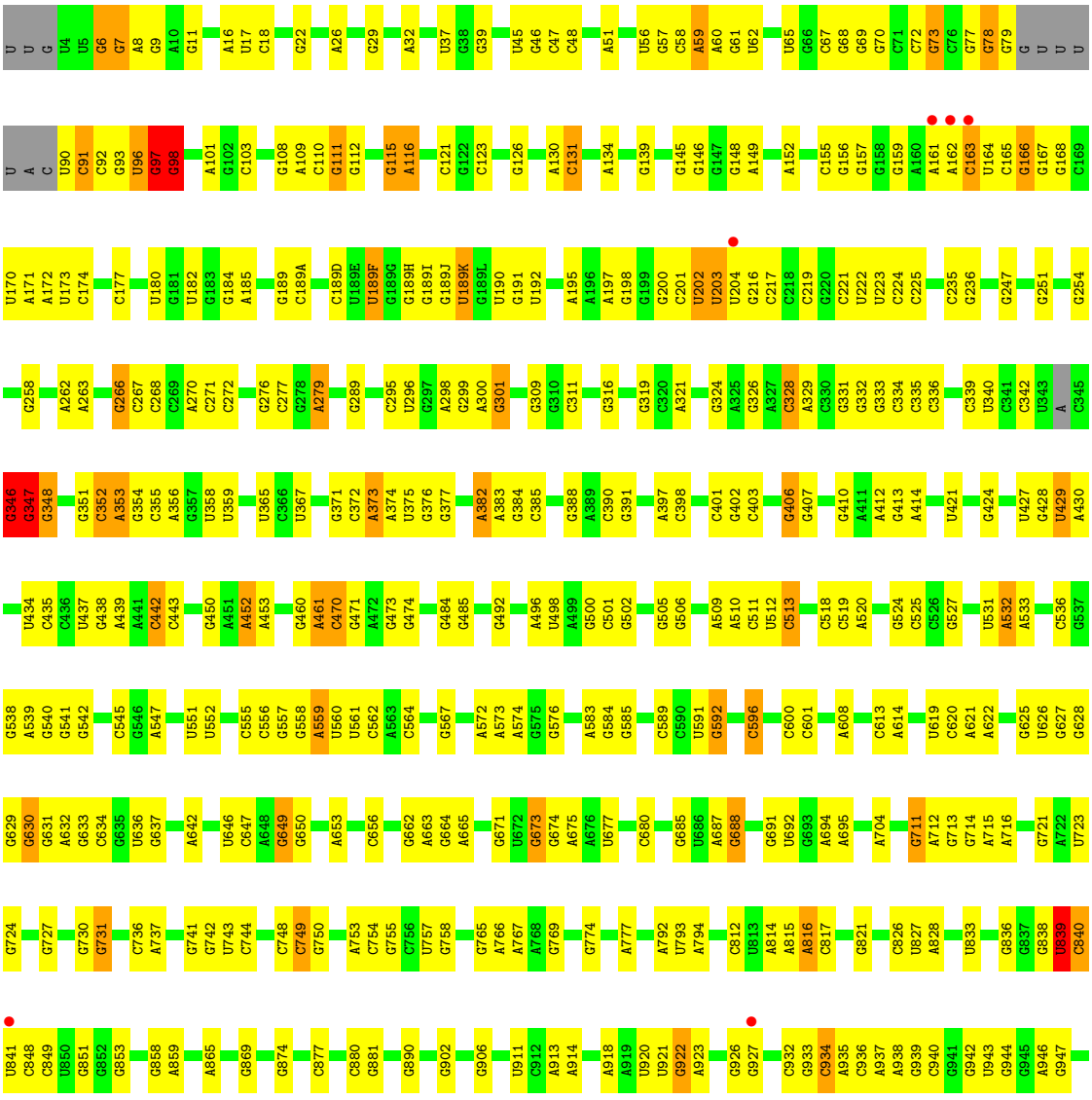
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	D3	1	Total O 1 1	0	0
61	D7	3	Total O 3 3	0	0
61	D8	4	Total O 4 4	0	0

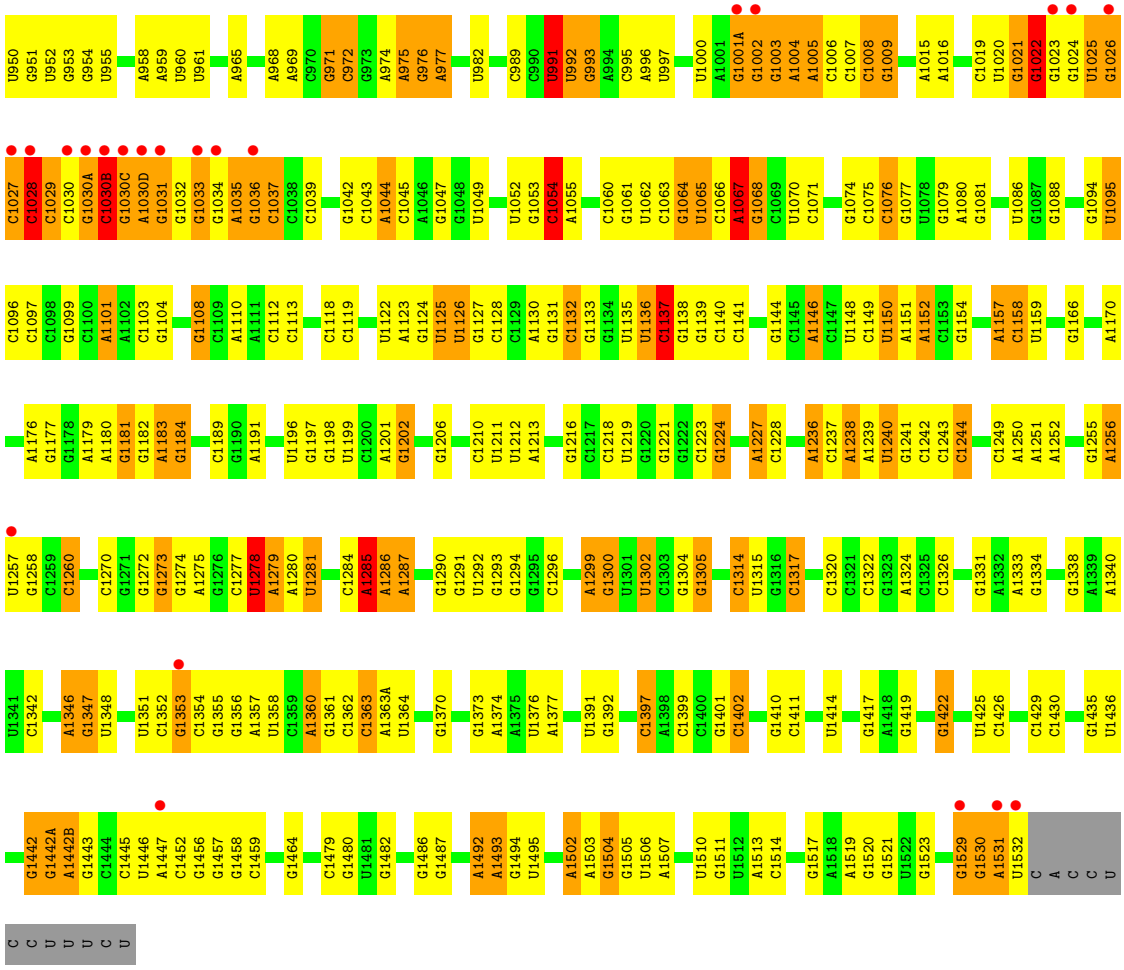
3 Residue-property plots (i)

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

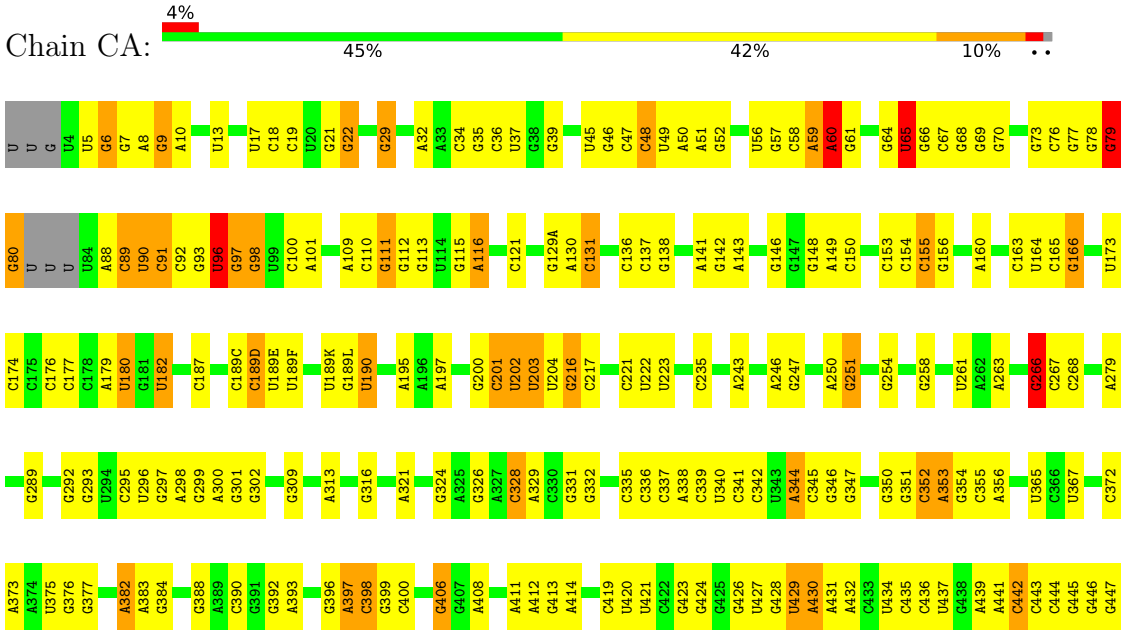
Chain AA: 2% 52% 37% 9%

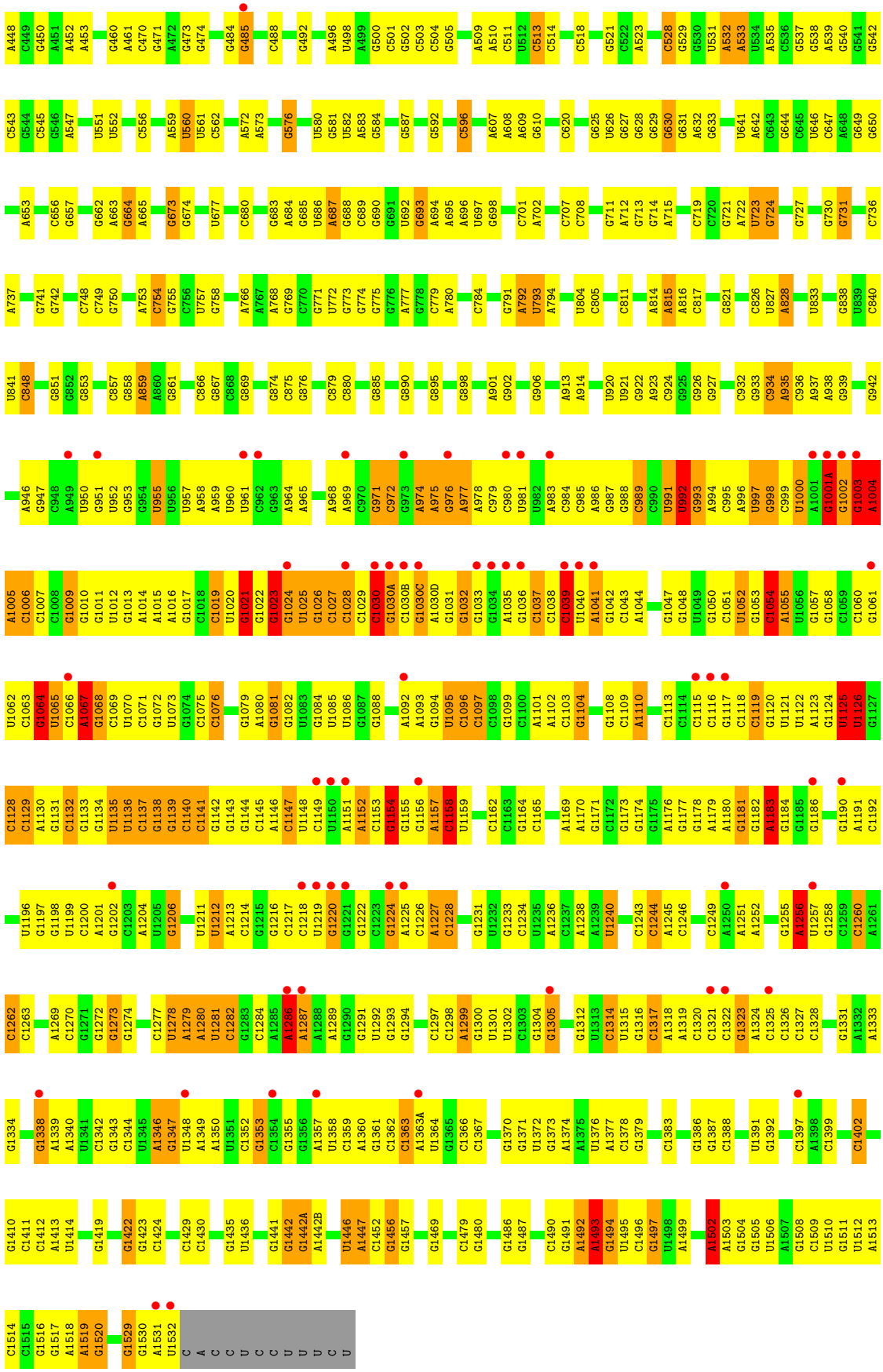




• Molecule 1: 16S Ribosomal RNA

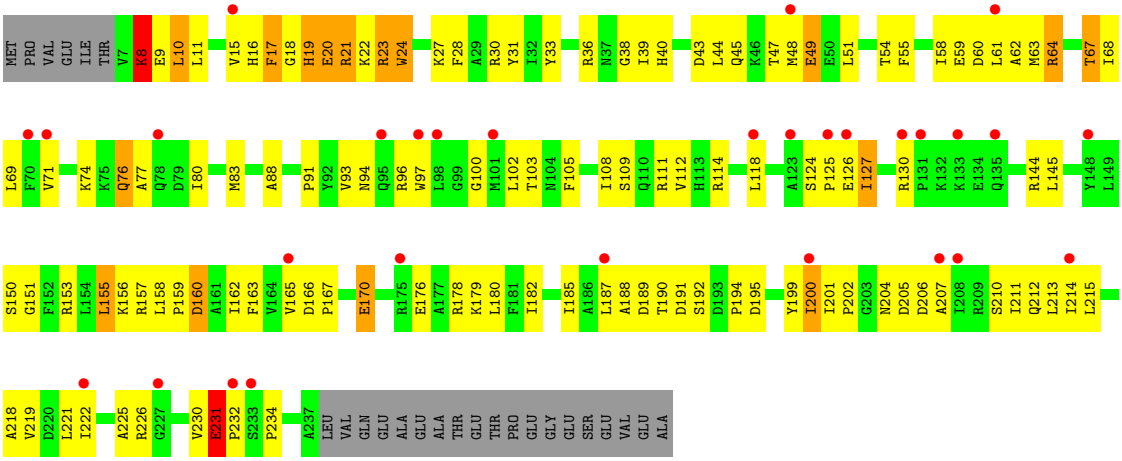
Chain CA:




A448 C449 G450 A451 A452 A453 G460 A461 C470 G471 A472 G473 G474 G484 G485 C488 G492 A496 U498 A499 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 C514 C518 G521 C522 A523 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542
C543 G544 C545 G546 A547 U551 U552 C556 A559 U560 U561 C562 A572 A573 G576 U580 G581 U582 A583 G584 G587 G592 C596 A607 A608 A609 G610 C620 G625 U626 G627 G628 G629 G630 G631 A632 G633 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650
A653 C656 G657 G662 A663 G664 A665 G673 G674 U677 C680 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C701 A702 C707 C708 G711 A712 G713 G714 A715 C719 C720 G721 A722 U723 G724 G727 G730 G731 C736
A737 G741 G742 C748 C749 G750 A753 C754 G755 C756 U757 G758 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 C784 G791 A792 U793 A794 U804 C805 C811 A814 A815 A816 C817 G821 C826 U827 A828 U833 G838 U839 C840
U841 C848 G851 G852 G853 C857 G858 A859 A860 G861 C866 G867 C868 G869 G874 C875 G876 C879 C880 G885 G890 G895 G898 A901 G902 G906 A913 A914 U920 U921 G922 A923 C924 G925 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 G942
A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004
A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061
U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1087 G1088 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 C1108 C1109 A1110 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127
C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 G1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 C1162 C1163 G1164 C1165 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1190 A1191 C1192
U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 U1211 U1212 A1213 C1214 C1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 C1243 C1244 A1245 C1246 C1249 A1250 A1251 A1252 G1255 A1256 U1257 G1258 C1259 C1260 A1261
C1262 C1263 A1269 C1270 G1271 G1272 G1273 G1274 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 C1297 C1298 A1299 G1300 U1301 U1302 G1303 G1304 G1305 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 G1331 A1332 A1333
G1334 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 U1355 G1356 A1357 U1358 C1359 A1360 U1361 C1362 C1363 A1363A U1364 G1365 C1366 C1367 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 C1383 G1386 G1387 C1388 U1391 G1392 C1397 A1398 C1399 C1402
G1410 C1411 C1412 A1413 U1414 G1419 G1422 G1423 C1424 C1429 C1430 G1435 U1436 G1441 G1442 G1442A A1442B U1446 A1447 C1452 G1456 G1457 G1469 C1479 G1480 G1486 G1487 C1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1502 A1503 G1504 G1505 U1506 A1507 G1508 C1509 U1510 G1511 U1512 A1513
C1514 C1515 G1516 G1517 A1518 A1519 G1520 G1529 G1530 A1531 U1532 C A C C U C C U U U C U

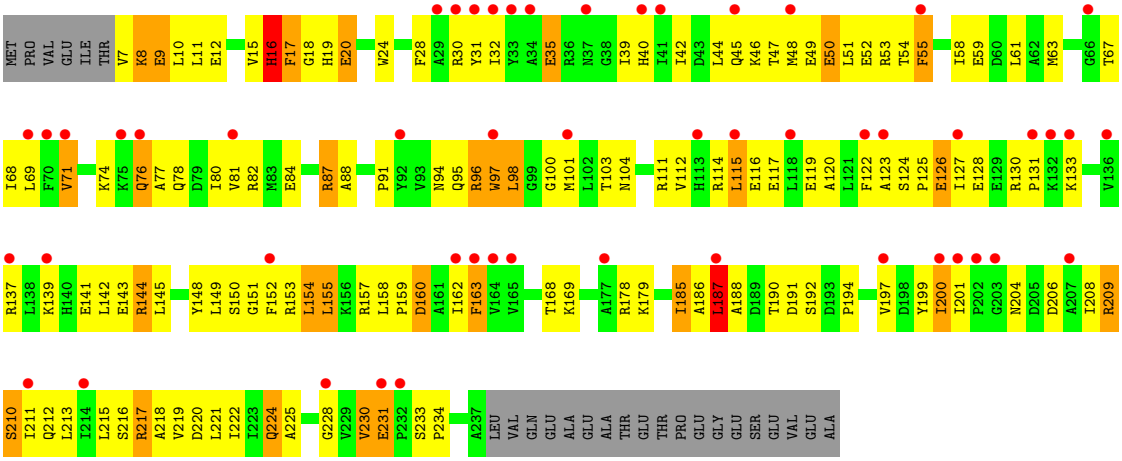
• Molecule 2: 30S ribosomal protein S2

Chain AB:



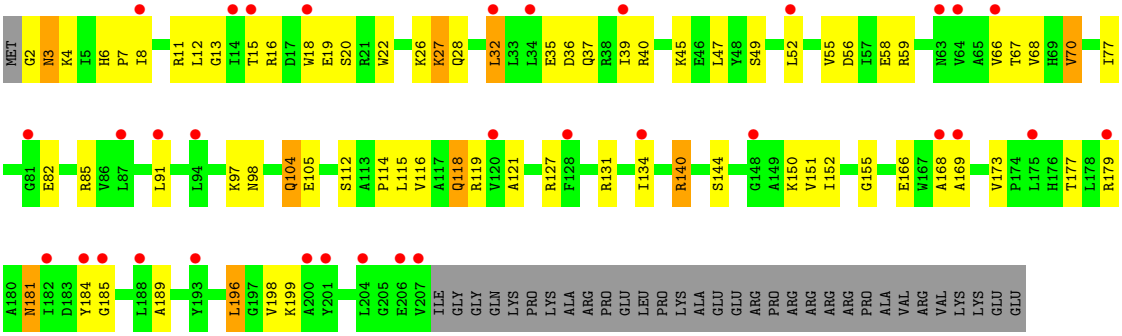
• Molecule 2: 30S ribosomal protein S2

Chain CB:



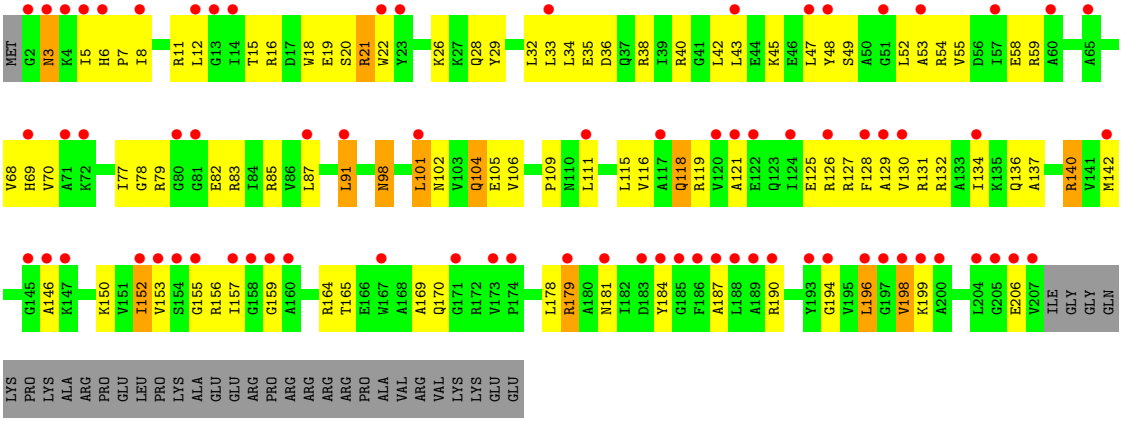
• Molecule 3: 30S ribosomal protein S3

Chain AC:



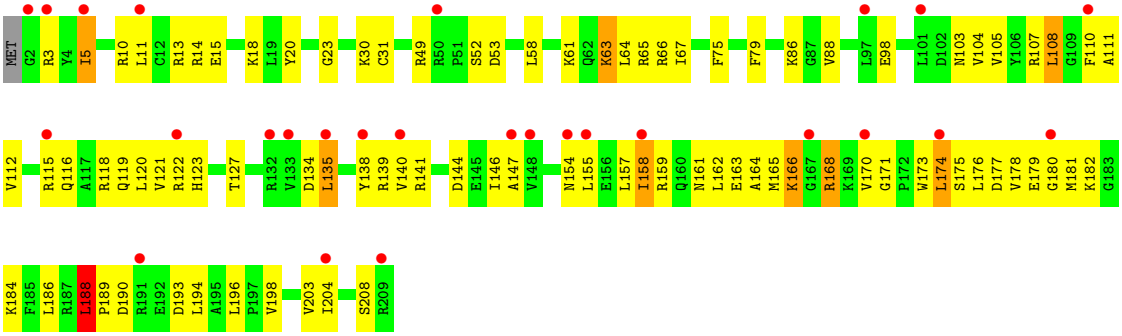
- Molecule 3: 30S ribosomal protein S3

Chain CC:



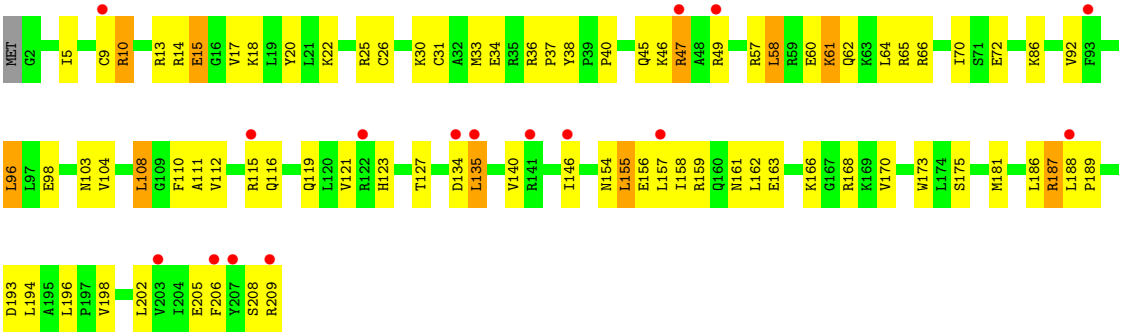
- Molecule 4: 30S ribosomal protein S4

Chain AD:



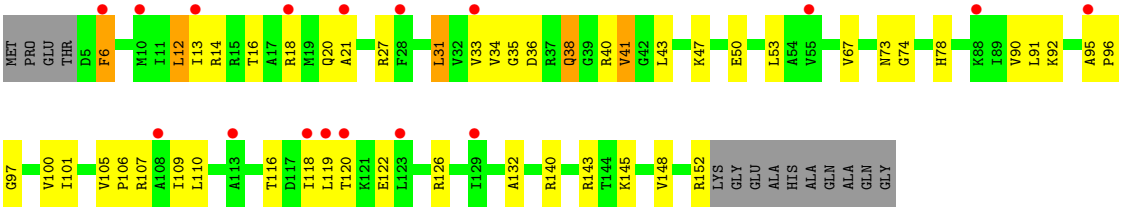
- Molecule 4: 30S ribosomal protein S4

Chain CD:



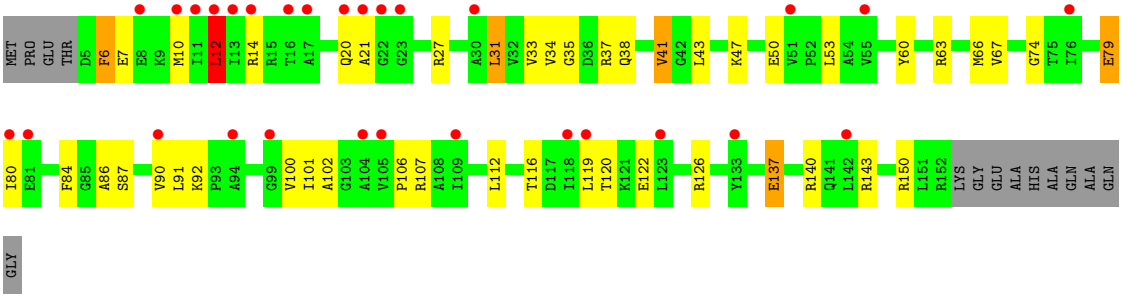
- Molecule 5: 30S ribosomal protein S5

Chain AE:



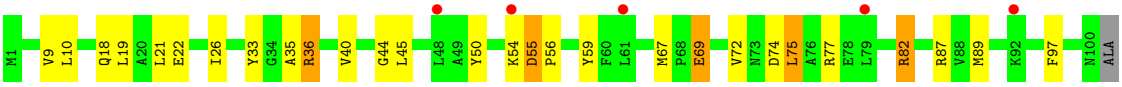
• Molecule 5: 30S ribosomal protein S5

Chain CE:



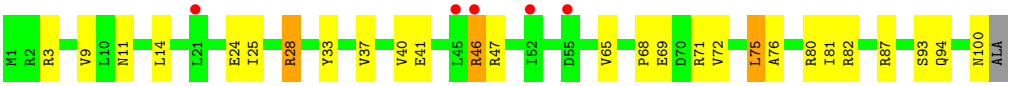
• Molecule 6: 30S ribosomal protein S6

Chain AF:



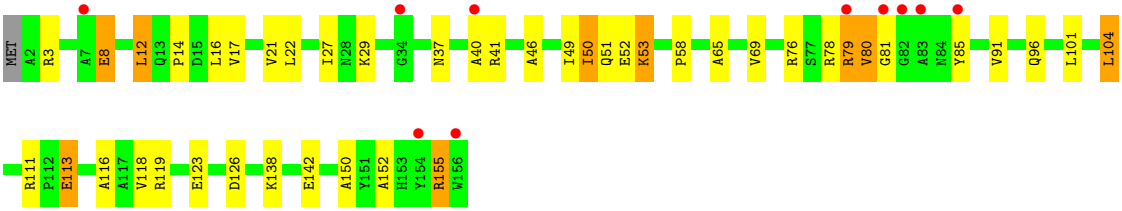
• Molecule 6: 30S ribosomal protein S6

Chain CF:



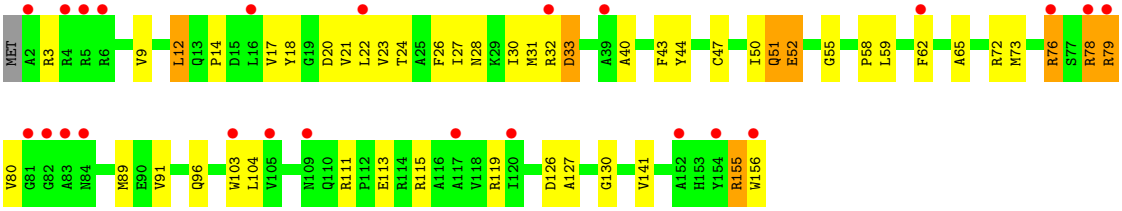
• Molecule 7: 30S ribosomal protein S7

Chain AG:



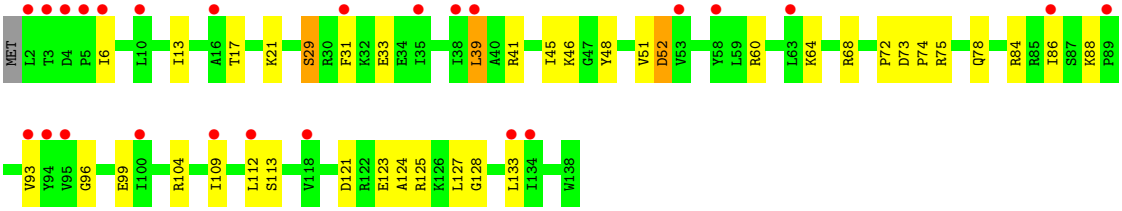
• Molecule 7: 30S ribosomal protein S7

Chain CG:



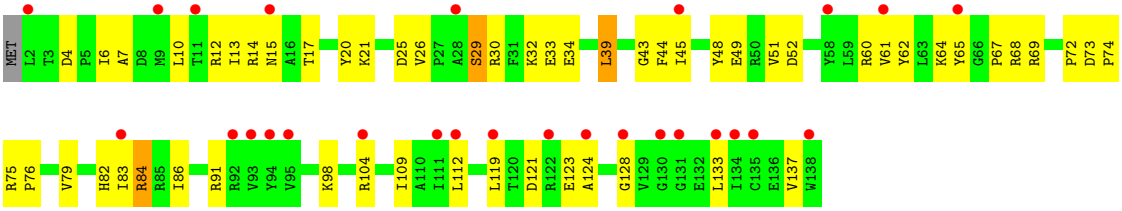
- Molecule 8: 30S ribosomal protein S8

Chain AH:



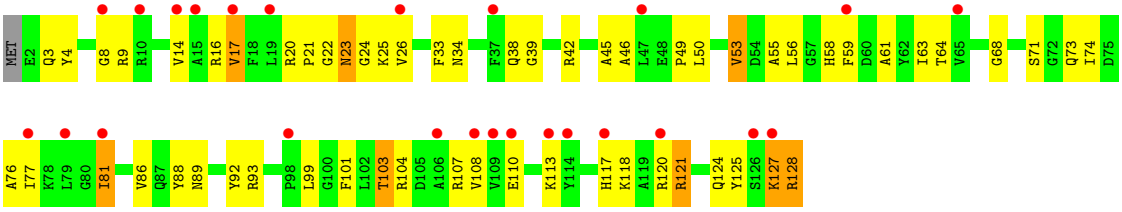
- Molecule 8: 30S ribosomal protein S8

Chain CH:



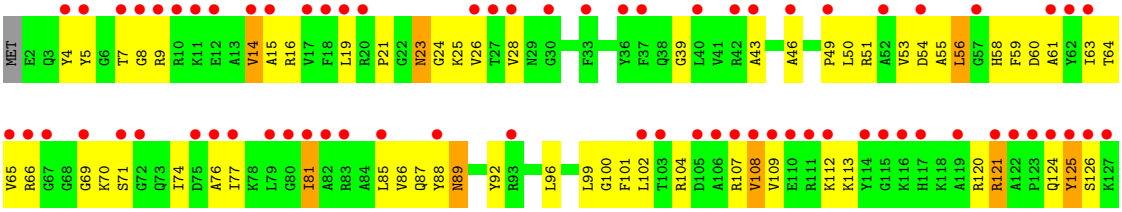
- Molecule 9: 30S ribosomal protein S9

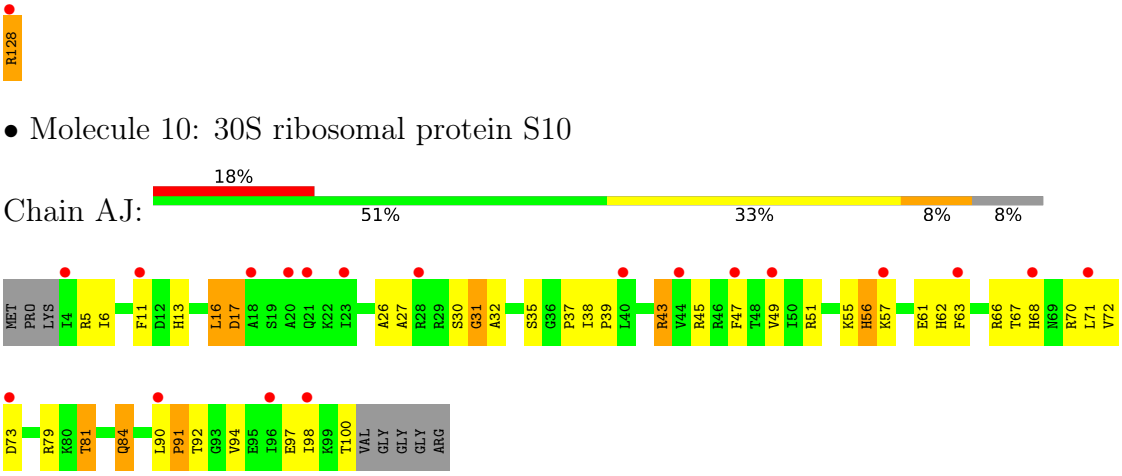
Chain AI:

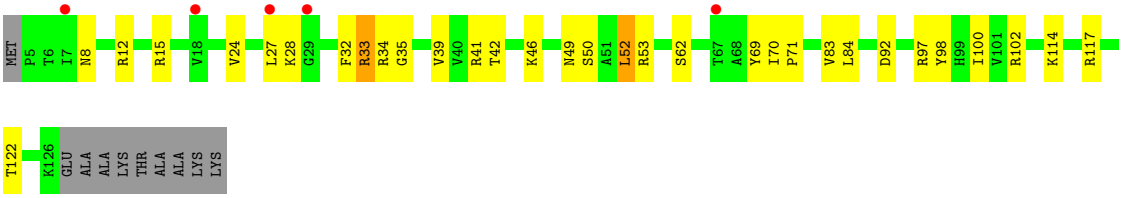


- Molecule 9: 30S ribosomal protein S9

Chain CI:

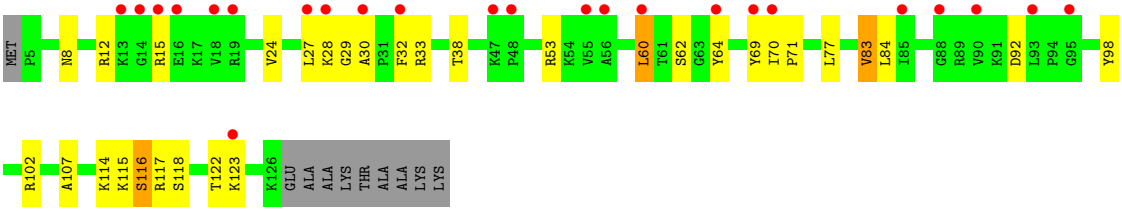



R128
• Molecule 10: 30S ribosomal protein S10
Chain AJ:
18%
51%
33%
8%
8%
MET PRO LYS I4 R5 I6 F11 D12 H13 L16 D17 A18 S19 A20 Q21 K22 I23 A26 A27 R28 R29 S30 G31 A32 S35 G36 P37 I38 P39 L40 R43 V44 R45 R46 F47 T48 V49 I50 R51 K55 H56 K57 E61 H62 F63 R66 T67 H68 N69 R70 L71 V72
D73 R79 K80 T81 Q84 L90 P91 T92 G93 V94 E95 T96 E97 I98 K99 T100 VAL GLY GLY GLY ARG
• Molecule 10: 30S ribosomal protein S10
Chain CJ:
33%
49%
36%
7%
9%
MET PRO LYS ILE R5 I6 K7 L8 R9 G10 H13 L16 D17 A18 S19 I23 A26 A27 R28 R29 S30 G31 A32 Q33 V34 S35 G36 P37 I38 P39 L40 P41 T42 R43 V44 R45 R46 F47 T48 V49 I50 R51 G52 P53 F54 K55 H56 K57 D58 S59 R60 E61 H62 F63 E64 L65
R66 T67 H68 N69 R70 L71 V72 D73 I74 P77 N78 R79 K80 T81 L85 L88 D89 L90 P91 T92 G93 V94 I98 K99 T100 VAL GLY GLY GLY ARG
• Molecule 11: 30S ribosomal protein S11
Chain AK:
6%
59%
28%
12%
MET ALA LYS LYS PRO SER LYS LYS LYS VAL LYS ARG Q13 V14 A15 S16 G17 R18 Y25 N26 I29 Y30 T31 I32 T33 D34 N38 P39 I40 T41 W42 S43 S44 G45 G46 V47 I48 G49 Y50 Y59 Q62 L63 L66 M73 A74 Y75 G76 S79 V80 D81 V82 I83
V84 T87 G88 A89 G90 R91 R96 A97 L98 Q99 A100 S101 G102 L103 Q104 V105 K106 S107 D111 N117 K123 R126 LYS ALA SER
• Molecule 11: 30S ribosomal protein S11
Chain CK:
6%
70%
16%
12%
MET ALA LYS LYS PRO SER LYS LYS LYS VAL LYS ARG Q13 Y20 S24 Y25 T31 D34 N38 P39 I40 G45 G46 V47 I48 G49 Y50 K51 R54 A68 D81 A89 Q93 R96 A97 L98 S101 Q104 V105 K106 D110 V114 P115
F125 R126 LYS ALA SER
• Molecule 12: 30S ribosomal protein S12
Chain AL:
4%
68%
23%
8%



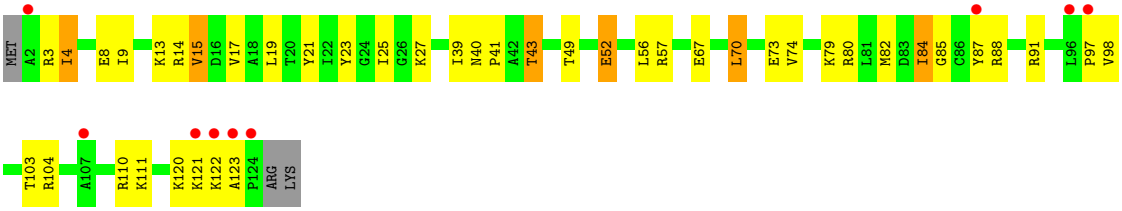
• Molecule 12: 30S ribosomal protein S12

Chain CL:



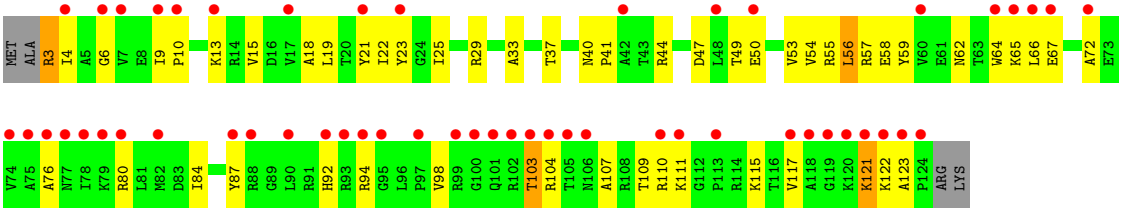
• Molecule 13: 30S ribosomal protein S13

Chain AM:



• Molecule 13: 30S ribosomal protein S13

Chain CM:

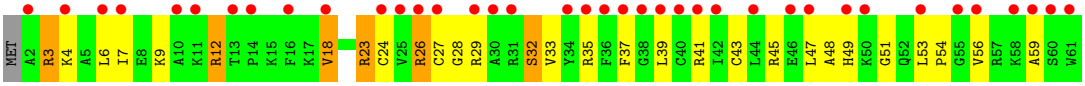


• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:

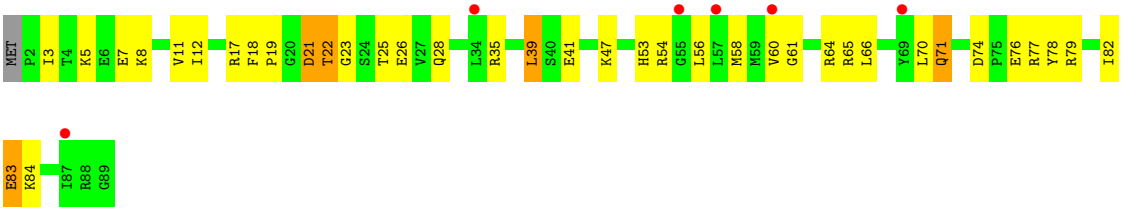
• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



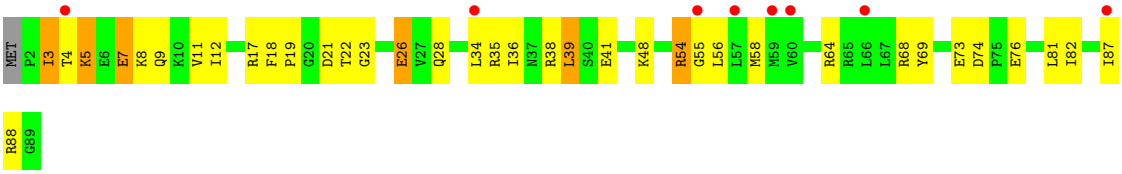
• Molecule 15: 30S ribosomal protein S15

Chain AO:



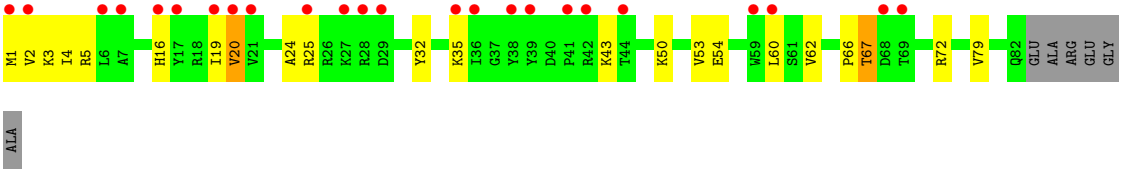
• Molecule 15: 30S ribosomal protein S15

Chain CO:



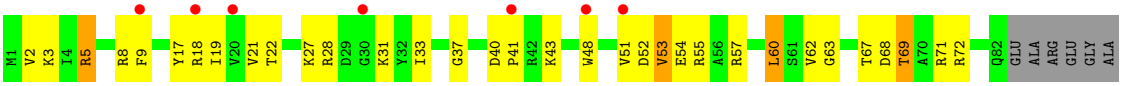
• Molecule 16: 30S ribosomal protein S16

Chain AP:



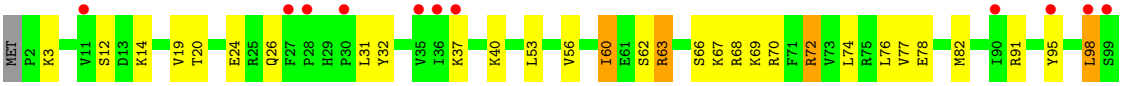
• Molecule 16: 30S ribosomal protein S16

Chain CP:



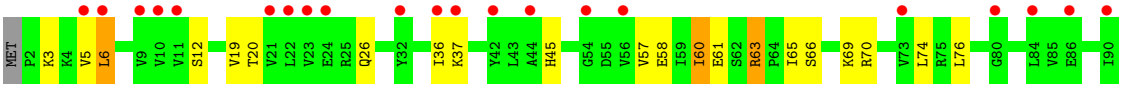
• Molecule 17: 30S ribosomal protein S17

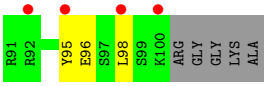
Chain AQ:



• Molecule 17: 30S ribosomal protein S17

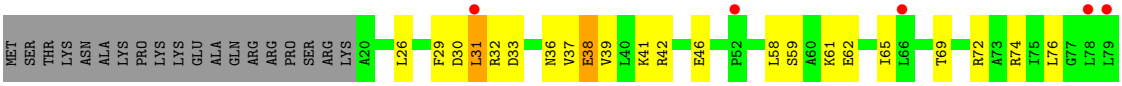
Chain CQ:





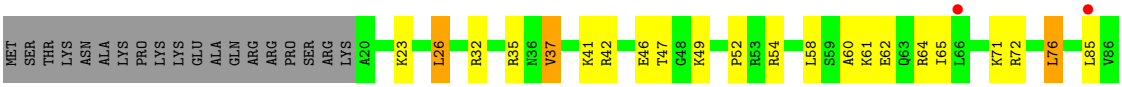
• Molecule 18: 30S ribosomal protein S18

Chain AR:



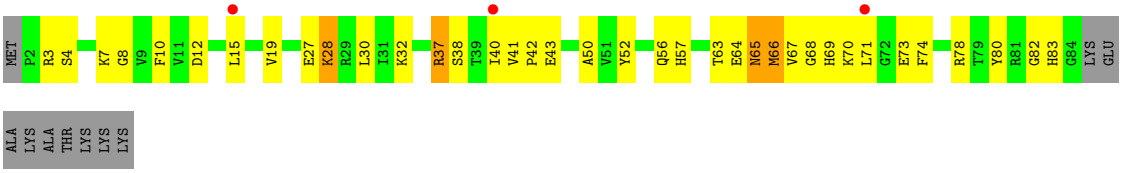
• Molecule 18: 30S ribosomal protein S18

Chain CR:



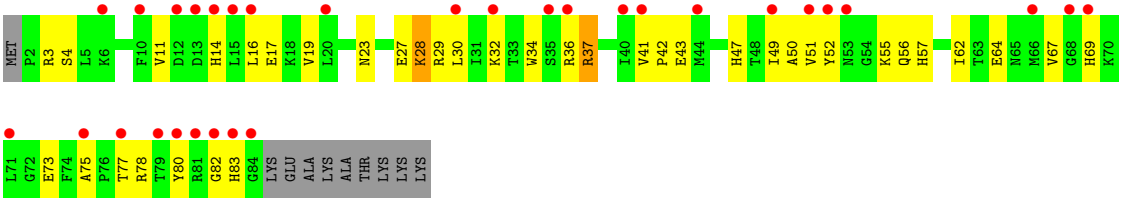
• Molecule 19: 30S ribosomal protein S19

Chain AS:



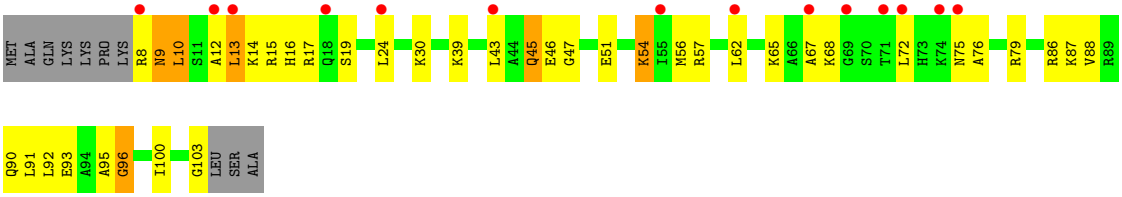
• Molecule 19: 30S ribosomal protein S19

Chain CS:



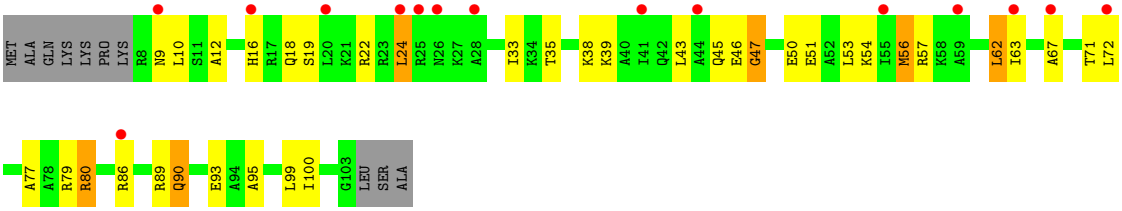
- Molecule 20: 30S ribosomal protein S20

Chain AT:



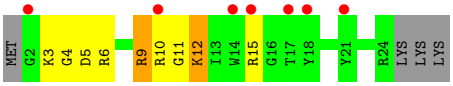
- Molecule 20: 30S ribosomal protein S20

Chain CT:



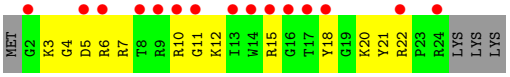
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



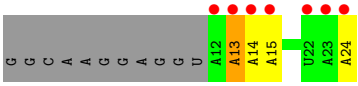
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



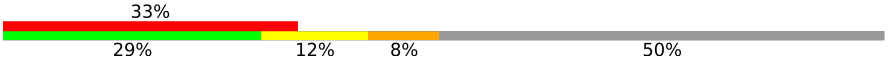
- Molecule 22: mRNA

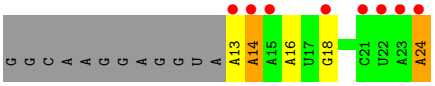
Chain AV:



• Molecule 22: mRNA

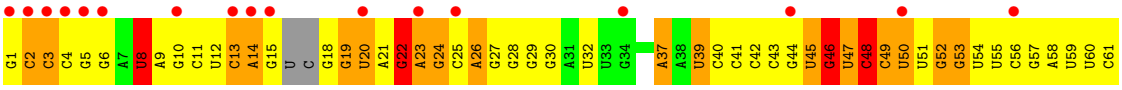
Chain CV:

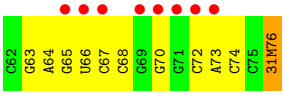




• Molecule 23: A-site tRNA

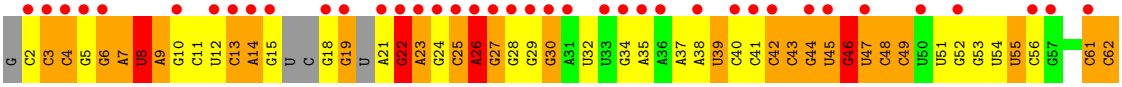
Chain AW:

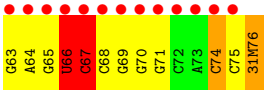




• Molecule 23: A-site tRNA

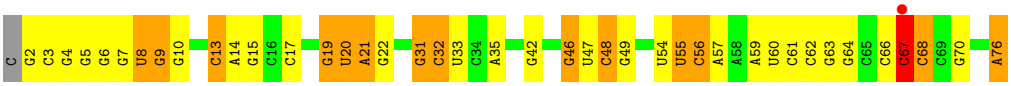
Chain CW:





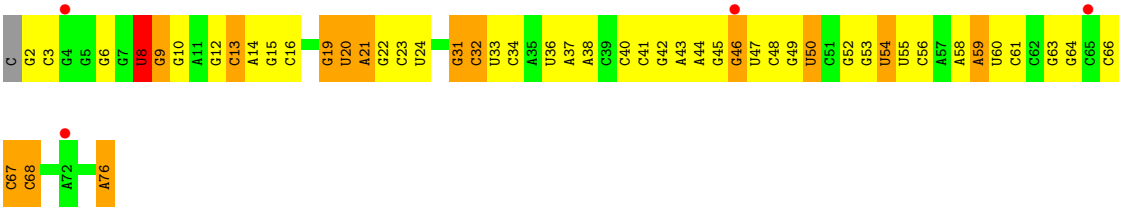
• Molecule 24: P-site tRNA

Chain AX:



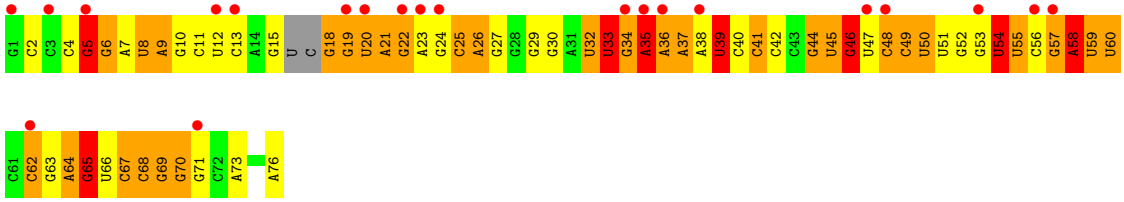
• Molecule 24: P-site tRNA

Chain CX:



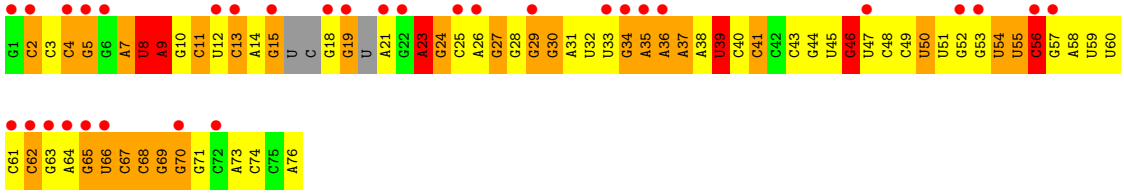
• Molecule 25: E-site tRNA

Chain AY:



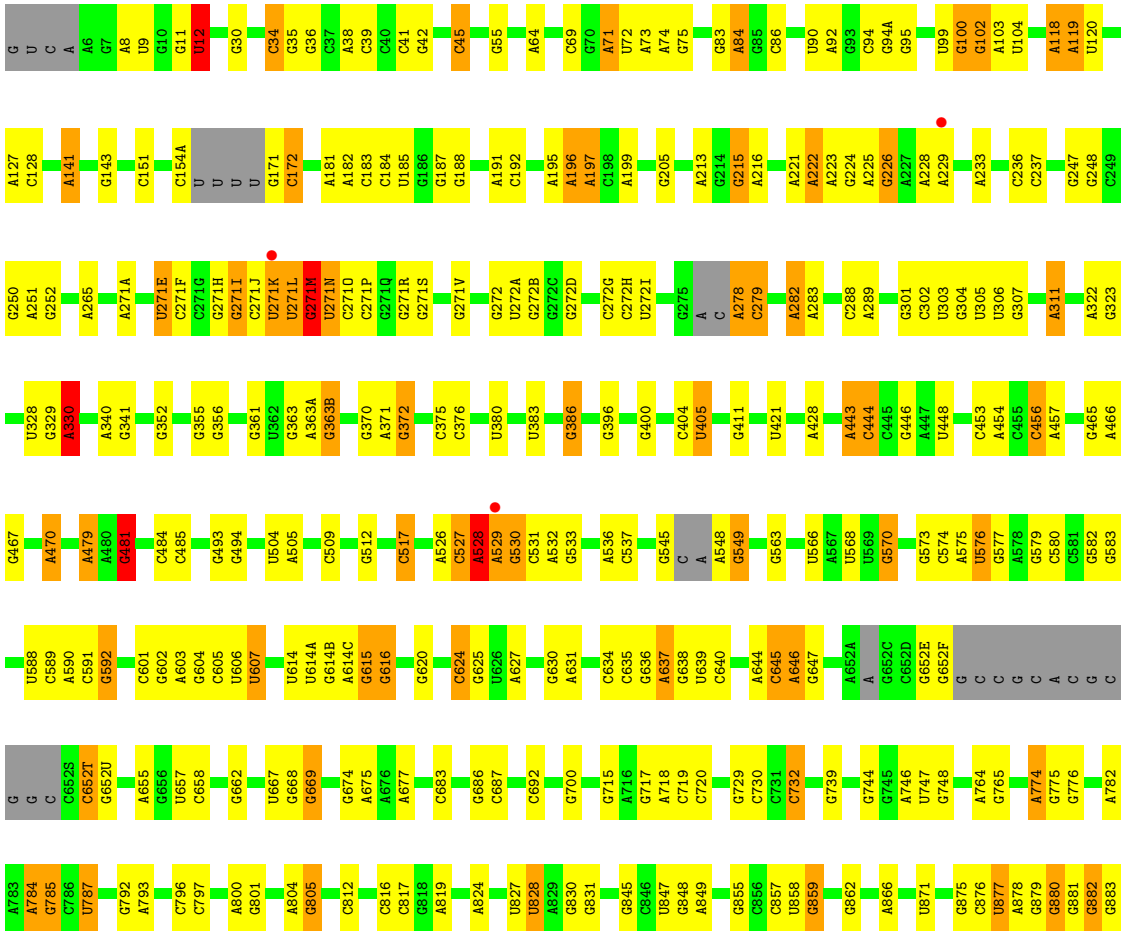
• Molecule 25: E-site tRNA

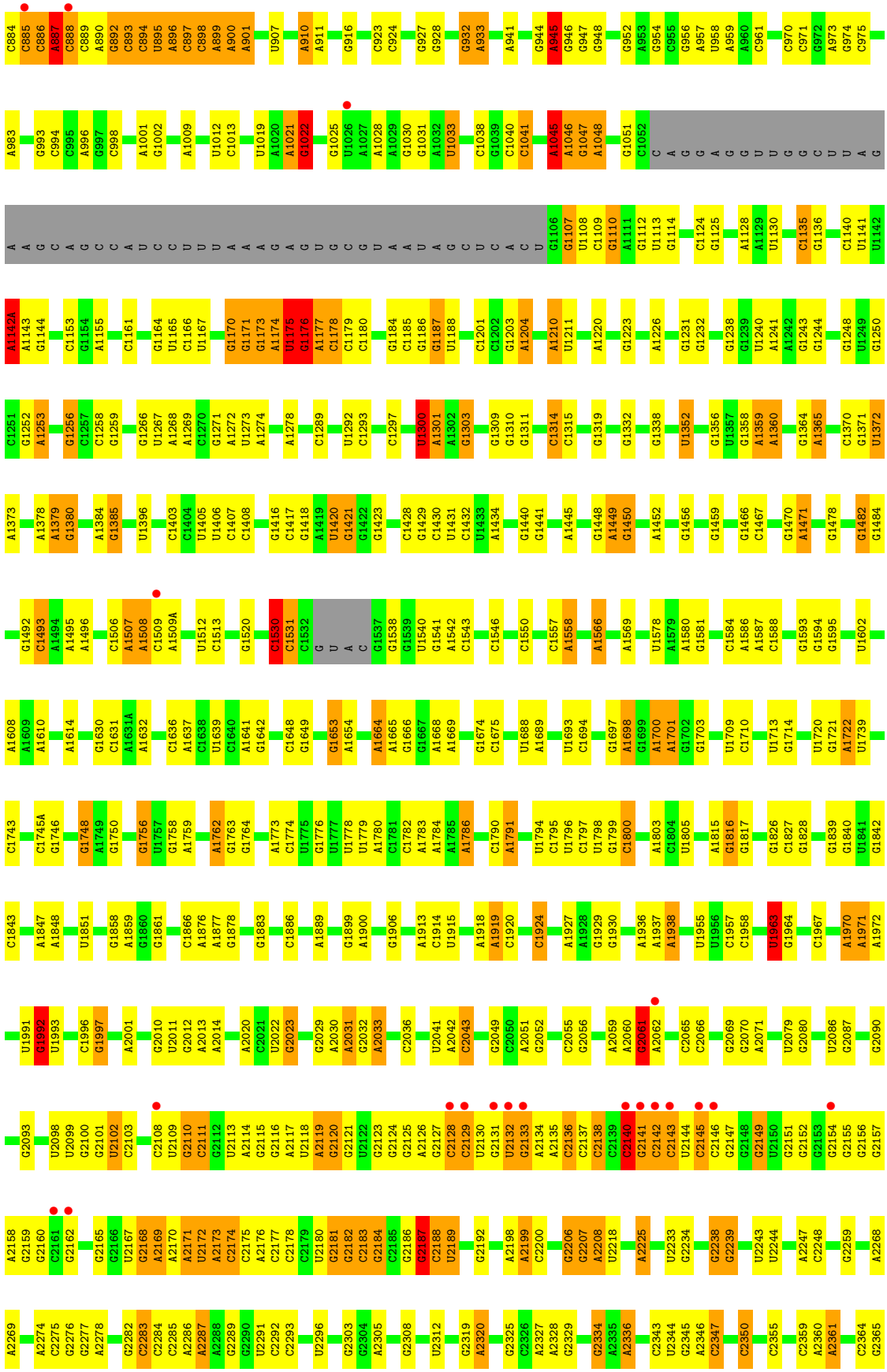
Chain CY:



• Molecule 26: 23S Ribosomal RNA

Chain BA:




C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 U907 A910 A911 G916 C923 C924 G927 G928 G932 A933 A941 G944 A945 G946 G947 G948 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 C970 C971 G972 A973 G974 C975
A983 G993 C994 G995 A996 G997 C998 A1001 G1002 A1009 U1012 C1013 U1019 A1020 A1021 G1022 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 C1038 G1039 C1040 C1041 A1045 A1046 G1047 A1048 G1051 C1052 C A G C A C A U C C U U U A A A G A G U G C G U A A U A G C U C A C U G G C U U A G
A A G C A G C C A U C C U U U A A A G A G U G C G U A A U A G C U C A C U G G C U U A G
A1142A A1143 G1144 C1153 G1154 A1155 C1161 G1164 U1165 C1166 U1167 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1184 C1185 G1186 G1187 U1188 C1201 C1202 G1203 A1204 A1210 U1211 A1220 G1223 A1226 G1231 G1232 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1248 U1249 G1250
C1251 G1252 A1253 G1256 C1257 C1258 G1259 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1278 C1289 U1292 C1293 C1297 U1300 A1301 A1302 G1303 G1309 G1310 G1311 C1314 C1315 G1319 G1332 G1338 U1352 G1356 U1357 G1358 A1359 A1360 G1364 A1365 C1370 G1371 U1372
A1373 A1378 A1379 G1380 A1384 G1385 U1396 C1403 C1404 U1405 U1406 C1407 C1408 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1440 G1441 A1445 G1448 A1449 G1450 A1452 G1456 G1459 G1466 C1467 G1470 A1471 G1478 G1482 G1484
G1492 C1493 A1494 A1495 A1496 C1506 A1507 A1508 C1509 A1509A U1512 C1513 G1520 C1530 C1531 C1532 G U A C G1537 G1538 G1539 U1540 G1541 A1542 C1543 C1546 C1550 C1557 A1558 A1566 A1569 U1578 A1579 A1580 G1581 C1584 A1586 A1587 C1588 G1593 G1594 G1595 U1602
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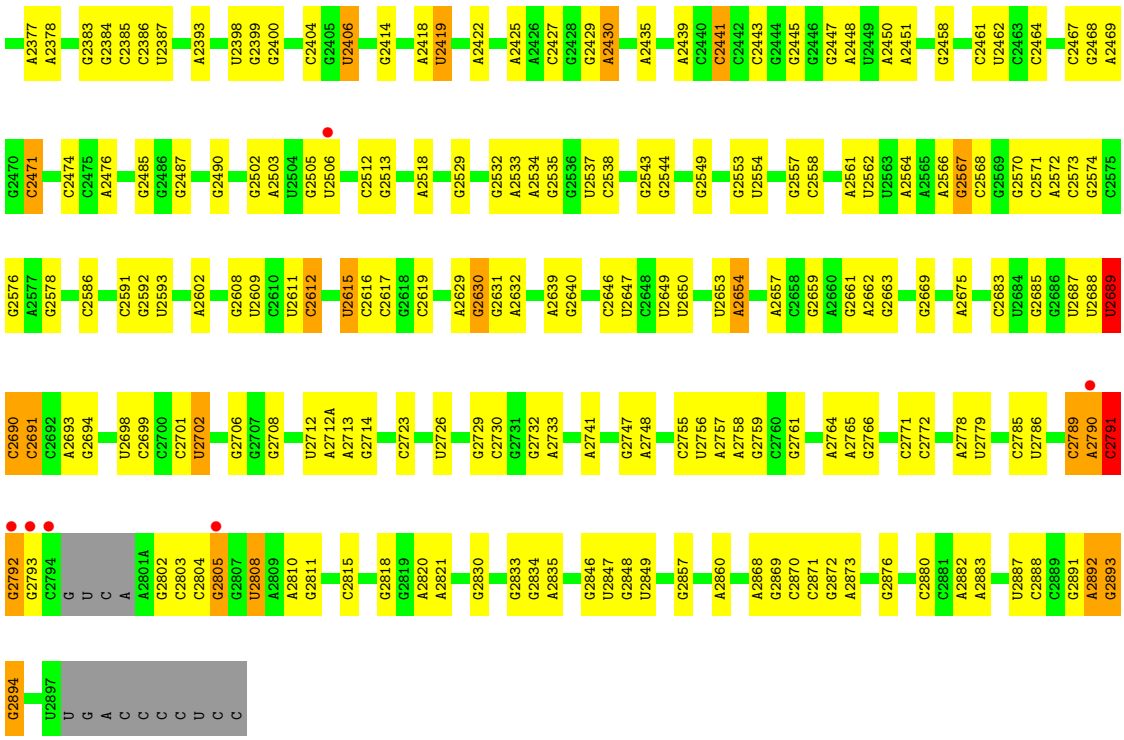
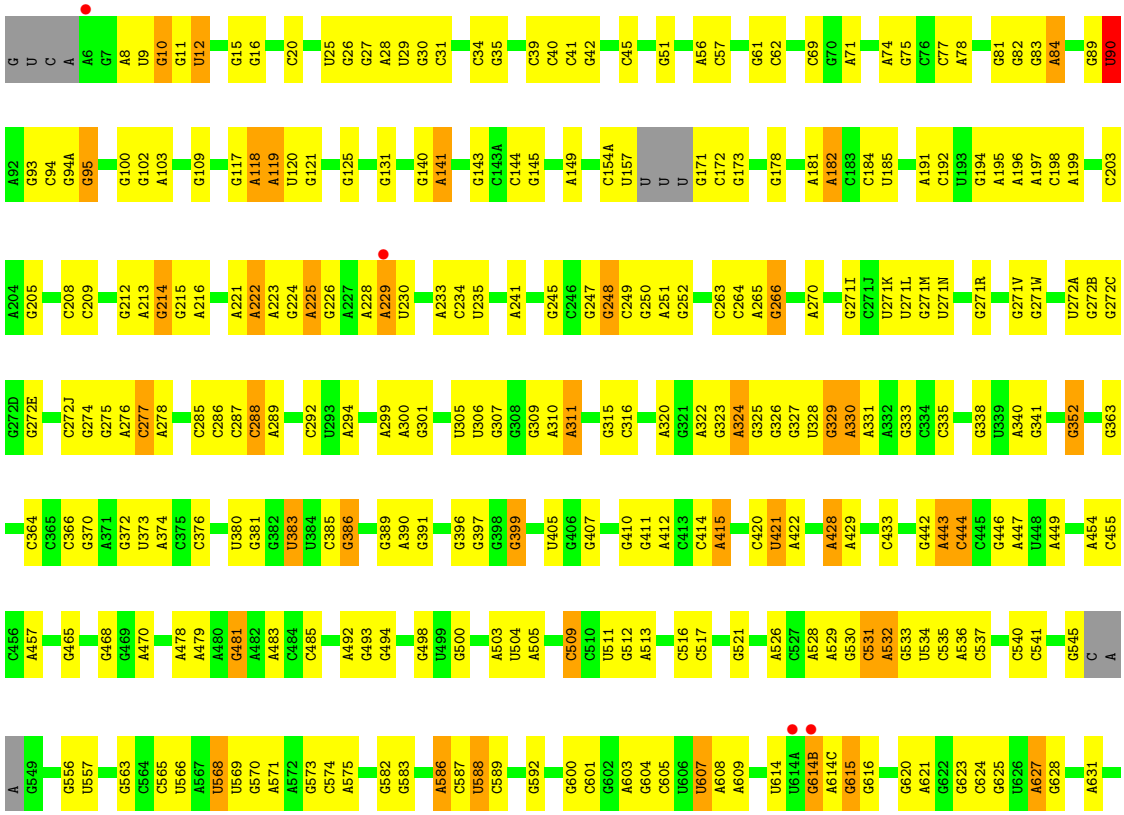
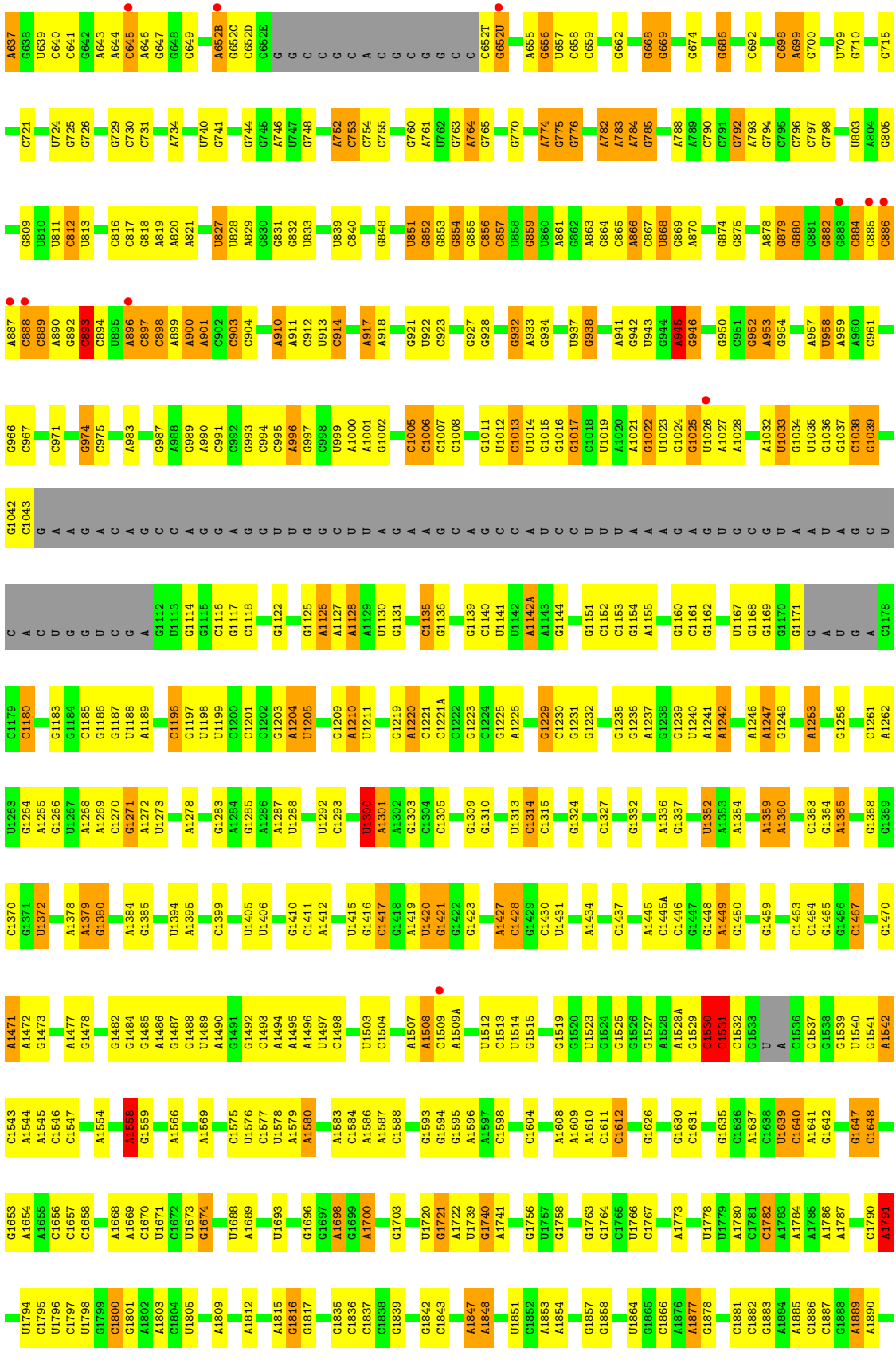


• Molecule 26: 23S Ribosomal RNA

Chain DA:

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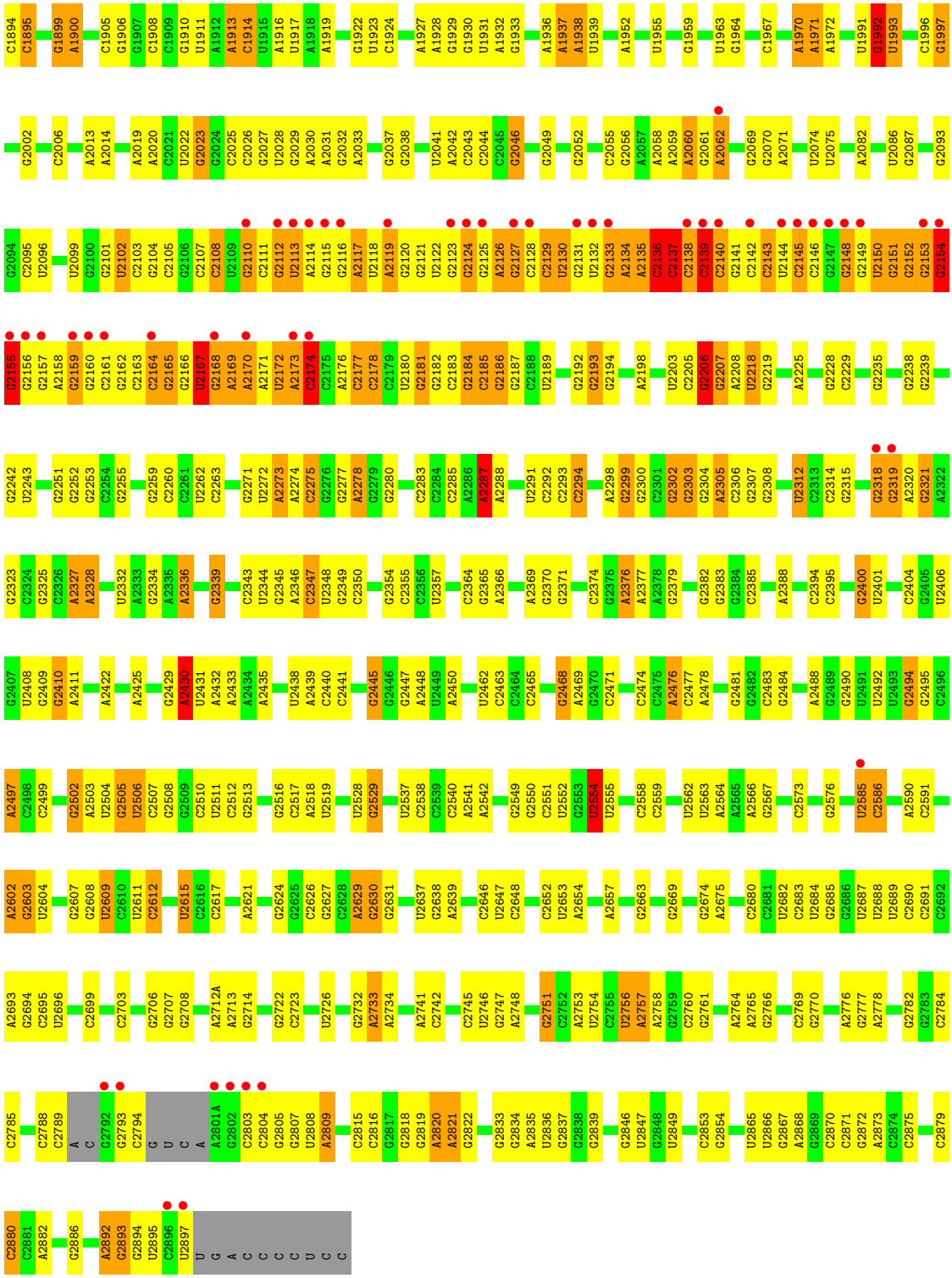
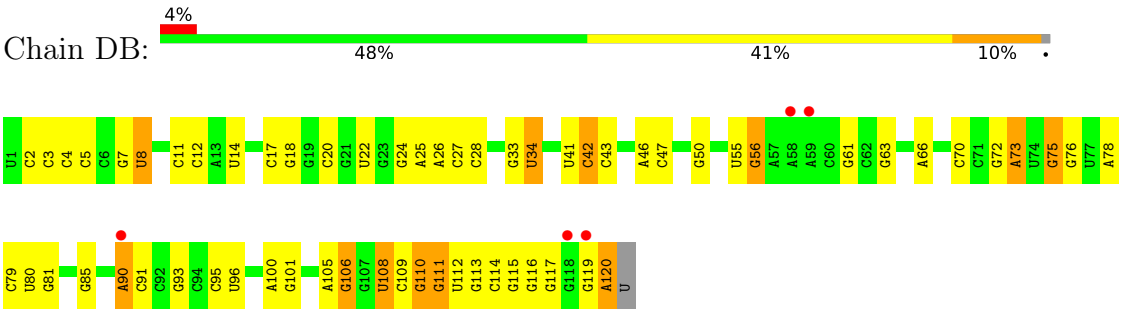


- Molecule 27: 5S Ribosomal RNA

Chain BB:

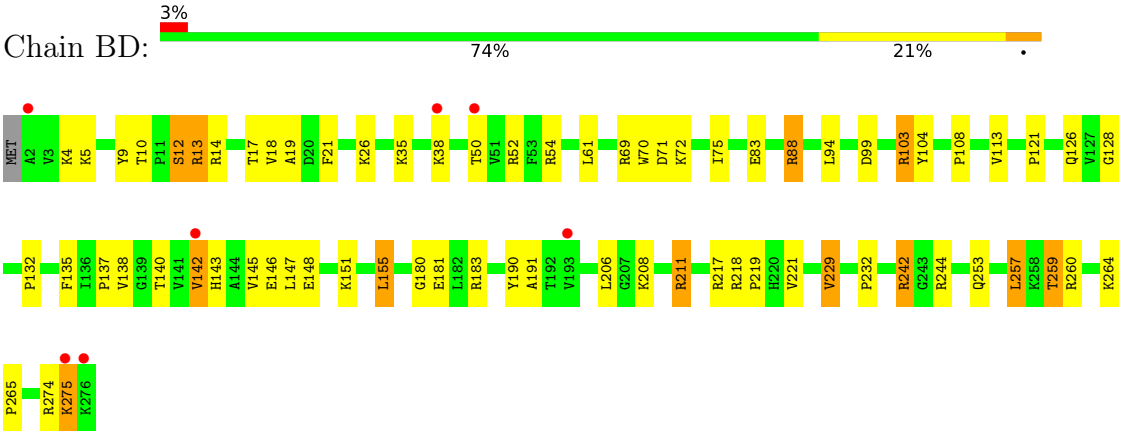
- Molecule 27: 5S Ribosomal RNA

Chain DB:



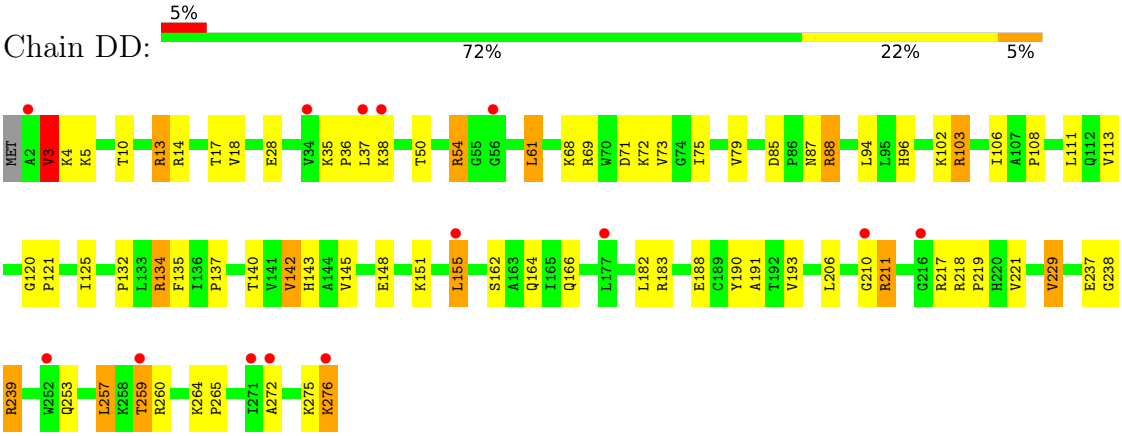
- Molecule 28: 50S ribosomal protein L2

Chain BD:



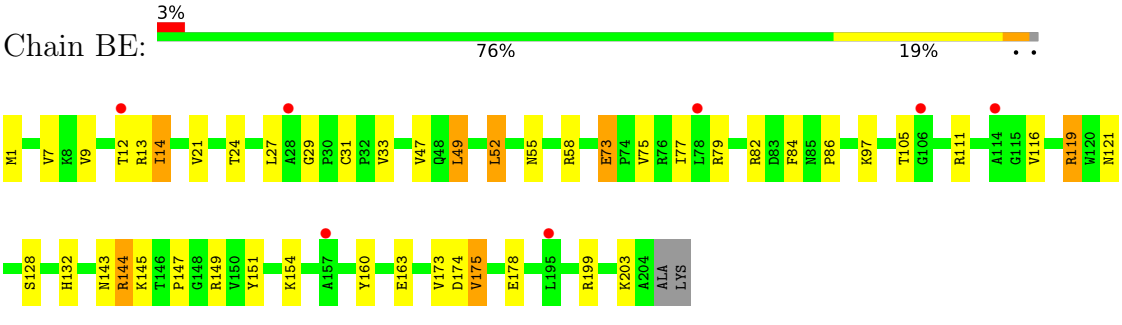
- Molecule 28: 50S ribosomal protein L2

Chain DD:



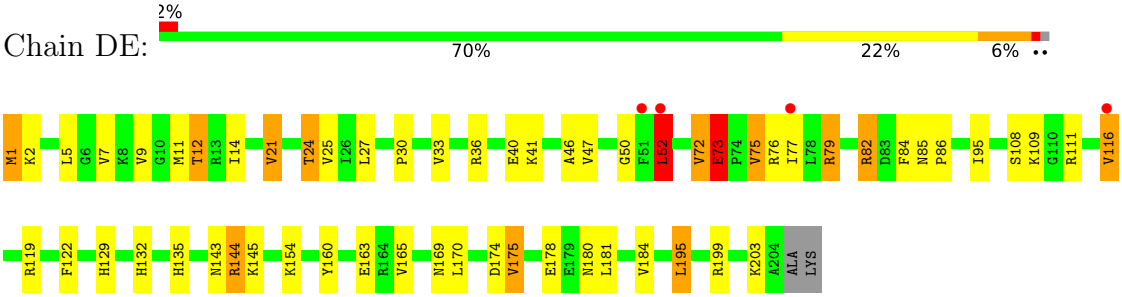
- Molecule 29: 50S ribosomal protein L3

Chain BE:



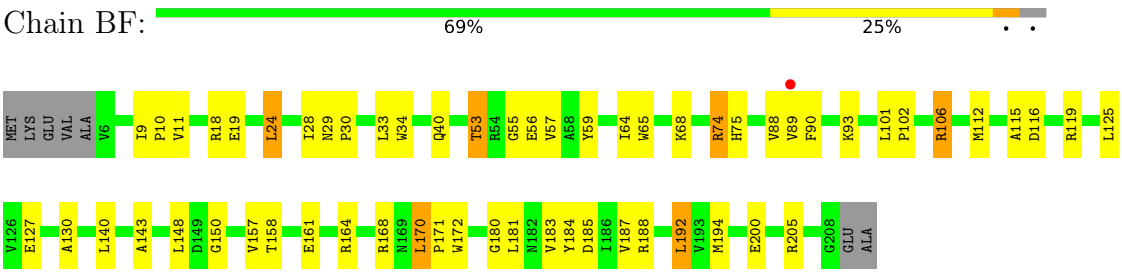
• Molecule 29: 50S ribosomal protein L3

Chain DE:



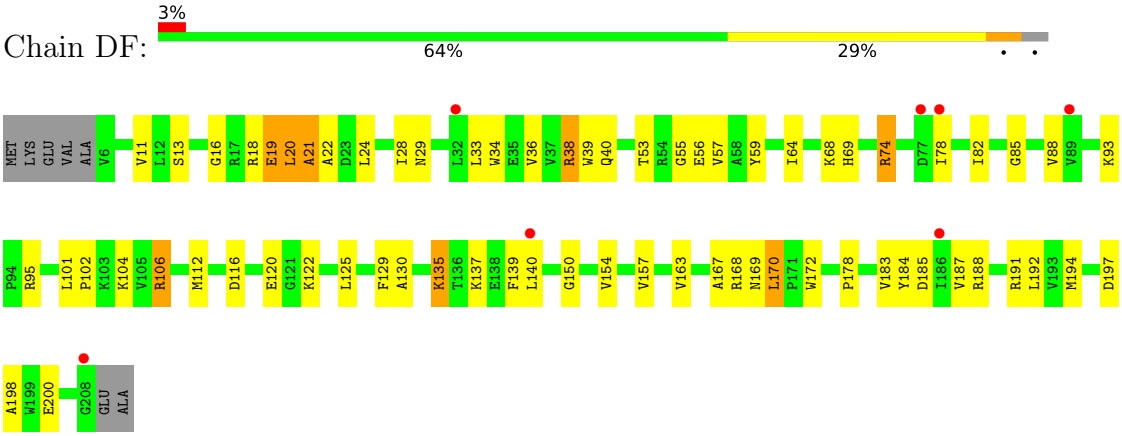
• Molecule 30: 50S ribosomal protein L4

Chain BF:



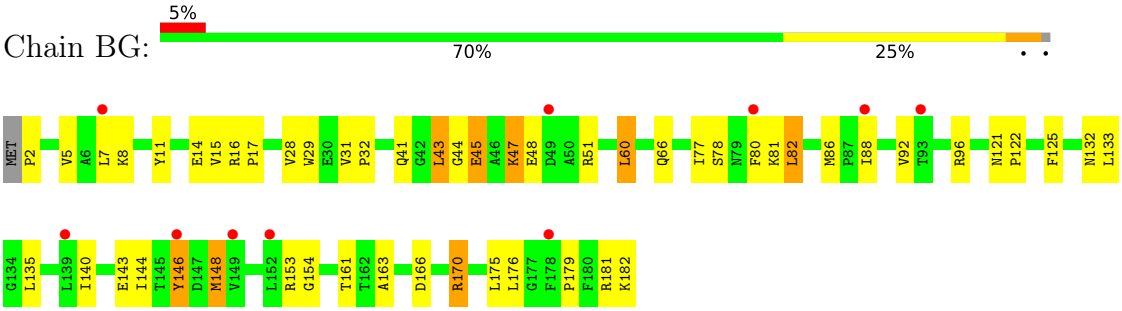
• Molecule 30: 50S ribosomal protein L4

Chain DF:



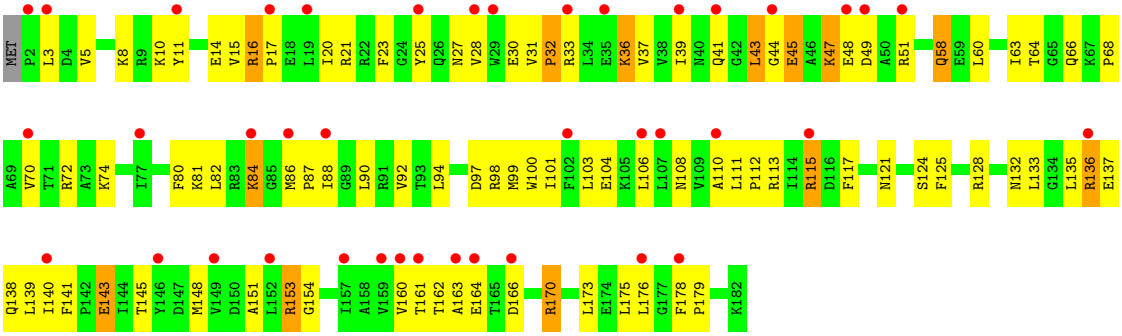
• Molecule 31: 50S ribosomal protein L5

Chain BG:



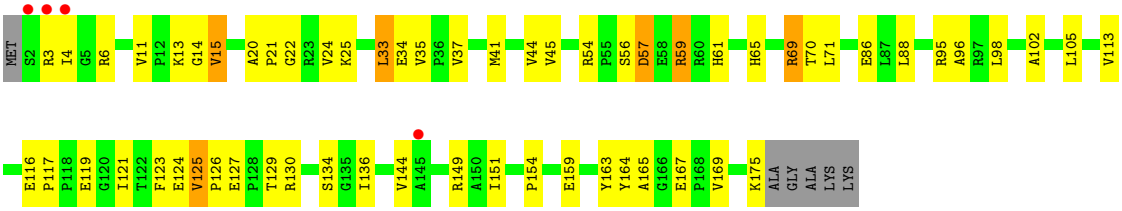
• Molecule 31: 50S ribosomal protein L5

Chain DG:



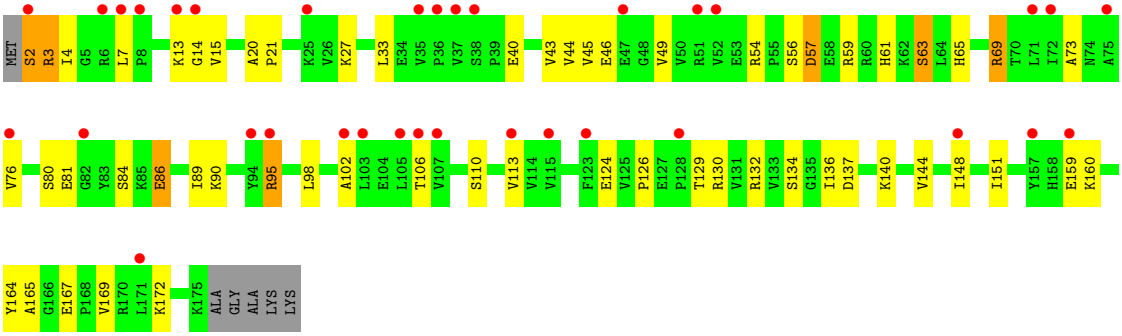
• Molecule 32: 50S ribosomal protein L6

Chain BH:



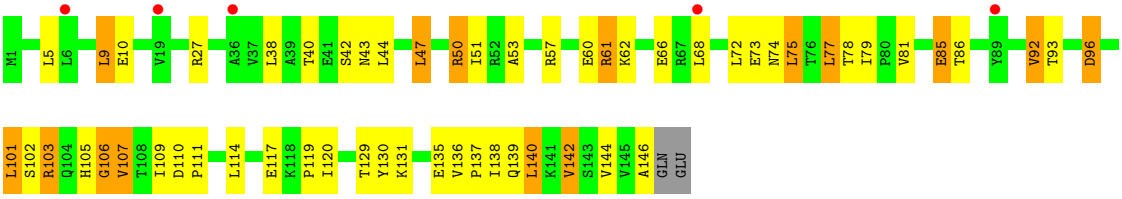
• Molecule 32: 50S ribosomal protein L6

Chain DH:



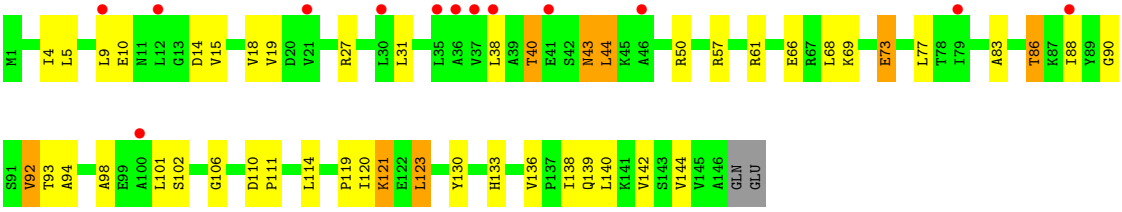
• Molecule 33: 50S ribosomal protein L9

Chain BI:



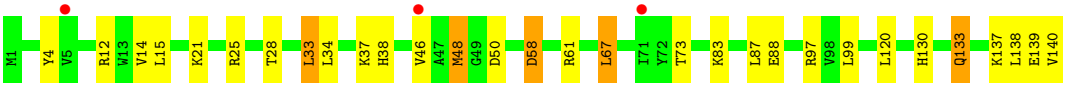
• Molecule 33: 50S ribosomal protein L9

Chain DI:



- Molecule 34: 50S ribosomal protein L13

Chain BN:

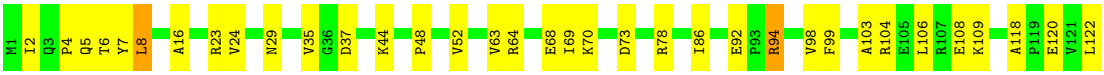


- Molecule 34: 50S ribosomal protein L13

Chain DN:

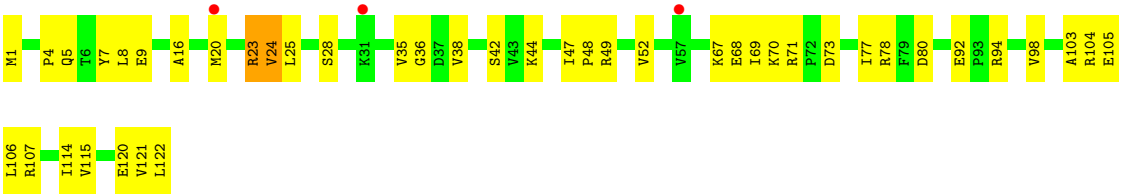
- Molecule 35: 50S ribosomal protein L14

Chain BO:



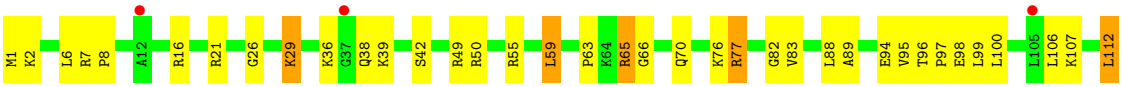
- Molecule 35: 50S ribosomal protein L14

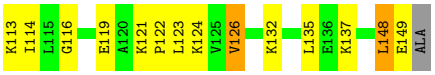
Chain DO:



- Molecule 36: 50S ribosomal protein L15

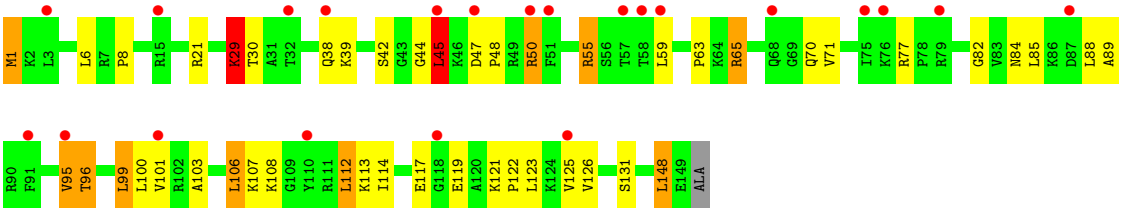
Chain BP:





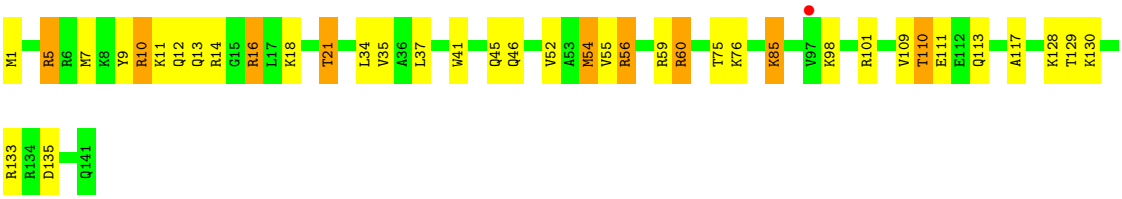
• Molecule 36: 50S ribosomal protein L15

Chain DP:



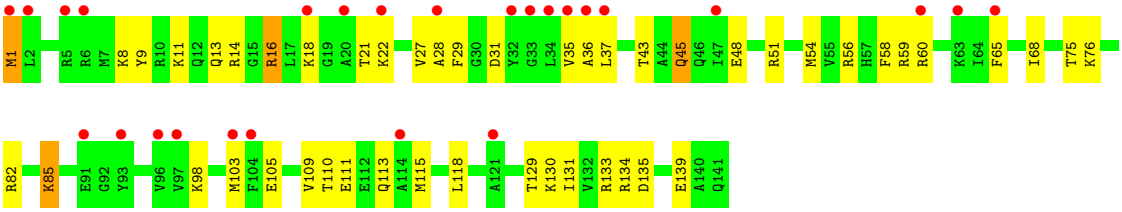
• Molecule 37: 50S ribosomal protein L16

Chain BQ:



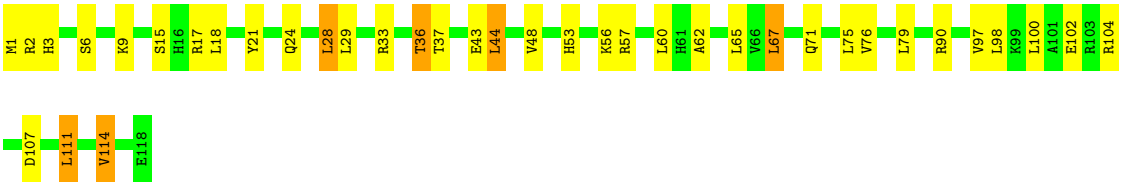
• Molecule 37: 50S ribosomal protein L16

Chain DQ:



• Molecule 38: 50S ribosomal protein L17

Chain BR:

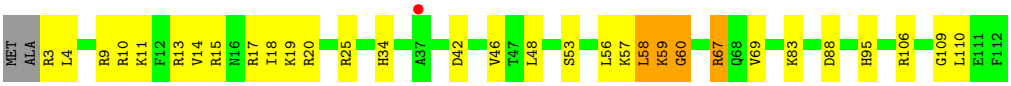


• Molecule 38: 50S ribosomal protein L17

Chain DR:

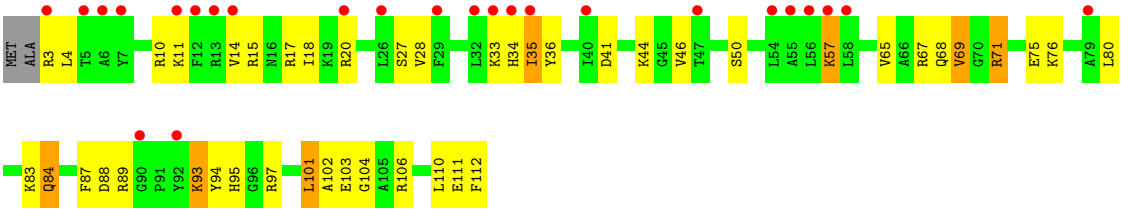
• Molecule 39: 50S ribosomal protein L18

Chain BS:



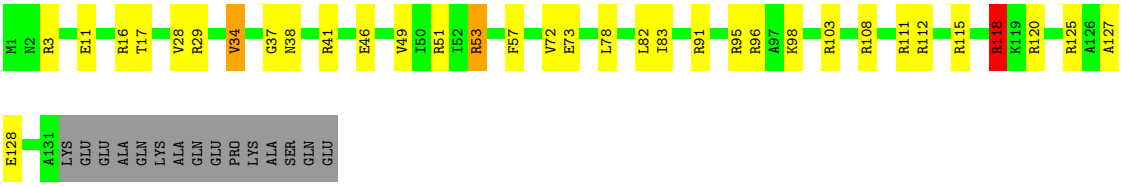
• Molecule 39: 50S ribosomal protein L18

Chain DS:



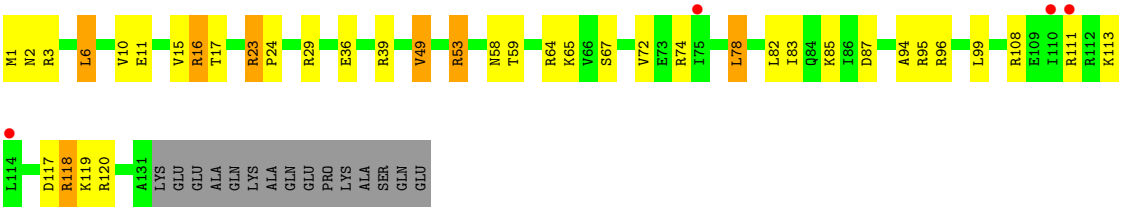
• Molecule 40: 50S ribosomal protein L19

Chain BT:



• Molecule 40: 50S ribosomal protein L19

Chain DT:

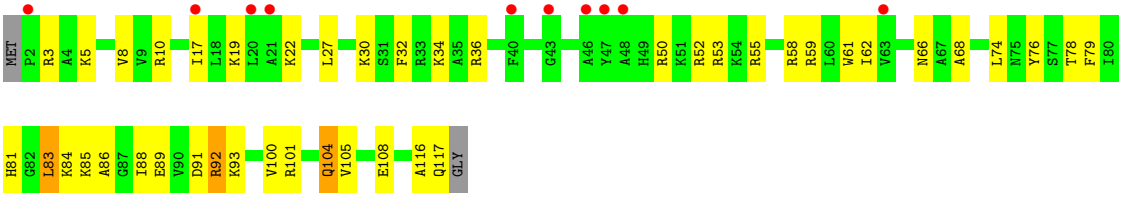


• Molecule 41: 50S ribosomal protein L20

Chain BU:

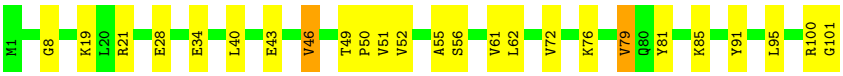
• Molecule 41: 50S ribosomal protein L20

Chain DU:



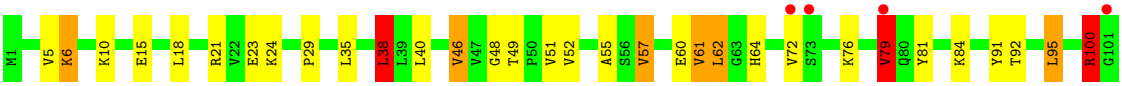
• Molecule 42: 50S ribosomal protein L21

Chain BV:



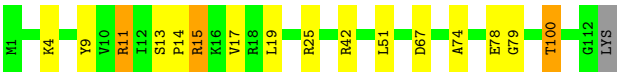
• Molecule 42: 50S ribosomal protein L21

Chain DV:



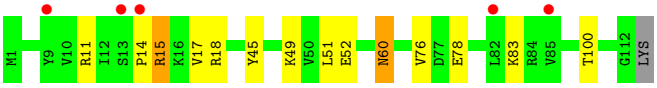
• Molecule 43: 50S ribosomal protein L22

Chain BW:



• Molecule 43: 50S ribosomal protein L22

Chain DW:

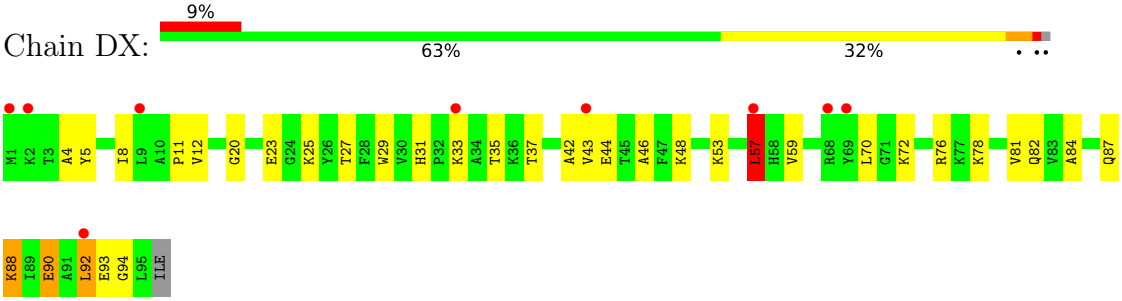


• Molecule 44: 50S ribosomal protein L23

Chain BX:

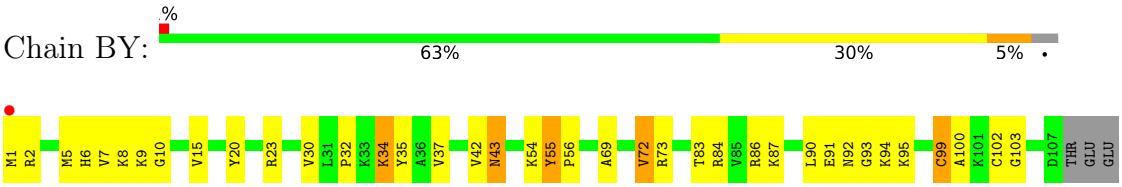
• Molecule 44: 50S ribosomal protein L23

Chain DX:



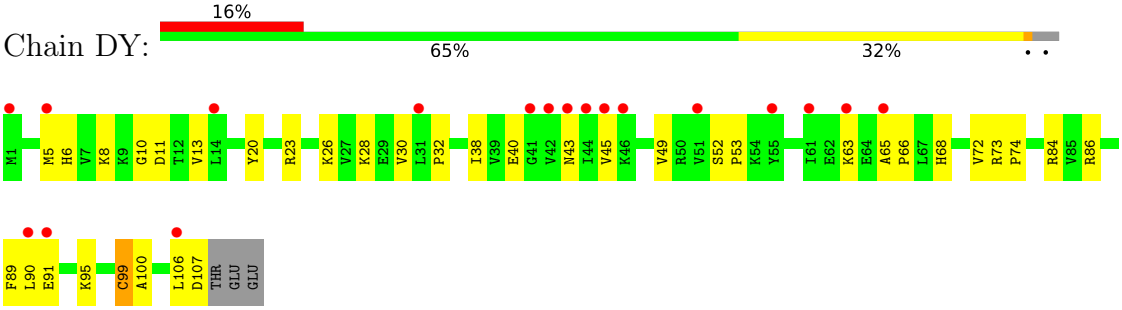
• Molecule 45: 50S ribosomal protein L24

Chain BY:



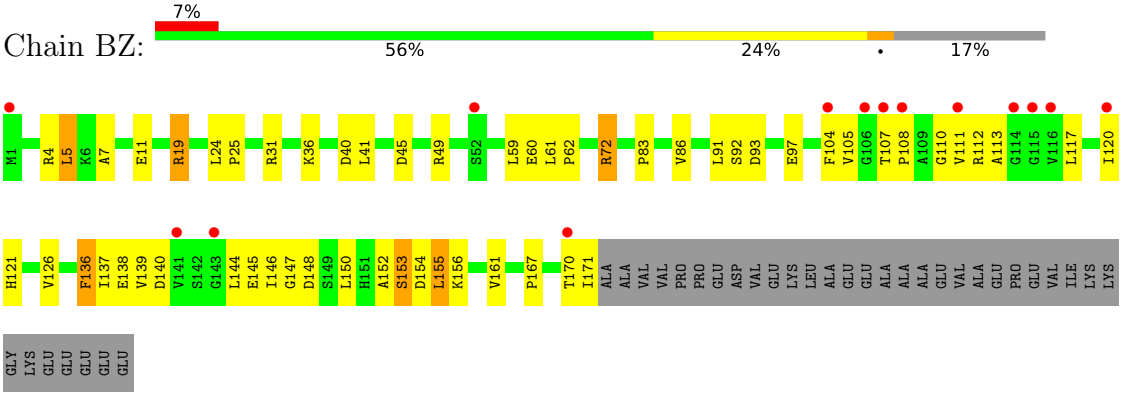
• Molecule 45: 50S ribosomal protein L24

Chain DY:



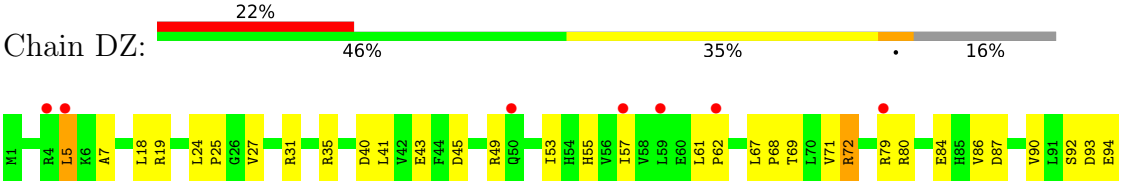
• Molecule 46: 50S ribosomal protein L25

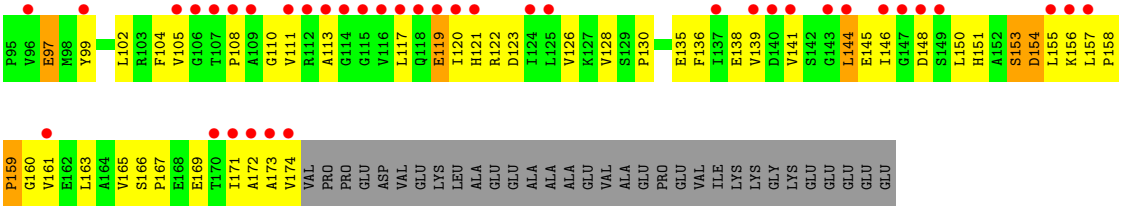
Chain BZ:



• Molecule 46: 50S ribosomal protein L25

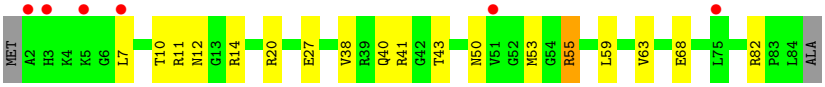
Chain DZ:





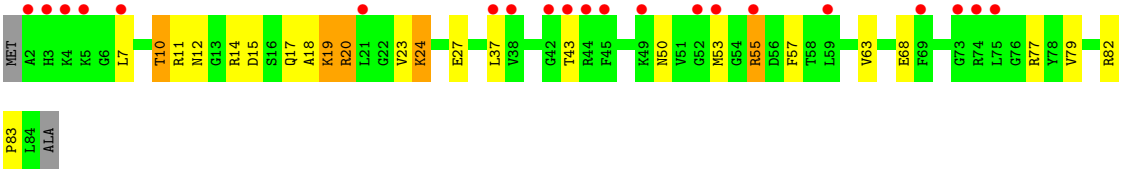
• Molecule 47: 50S ribosomal protein L27

Chain B0:



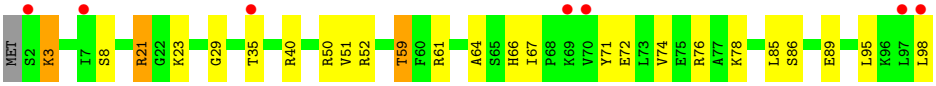
• Molecule 47: 50S ribosomal protein L27

Chain D0:



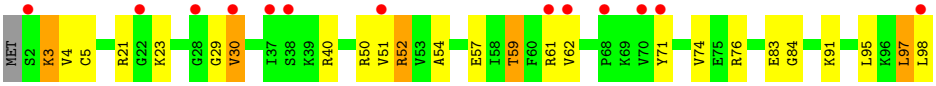
• Molecule 48: 50S ribosomal protein L28

Chain B1:



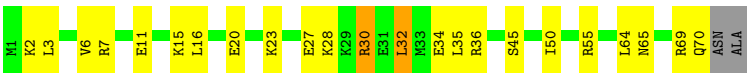
• Molecule 48: 50S ribosomal protein L28

Chain D1:



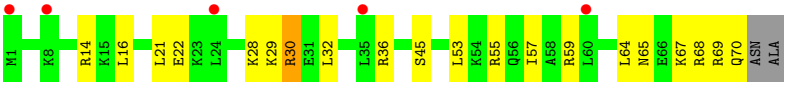
• Molecule 49: 50S ribosomal protein L29

Chain B2:



• Molecule 49: 50S ribosomal protein L29

Chain D2:

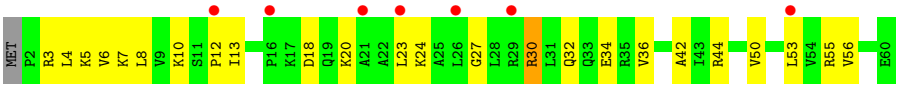


• Molecule 50: 50S ribosomal protein L30

Chain B3:

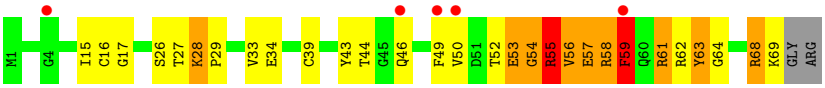
• Molecule 50: 50S ribosomal protein L30

Chain D3:



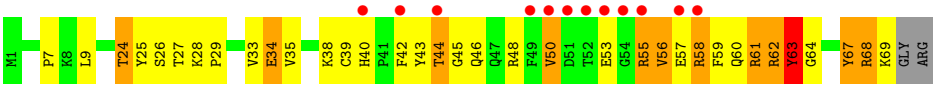
• Molecule 51: 50S ribosomal protein L31

Chain B4:



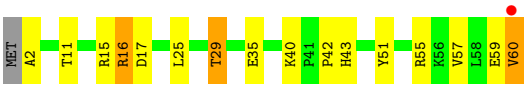
• Molecule 51: 50S ribosomal protein L31

Chain D4:



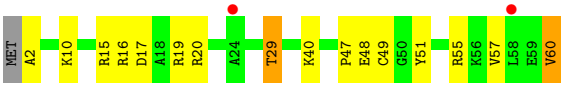
• Molecule 52: 50S ribosomal protein L32

Chain B5:



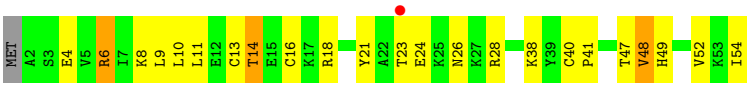
• Molecule 52: 50S ribosomal protein L32

Chain D5:



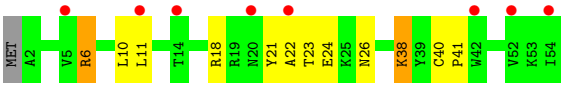
• Molecule 53: 50S ribosomal protein L33

Chain B6:



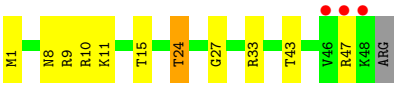
- Molecule 53: 50S ribosomal protein L33

Chain D6:



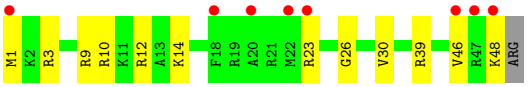
- Molecule 54: 50S ribosomal protein L34

Chain B7:



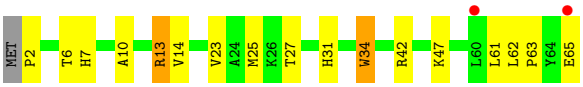
- Molecule 54: 50S ribosomal protein L34

Chain D7:



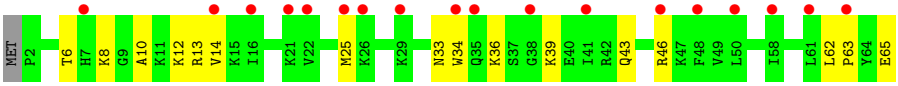
- Molecule 55: 50S ribosomal protein L35

Chain B8:



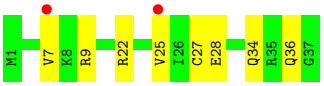
- Molecule 55: 50S ribosomal protein L35

Chain D8:



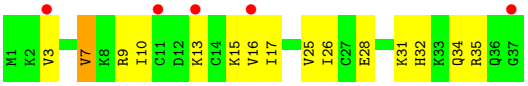
- Molecule 56: 50S ribosomal protein L36

Chain B9:



• Molecule 56: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 255.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (255.92-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.280 0.233 , 0.280	Depositor DCC
R_{free} test set	90444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	297141	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5MC, 5MU, SF4, 31M, K, MG, MIA, 4SU, 7MG, PSU

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	0.37	0/36049	0.91	42/56261 (0.1%)
1	CA	0.40	6/36170 (0.0%)	1.00	88/56452 (0.2%)
2	AB	0.31	0/1881	0.60	0/2542
2	CB	0.33	0/1860	0.65	1/2518 (0.0%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.32	0/1566	0.61	0/2119
4	AD	0.29	0/1689	0.58	2/2267 (0.1%)
4	CD	0.30	0/1704	0.54	0/2284
5	AE	0.30	0/1145	0.55	0/1543
5	CE	0.31	0/1149	0.62	1/1548 (0.1%)
6	AF	0.28	0/819	0.49	0/1111
6	CF	0.31	0/829	0.52	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.28	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.50	0/1494
8	CH	0.27	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.59	0/1346
9	CI	0.30	0/997	0.57	0/1343
10	AJ	0.28	0/722	0.59	0/982
10	CJ	0.31	0/727	0.59	0/988
11	AK	0.28	0/844	0.60	1/1145 (0.1%)
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.30	0/946	0.52	0/1274
12	CL	0.30	0/946	0.55	0/1274
13	AM	0.28	0/969	0.61	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.55	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.28	0/697	0.52	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.28	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.56	0/746
18	CR	0.28	0/560	0.56	0/746
19	AS	0.29	0/667	0.58	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.28	0/730	0.58	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.26	0/203	0.52	0/266
21	CU	0.35	0/203	0.52	0/266
22	AV	0.41	0/310	0.94	0/480
22	CV	0.45	0/282	1.06	1/437 (0.2%)
23	AW	0.47	0/1577	1.18	6/2454 (0.2%)
23	CW	0.59	0/1531	1.46	25/2379 (1.1%)
24	AX	0.51	0/1725	1.17	14/2689 (0.5%)
24	CX	0.44	0/1725	1.12	10/2689 (0.4%)
25	AY	0.62	0/1602	1.43	22/2493 (0.9%)
25	CY	0.64	0/1579	1.46	32/2455 (1.3%)
26	BA	0.48	2/68013 (0.0%)	0.95	84/106165 (0.1%)
26	DA	0.42	1/67542 (0.0%)	0.94	72/105428 (0.1%)
27	BB	0.41	0/2878	0.88	0/4490
27	DB	0.44	0/2878	0.94	0/4490
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2186	0.55	0/2944
29	BE	0.36	0/1592	0.57	0/2149
29	DE	0.34	0/1592	0.60	1/2149 (0.0%)
30	BF	0.35	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.58	0/2188
31	BG	0.31	0/1450	0.54	0/1959
31	DG	0.33	0/1449	0.57	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.30	0/1356	0.52	0/1834
33	BI	0.29	0/1100	0.60	0/1501
33	DI	0.28	0/1076	0.57	0/1471
34	BN	0.32	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.54	0/1543
35	BO	0.34	0/943	0.58	1/1269 (0.1%)
35	DO	0.31	0/943	0.51	0/1269
36	BP	0.34	0/1152	0.58	0/1533
36	DP	0.31	0/1152	0.59	0/1533
37	BQ	0.34	0/1143	0.53	0/1527
37	DQ	0.31	0/1143	0.52	0/1527
38	BR	0.35	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DR	0.29	0/982	0.52	0/1312
39	BS	0.31	0/887	0.63	2/1180 (0.2%)
39	DS	0.29	0/880	0.61	0/1172
40	BT	0.33	0/1105	0.59	1/1477 (0.1%)
40	DT	0.29	0/1097	0.56	0/1468
41	BU	0.37	0/977	0.56	0/1301
41	DU	0.31	0/977	0.50	0/1301
42	BV	0.39	0/782	0.58	0/1049
42	DV	0.32	0/782	0.64	2/1049 (0.2%)
43	BW	0.38	0/897	0.57	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.39	0/764	0.59	1/1025 (0.1%)
44	DX	0.32	0/764	0.56	1/1025 (0.1%)
45	BY	0.34	0/819	0.57	0/1095
45	DY	0.31	0/819	0.55	0/1095
46	BZ	0.31	0/1379	0.61	0/1873
46	DZ	0.29	0/1390	0.57	0/1890
47	B0	0.35	0/662	0.57	0/881
47	D0	0.29	0/662	0.49	0/881
48	B1	0.34	0/762	0.56	0/1014
48	D1	0.32	0/762	0.54	0/1014
49	B2	0.32	0/590	0.56	0/781
49	D2	0.27	0/590	0.46	0/781
50	B3	0.36	0/474	0.58	0/635
50	D3	0.27	0/469	0.50	0/630
51	B4	0.35	0/571	0.71	0/768
51	D4	0.34	0/545	0.70	0/737
52	B5	0.38	0/469	0.60	0/635
52	D5	0.33	0/469	0.52	0/635
53	B6	0.36	0/460	0.51	0/613
53	D6	0.30	0/456	0.48	0/608
54	B7	0.39	0/426	0.55	0/561
54	D7	0.33	0/426	0.59	0/561
55	B8	0.36	0/519	0.58	0/684
55	D8	0.32	0/525	0.52	0/691
56	B9	0.35	0/310	0.51	0/407
56	D9	0.31	0/310	0.56	0/407
All	All	0.40	9/316594 (0.0%)	0.88	410/473970 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-11.01	1.28	1.37
1	CA	1154	G	C6-N1	-10.68	1.32	1.39
1	CA	1119	C	N3-C4	-9.86	1.27	1.33
1	CA	1154	G	N7-C5	-7.17	1.34	1.39
26	BA	330	A	N9-C4	-6.79	1.33	1.37

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1119	C	N1-C2-O2	32.18	138.21	118.90
1	CA	1154	G	N3-C2-N2	24.48	137.03	119.90
1	CA	1154	G	C5-C6-O6	24.01	143.00	128.60
1	CA	1154	G	N1-C2-N2	-21.95	96.45	116.20
1	CA	1119	C	N3-C2-O2	-20.26	107.72	121.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	495	0
1	CA	32312	0	16307	663	0
2	AB	1846	0	1867	92	0
2	CB	1825	0	1828	102	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	61	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	33	0
6	AF	806	0	793	24	0
6	CF	816	0	808	18	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	42	0
9	AI	983	0	986	47	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	14	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	39	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	20	0
15	CO	728	0	760	31	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	17	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	42	0
20	AT	728	0	798	32	0
20	CT	727	0	796	25	0
21	AU	199	0	208	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	10	0
22	AV	277	0	140	2	0
22	CV	252	0	130	7	0
23	AW	1607	0	839	55	0
23	CW	1560	0	803	55	0
24	AX	1625	0	828	34	0
24	CX	1625	0	828	33	0
25	AY	1581	0	805	96	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	669	0
26	DA	60311	0	30409	876	0
27	BB	2573	0	1306	19	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	51	0
28	DD	2136	0	2218	61	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	45	0
30	BF	1584	0	1625	47	0
30	DF	1580	0	1619	50	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	66	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	41	0
33	DI	1061	0	1080	25	0
34	BN	1117	0	1183	17	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	20	0
35	DO	933	0	996	29	0
36	BP	1135	0	1212	38	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	31	0
37	DQ	1122	0	1179	35	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	27	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	17	0
41	DU	959	0	1019	38	0
42	BV	771	0	830	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DV	771	0	830	25	0
43	BW	886	0	939	12	0
43	DW	886	0	940	9	0
44	BX	750	0	814	16	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	26	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	61	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	18	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	12	0
51	B4	558	0	544	22	0
51	D4	532	0	503	31	0
52	B5	455	0	465	11	0
52	D5	455	0	465	12	0
53	B6	453	0	473	13	0
53	D6	449	0	469	9	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	21	0
55	D8	517	0	582	10	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0
61	DX	3	0	0	0	0
61	DY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	297141	0	196251	5228	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 11.

The worst 5 of 5228 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)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12

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	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	4 3
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	4 3
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	29 40
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100 100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	15 22
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29 40
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100 100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100 100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	5	5
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	30
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	19	27
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	1
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	0
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	10
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	10
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	12	16
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	13	17
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	1
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	4	3
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	34	46
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	22	30
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	40
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	15	22
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	29	40
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	15	22
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	34
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	9	11
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	25	34
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	25	34
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	7	7
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	30
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	30
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	30
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	15
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	30
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	24
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	24
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	22
43	BW	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	25	34
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	14	19
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	19
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	7
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	22	30

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU

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Mol	Chain	Res	Type
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	BD	275	LYS

5.3.2 Protein sidechains (i)

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	192/220 (87%)	163 (85%)	29 (15%)	3	2
2	CB	187/220 (85%)	149 (80%)	38 (20%)	1	1
3	AC	143/188 (76%)	121 (85%)	22 (15%)	2	2
3	CC	140/188 (74%)	124 (89%)	16 (11%)	5	5
4	AD	170/181 (94%)	152 (89%)	18 (11%)	6	7
4	CD	173/181 (96%)	152 (88%)	21 (12%)	5	4
5	AE	113/123 (92%)	105 (93%)	8 (7%)	14	19
5	CE	114/123 (93%)	101 (89%)	13 (11%)	5	5
6	AF	83/90 (92%)	76 (92%)	7 (8%)	11	13
6	CF	85/90 (94%)	80 (94%)	5 (6%)	19	25
7	AG	119/127 (94%)	108 (91%)	11 (9%)	9	11
7	CG	120/127 (94%)	109 (91%)	11 (9%)	9	11
8	AH	114/119 (96%)	105 (92%)	9 (8%)	12	15
8	CH	114/119 (96%)	107 (94%)	7 (6%)	18	24
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	2
9	CI	89/99 (90%)	76 (85%)	13 (15%)	3	2
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	5	4
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	10	12
11	AK	82/99 (83%)	77 (94%)	5 (6%)	18	24
11	CK	83/99 (84%)	76 (92%)	7 (8%)	11	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	93 (96%)	4 (4%)	30	41
12	CL	97/109 (89%)	93 (96%)	4 (4%)	30	41
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5	5
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	3
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	3
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	2
15	AO	78/80 (98%)	64 (82%)	14 (18%)	2	1
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5	5
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	3
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7	7
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	9
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	18
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	13
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5	5
19	AS	69/80 (86%)	64 (93%)	5 (7%)	14	18
19	CS	67/80 (84%)	63 (94%)	4 (6%)	19	25
20	AT	70/82 (85%)	62 (89%)	8 (11%)	5	5
20	CT	70/82 (85%)	62 (89%)	8 (11%)	5	5
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	2
21	CU	18/22 (82%)	17 (94%)	1 (6%)	21	28
28	BD	215/218 (99%)	195 (91%)	20 (9%)	9	10
28	DD	215/218 (99%)	193 (90%)	22 (10%)	7	8
29	BE	164/166 (99%)	146 (89%)	18 (11%)	6	6
29	DE	164/166 (99%)	145 (88%)	19 (12%)	5	5
30	BF	160/166 (96%)	149 (93%)	11 (7%)	15	20
30	DF	159/166 (96%)	144 (91%)	15 (9%)	8	10
31	BG	143/156 (92%)	128 (90%)	15 (10%)	7	7
31	DG	142/156 (91%)	122 (86%)	20 (14%)	3	3
32	BH	144/148 (97%)	126 (88%)	18 (12%)	4	4
32	DH	144/148 (97%)	126 (88%)	18 (12%)	4	4
33	BI	110/124 (89%)	86 (78%)	24 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	88 (85%)	16 (15%)	2	2
34	BN	118/119 (99%)	103 (87%)	15 (13%)	4	4
34	DN	118/119 (99%)	106 (90%)	12 (10%)	7	8
35	BO	100/100 (100%)	93 (93%)	7 (7%)	15	19
35	DO	100/100 (100%)	93 (93%)	7 (7%)	15	19
36	BP	115/116 (99%)	98 (85%)	17 (15%)	3	2
36	DP	115/116 (99%)	100 (87%)	15 (13%)	4	3
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	3
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	6
38	BR	101/101 (100%)	82 (81%)	19 (19%)	1	1
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	1
39	BS	87/88 (99%)	81 (93%)	6 (7%)	15	20
39	DS	85/88 (97%)	75 (88%)	10 (12%)	5	5
40	BT	115/127 (91%)	106 (92%)	9 (8%)	12	16
40	DT	113/127 (89%)	103 (91%)	10 (9%)	10	12
41	BU	93/94 (99%)	84 (90%)	9 (10%)	8	9
41	DU	93/94 (99%)	85 (91%)	8 (9%)	10	13
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	2
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	2
43	BW	90/92 (98%)	83 (92%)	7 (8%)	12	16
43	DW	90/92 (98%)	83 (92%)	7 (8%)	12	16
44	BX	77/78 (99%)	71 (92%)	6 (8%)	12	16
44	DX	77/78 (99%)	71 (92%)	6 (8%)	12	16
45	BY	85/91 (93%)	75 (88%)	10 (12%)	5	5
45	DY	85/91 (93%)	79 (93%)	6 (7%)	14	19
46	BZ	145/179 (81%)	133 (92%)	12 (8%)	11	14
46	DZ	145/179 (81%)	129 (89%)	16 (11%)	6	6
47	B0	65/67 (97%)	62 (95%)	3 (5%)	27	36
47	D0	65/67 (97%)	60 (92%)	5 (8%)	13	16
48	B1	80/83 (96%)	73 (91%)	7 (9%)	10	12
48	D1	80/83 (96%)	71 (89%)	9 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	57 (88%)	8 (12%)	4	4
49	D2	65/67 (97%)	59 (91%)	6 (9%)	9	11
50	B3	51/52 (98%)	46 (90%)	5 (10%)	8	9
50	D3	50/52 (96%)	44 (88%)	6 (12%)	5	5
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	1
51	D4	53/63 (84%)	43 (81%)	10 (19%)	1	1
52	B5	50/52 (96%)	45 (90%)	5 (10%)	7	8
52	D5	50/52 (96%)	46 (92%)	4 (8%)	12	15
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	3
53	D6	50/52 (96%)	48 (96%)	2 (4%)	31	43
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14	18
54	D7	41/42 (98%)	38 (93%)	3 (7%)	14	18
55	B8	53/55 (96%)	49 (92%)	4 (8%)	13	17
55	D8	54/55 (98%)	51 (94%)	3 (6%)	21	28
56	B9	34/34 (100%)	34 (100%)	0	100	100
56	D9	34/34 (100%)	32 (94%)	2 (6%)	19	25
All	All	9320/10066 (93%)	8304 (89%)	1016 (11%)	6	6

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	B1	59	THR
38	DR	100	LEU
4	CD	86	LYS
38	DR	29	LEU
45	DY	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
31	DG	40	ASN
40	DT	58	ASN
30	BF	203	GLN
30	BF	169	ASN
41	DU	117	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	304 (20%)	25 (1%)
1	CA	1501/1521 (98%)	316 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	70/76 (92%)	30 (42%)	2 (2%)
23	CW	67/76 (88%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	71/76 (93%)	35 (49%)	4 (5%)
25	CY	69/76 (90%)	32 (46%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	552 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9286/9620 (96%)	1824 (19%)	126 (1%)

5 of 1824 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2181	G
26	DA	1427	A
1	CA	532	A
26	DA	1420	U
26	DA	2126	A

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

38 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	$\#\|Z\| > 2$
23	PSU	CW	39	23	18,21,22	1.33	2 (11%)	22,30,33	1.73	3 (13%)
24	5MC	AX	32	24	18,22,23	0.98	2 (11%)	26,32,35	1.29	3 (11%)
23	7MG	CW	46	23	22,26,27	1.43	4 (18%)	29,39,42	2.41	6 (20%)
25	PSU	CY	39	25	18,21,22	1.41	2 (11%)	22,30,33	2.15	3 (13%)
23	PSU	CW	32	23	18,21,22	1.31	2 (11%)	22,30,33	1.84	3 (13%)
23	PSU	AW	55	23	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
23	PSU	AW	32	23	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
25	PSU	CY	32	25	18,21,22	1.35	2 (11%)	22,30,33	1.84	4 (18%)
23	MIA	AW	37	23	24,31,32	2.19	4 (16%)	26,44,47	2.60	10 (38%)
24	5MU	AX	54	57,24	19,22,23	1.43	5 (26%)	28,32,35	1.93	5 (17%)
25	PSU	AY	55	25	18,21,22	1.34	3 (16%)	22,30,33	2.16	5 (22%)
23	4SU	AW	8	23	18,21,22	1.71	4 (22%)	26,30,33	2.08	5 (19%)
25	4SU	CY	8	25	18,21,22	1.62	4 (22%)	26,30,33	2.95	6 (23%)
25	5MU	AY	54	25	19,22,23	1.49	5 (26%)	28,32,35	2.13	7 (25%)
23	31M	CW	76	23	38,44,45	1.41	5 (13%)	38,61,64	1.23	3 (7%)
25	5MU	CY	54	25	19,22,23	1.34	4 (21%)	28,32,35	2.18	6 (21%)
23	PSU	CW	55	23	18,21,22	1.35	2 (11%)	22,30,33	1.95	3 (13%)
25	PSU	CY	55	25	18,21,22	1.43	4 (22%)	22,30,33	2.30	5 (22%)
24	PSU	CX	55	24	18,21,22	1.32	2 (11%)	22,30,33	1.85	4 (18%)
25	PSU	AY	39	25	18,21,22	1.54	4 (22%)	22,30,33	1.82	5 (22%)
24	4SU	CX	8	24	18,21,22	1.95	6 (33%)	26,30,33	1.35	4 (15%)
24	5MU	CX	54	24	19,22,23	1.39	4 (21%)	28,32,35	2.26	6 (21%)
25	7MG	CY	46	25	22,26,27	1.44	5 (22%)	29,39,42	2.56	8 (27%)
25	7MG	AY	46	25	22,26,27	1.29	3 (13%)	29,39,42	2.81	7 (24%)
24	5MC	CX	32	24	18,22,23	0.96	2 (11%)	26,32,35	1.17	3 (11%)
23	5MU	AW	54	23	19,22,23	1.40	5 (26%)	28,32,35	1.90	6 (21%)
23	MIA	CW	37	23	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
23	7MG	AW	46	23	22,26,27	1.36	4 (18%)	29,39,42	2.52	6 (20%)
25	4SU	AY	8	25	18,21,22	1.78	5 (27%)	26,30,33	2.00	5 (19%)
25	PSU	AY	32	25	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
25	MIA	CY	37	25	18,24,32	1.16	2 (11%)	18,35,47	1.25	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	MIA	AY	37	25	18,24,32	1.14	2 (11%)	18,35,47	1.22	2 (11%)
23	4SU	CW	8	23	18,21,22	1.58	4 (22%)	26,30,33	2.33	5 (19%)
23	5MU	CW	54	23	19,22,23	1.34	4 (21%)	28,32,35	1.97	7 (25%)
23	31M	AW	76	23	38,44,45	1.40	5 (13%)	38,61,64	1.39	4 (10%)
24	4SU	AX	8	24	18,21,22	2.17	5 (27%)	26,30,33	1.70	6 (23%)
24	PSU	AX	55	57,24	18,21,22	1.31	2 (11%)	22,30,33	1.90	4 (18%)
23	PSU	AW	39	23	18,21,22	1.38	2 (11%)	22,30,33	1.70	3 (13%)

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
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
25	PSU	CY	39	25	-	2/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	1/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
24	5MU	AX	54	57,24	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	2/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	4SU	CY	8	25	-	2/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	2/7/25/26	0/2/2/2
23	31M	CW	76	23	-	11/27/49/50	0/4/4/4
25	5MU	CY	54	25	-	2/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
25	PSU	CY	55	25	-	4/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2
25	PSU	AY	39	25	-	2/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	4/7/37/38	0/3/3/3
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
25	4SU	AY	8	25	-	2/7/25/26	0/2/2/2
25	PSU	AY	32	25	-	1/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/3/25/34	0/3/3/3
25	MIA	AY	37	25	-	3/3/25/34	0/3/3/3
23	4SU	CW	8	23	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
23	31M	AW	76	23	-	9/27/49/50	0/4/4/4
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	57,24	-	0/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.24	1.53	1.32
23	AW	37	MIA	C2-S10	-6.30	1.70	1.75
24	AX	8	4SU	C4-N3	-5.19	1.32	1.37
23	AW	76	31M	CB-CG	-5.03	1.39	1.51
23	CW	76	31M	CB-CG	-4.85	1.39	1.51

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	46	7MG	N9-C4-N3	10.08	140.54	125.47
23	AW	46	7MG	N9-C4-N3	8.92	138.81	125.47
25	CY	8	4SU	C4-N3-C2	-8.84	118.75	127.34
23	AW	37	MIA	C12-C13-C14	-8.47	110.65	127.14
23	CW	46	7MG	N9-C4-N3	8.10	137.58	125.47

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
23	AW	76	31M	NM-CAM-CTM-N
23	AW	76	31M	CBM-CAM-CTM-N

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Mol	Chain	Res	Type	Atoms
23	AW	76	31M	CBM-CAM-CTM-OTM
25	AY	39	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CW	39	PSU	3	0
24	AX	32	5MC	3	0
23	CW	46	7MG	1	0
25	CY	39	PSU	4	0
23	AW	37	MIA	1	0
25	AY	55	PSU	4	0
23	AW	8	4SU	1	0
25	CY	8	4SU	5	0
25	AY	54	5MU	2	0
23	CW	76	31M	7	0
23	CW	55	PSU	1	0
25	CY	55	PSU	4	0
25	AY	39	PSU	4	0
24	CX	8	4SU	2	0
24	CX	54	5MU	2	0
25	CY	46	7MG	1	0
25	AY	46	7MG	3	0
24	CX	32	5MC	2	0
23	AW	46	7MG	1	0
25	AY	8	4SU	1	0
25	AY	32	PSU	2	0
25	CY	37	MIA	2	0
25	AY	37	MIA	3	0
23	CW	8	4SU	2	0
23	AW	76	31M	4	0
24	AX	8	4SU	2	0
24	AX	55	PSU	1	0
23	AW	39	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2093 ligands modelled in this entry, 2091 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	SF4	CD	302	4	0,12,12	-	-	-		
58	SF4	AD	501	4	0,12,12	-	-	-		

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	SF4	CD	302	4	-	-	0/6/5/5
58	SF4	AD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	1498/1521 (98%)	0.35	28 (1%)	66	73	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.38	63 (4%)	36	42	44, 74, 94, 109	0
2	AB	231/256 (90%)	0.77	30 (12%)	3	4	72, 82, 90, 94	0
2	CB	231/256 (90%)	1.43	52 (22%)	0	0	73, 84, 90, 95	0
3	AC	206/239 (86%)	0.96	33 (16%)	1	2	68, 79, 87, 94	0
3	CC	206/239 (86%)	1.84	76 (36%)	0	0	71, 81, 89, 94	0
4	AD	208/209 (99%)	0.97	27 (12%)	3	4	57, 72, 81, 90	0
4	CD	208/209 (99%)	0.80	16 (7%)	13	17	58, 71, 80, 91	0
5	AE	148/162 (91%)	1.01	17 (11%)	4	6	58, 71, 80, 85	0
5	CE	148/162 (91%)	1.21	29 (19%)	1	1	60, 73, 81, 86	0
6	AF	100/101 (99%)	0.56	5 (5%)	28	34	56, 69, 78, 82	0
6	CF	100/101 (99%)	0.43	5 (5%)	28	34	57, 70, 78, 82	0
7	AG	155/156 (99%)	0.84	10 (6%)	18	22	65, 75, 83, 91	0
7	CG	155/156 (99%)	1.13	24 (15%)	2	2	66, 76, 84, 92	0
8	AH	137/138 (99%)	0.96	25 (18%)	1	1	62, 72, 79, 87	0
8	CH	137/138 (99%)	1.09	27 (19%)	1	1	64, 74, 80, 87	0
9	AI	127/128 (99%)	1.11	25 (19%)	1	1	65, 80, 86, 89	0
9	CI	127/128 (99%)	2.49	72 (56%)	0	0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	1.18	19 (19%)	1	1	64, 82, 90, 93	0
10	CJ	96/105 (91%)	1.72	35 (36%)	0	0	67, 84, 91, 93	0
11	AK	114/129 (88%)	0.83	8 (7%)	16	19	48, 70, 79, 84	0
11	CK	114/129 (88%)	0.76	8 (7%)	16	19	51, 71, 79, 84	0
12	AL	122/132 (92%)	0.77	5 (4%)	37	44	50, 65, 73, 78	0
12	CL	122/132 (92%)	1.17	24 (19%)	1	1	53, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.70	9 (7%)	15	18	55, 70, 81, 89	0
13	CM	122/126 (96%)	2.06	53 (43%)	0	0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.20	9 (15%)	2	2	67, 74, 83, 84	0
14	CN	60/61 (98%)	3.00	38 (63%)	0	0	69, 77, 84, 88	0
15	AO	88/89 (98%)	0.67	6 (6%)	17	20	56, 67, 80, 81	0
15	CO	88/89 (98%)	0.92	8 (9%)	9	11	59, 69, 80, 83	0
16	AP	82/88 (93%)	1.57	24 (29%)	0	0	57, 71, 80, 84	0
16	CP	82/88 (93%)	0.97	7 (8%)	10	12	58, 70, 80, 84	0
17	AQ	99/105 (94%)	0.81	11 (11%)	5	7	59, 71, 80, 84	0
17	CQ	99/105 (94%)	1.29	25 (25%)	0	0	61, 71, 81, 85	0
18	AR	68/88 (77%)	0.75	5 (7%)	14	18	59, 68, 81, 83	0
18	CR	68/88 (77%)	0.60	3 (4%)	34	41	61, 70, 80, 84	0
19	AS	83/93 (89%)	0.60	3 (3%)	42	49	71, 80, 86, 95	0
19	CS	83/93 (89%)	1.93	31 (37%)	0	0	74, 82, 89, 96	0
20	AT	96/106 (90%)	0.94	14 (14%)	2	3	57, 71, 81, 85	0
20	CT	96/106 (90%)	1.15	15 (15%)	2	2	58, 70, 82, 85	0
21	AU	23/27 (85%)	1.65	7 (30%)	0	0	67, 74, 77, 81	0
21	CU	23/27 (85%)	2.78	15 (65%)	0	0	70, 75, 80, 84	0
22	AV	13/24 (54%)	2.86	7 (53%)	0	0	58, 81, 96, 99	0
22	CV	12/24 (50%)	3.67	8 (66%)	0	0	63, 84, 93, 94	0
23	AW	66/76 (86%)	1.96	25 (37%)	0	0	68, 96, 103, 105	0
23	CW	64/76 (84%)	3.61	52 (81%)	0	0	73, 97, 103, 106	0
24	AX	72/77 (93%)	0.44	1 (1%)	75	81	39, 68, 87, 91	0
24	CX	72/77 (93%)	0.73	4 (5%)	24	29	53, 82, 93, 97	0
25	AY	67/76 (88%)	1.42	21 (31%)	0	0	44, 97, 102, 105	0
25	CY	66/76 (86%)	2.35	32 (48%)	0	0	47, 97, 102, 105	0
26	BA	2819/2915 (96%)	0.67	29 (1%)	82	86	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.18	65 (2%)	60	67	30, 49, 90, 108	0
27	BB	120/121 (99%)	0.55	0	100	100	40, 64, 73, 86	0
27	DB	120/121 (99%)	0.20	5 (4%)	36	42	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.81	7 (2%)	57	63	27, 43, 58, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DD	275/276 (99%)	0.69	14 (5%) 28 33	29, 45, 61, 81	0
29	BE	204/206 (99%)	0.79	7 (3%) 45 52	25, 48, 66, 80	0
29	DE	204/206 (99%)	0.57	4 (1%) 65 72	29, 52, 67, 81	0
30	BF	203/210 (96%)	0.75	1 (0%) 91 94	26, 53, 76, 87	0
30	DF	203/210 (96%)	0.57	7 (3%) 45 52	30, 58, 77, 87	0
31	BG	181/182 (99%)	0.81	10 (5%) 25 30	51, 69, 81, 88	0
31	DG	181/182 (99%)	1.26	40 (22%) 0 0	56, 73, 82, 90	0
32	BH	174/180 (96%)	0.75	4 (2%) 60 67	51, 65, 75, 88	0
32	DH	174/180 (96%)	1.09	34 (19%) 1 1	55, 70, 78, 88	0
33	BI	146/148 (98%)	0.56	5 (3%) 45 52	50, 74, 82, 87	0
33	DI	146/148 (98%)	0.60	13 (8%) 9 11	52, 75, 82, 86	0
34	BN	140/140 (100%)	0.90	3 (2%) 63 70	32, 50, 67, 76	0
34	DN	140/140 (100%)	0.68	8 (5%) 23 28	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.58	0 100 100	30, 43, 59, 70	0
35	DO	122/122 (100%)	0.75	3 (2%) 57 63	45, 59, 73, 78	0
36	BP	149/150 (99%)	0.82	3 (2%) 65 72	26, 55, 75, 83	0
36	DP	149/150 (99%)	0.95	22 (14%) 2 2	30, 59, 77, 85	0
37	BQ	141/141 (100%)	0.83	1 (0%) 87 90	36, 52, 67, 80	0
37	DQ	141/141 (100%)	1.25	26 (18%) 1 1	41, 57, 70, 82	0
38	BR	118/118 (100%)	0.68	0 100 100	25, 36, 54, 59	0
38	DR	118/118 (100%)	0.64	2 (1%) 70 76	40, 54, 65, 72	0
39	BS	110/112 (98%)	0.50	1 (0%) 84 88	38, 51, 65, 72	0
39	DS	110/112 (98%)	1.22	25 (22%) 0 0	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.51	0 100 100	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.66	4 (3%) 49 56	48, 63, 79, 85	0
41	BU	116/118 (98%)	0.80	1 (0%) 84 88	18, 33, 49, 59	0
41	DU	116/118 (98%)	0.82	10 (8%) 10 12	42, 61, 78, 84	0
42	BV	101/101 (100%)	0.55	0 100 100	21, 41, 58, 67	0
42	DV	101/101 (100%)	0.63	4 (3%) 38 45	41, 71, 83, 91	0
43	BW	112/113 (99%)	0.73	0 100 100	23, 34, 54, 79	0
43	DW	112/113 (99%)	0.69	5 (4%) 33 40	39, 50, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BX	95/96 (98%)	0.56	0 100 100	23, 38, 61, 84	0
44	DX	95/96 (98%)	0.97	9 (9%) 8 10	43, 60, 76, 79	0
45	BY	107/110 (97%)	0.51	1 (0%) 84 88	32, 50, 69, 83	0
45	DY	107/110 (97%)	1.19	18 (16%) 1 1	57, 71, 81, 88	0
46	BZ	171/206 (83%)	0.70	14 (8%) 11 14	39, 64, 91, 95	0
46	DZ	174/206 (84%)	1.53	46 (26%) 0 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	0.88	6 (7%) 15 18	27, 39, 61, 73	0
47	D0	83/85 (97%)	1.49	21 (25%) 0 0	46, 66, 75, 82	0
48	B1	97/98 (98%)	0.80	7 (7%) 15 18	30, 48, 70, 76	0
48	D1	97/98 (98%)	0.95	13 (13%) 3 4	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.57	0 100 100	34, 50, 64, 79	0
49	D2	70/72 (97%)	0.66	5 (7%) 16 19	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.63	0 100 100	24, 37, 63, 71	0
50	D3	59/60 (98%)	0.96	7 (11%) 4 5	49, 64, 79, 85	0
51	B4	69/71 (97%)	0.48	5 (7%) 15 18	54, 73, 87, 92	0
51	D4	69/71 (97%)	1.13	12 (17%) 1 1	74, 88, 94, 99	0
52	B5	59/60 (98%)	0.63	1 (1%) 70 76	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.55	2 (3%) 45 52	36, 51, 67, 73	0
53	B6	53/54 (98%)	0.60	1 (1%) 66 73	31, 44, 61, 68	0
53	D6	53/54 (98%)	1.10	8 (15%) 2 2	52, 63, 76, 79	0
54	B7	48/49 (97%)	1.03	3 (6%) 20 23	21, 30, 62, 76	0
54	D7	48/49 (97%)	1.31	8 (16%) 1 1	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.74	2 (3%) 49 56	25, 36, 45, 60	0
55	D8	64/65 (98%)	1.51	18 (28%) 0 0	46, 58, 66, 72	0
56	B9	37/37 (100%)	1.07	2 (5%) 25 30	31, 49, 73, 74	0
56	D9	37/37 (100%)	1.27	5 (13%) 3 4	46, 57, 73, 76	0
All	All	20897/21748 (96%)	0.73	1673 (8%) 12 15	18, 64, 89, 109	0

The worst 5 of 1673 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	12.7
2	CB	165	VAL	12.6

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Mol	Chain	Res	Type	RSRZ
13	AM	124	PRO	11.3
23	CW	71	G	10.9
7	CG	83	ALA	10.6

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
25	7MG	CY	46	24/25	0.48	0.37	86,105,111,137	0
25	MIA	CY	37	22/30	0.61	0.38	72,95,113,138	0
25	5MU	CY	54	21/22	0.63	0.53	78,94,109,140	0
23	7MG	CW	46	24/25	0.66	0.27	79,96,109,133	0
25	PSU	CY	55	20/21	0.67	0.49	94,102,110,124	0
25	4SU	CY	8	20/21	0.68	0.22	93,103,113,128	0
23	4SU	CW	8	20/21	0.69	0.30	81,98,120,127	0
25	PSU	AY	55	20/21	0.70	0.29	93,101,108,122	0
23	7MG	AW	46	24/25	0.72	0.23	84,99,117,133	0
25	5MU	AY	54	21/22	0.73	0.26	80,96,105,131	0
25	7MG	AY	46	24/25	0.76	0.27	75,101,111,123	0
25	PSU	AY	39	20/21	0.76	0.30	78,90,117,123	0
25	PSU	CY	39	20/21	0.77	0.30	79,90,116,130	0
25	4SU	AY	8	20/21	0.78	0.16	82,96,103,118	0
25	PSU	CY	32	20/21	0.79	0.21	80,92,101,107	0
23	PSU	CW	55	20/21	0.79	0.30	79,89,99,104	0
25	MIA	AY	37	22/30	0.80	0.22	77,90,111,119	0
23	4SU	AW	8	20/21	0.81	0.20	86,95,112,128	0
25	PSU	AY	32	20/21	0.83	0.24	78,93,100,106	0
23	5MU	CW	54	21/22	0.84	0.24	74,88,99,101	0
23	MIA	CW	37	22/30	0.84	0.32	75,85,92,100	0
23	PSU	AW	55	20/21	0.84	0.27	77,90,98,104	0
23	PSU	CW	39	20/21	0.87	0.42	78,84,97,98	0
23	PSU	AW	32	20/21	0.88	0.25	77,83,92,98	0
23	PSU	CW	32	20/21	0.88	0.45	81,87,94,103	0
24	PSU	CX	55	20/21	0.89	0.15	70,80,91,96	0
23	31M	CW	76	41/42	0.89	0.41	50,63,73,88	20
23	5MU	AW	54	21/22	0.91	0.20	65,82,91,93	0
24	4SU	CX	8	20/21	0.91	0.17	77,87,95,97	0
24	5MU	CX	54	21/22	0.92	0.22	70,81,89,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PSU	AW	39	20/21	0.93	0.23	73,82,95,97	0
23	31M	AW	76	41/42	0.94	0.33	37,54,66,83	9
24	4SU	AX	8	20/21	0.94	0.18	54,66,82,89	0
23	MIA	AW	37	29/30	0.94	0.26	59,71,81,86	0
24	5MU	AX	54	21/22	0.95	0.20	49,68,79,84	0
24	PSU	AX	55	20/21	0.95	0.21	50,63,73,83	0
24	5MC	AX	32	21/22	0.95	0.21	43,53,62,78	0
24	5MC	CX	32	21/22	0.96	0.21	63,76,86,88	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	BA	3730	1/1	0.31	0.19	71,71,71,71	0
57	MG	BA	3427	1/1	0.41	0.20	61,61,61,61	0
57	MG	BA	3670	1/1	0.43	0.26	61,61,61,61	0
57	MG	DA	3448	1/1	0.43	0.20	70,70,70,70	0
57	MG	DA	3403	1/1	0.45	0.14	57,57,57,57	0
57	MG	BA	3721	1/1	0.46	0.32	82,82,82,82	0
57	MG	DA	3651	1/1	0.48	0.53	75,75,75,75	0
57	MG	DA	3530	1/1	0.51	0.13	74,74,74,74	0
57	MG	DA	3329	1/1	0.54	0.13	54,54,54,54	0
57	MG	DA	3563	1/1	0.57	0.15	74,74,74,74	0
57	MG	AW	3004	1/1	0.57	0.14	49,49,49,49	0
57	MG	BA	3636	1/1	0.58	0.14	64,64,64,64	0
57	MG	CT	3001	1/1	0.58	0.12	56,56,56,56	0
57	MG	DA	3259	1/1	0.58	0.21	43,43,43,43	0
57	MG	DR	5001	1/1	0.58	0.24	70,70,70,70	0
57	MG	BB	215	1/1	0.59	0.18	73,73,73,73	0
57	MG	DA	3673	1/1	0.60	0.14	69,69,69,69	0
57	MG	CA	3070	1/1	0.61	0.15	63,63,63,63	0
57	MG	DA	3320	1/1	0.61	0.15	55,55,55,55	0
57	MG	CA	3088	1/1	0.62	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3616	1/1	0.62	0.21	65,65,65,65	0
57	MG	BA	3568	1/1	0.63	0.10	59,59,59,59	0
57	MG	AA	3004	1/1	0.63	0.15	67,67,67,67	0
57	MG	DA	3566	1/1	0.64	0.12	69,69,69,69	0
57	MG	DA	3213	1/1	0.64	0.32	63,63,63,63	0
57	MG	BA	3470	1/1	0.65	0.13	62,62,62,62	0
57	MG	D8	5001	1/1	0.65	0.23	66,66,66,66	0
57	MG	AA	3153	1/1	0.66	0.18	74,74,74,74	0
57	MG	DA	3518	1/1	0.66	0.24	54,54,54,54	0
57	MG	CA	3051	1/1	0.66	0.19	81,81,81,81	0
57	MG	DA	3532	1/1	0.66	0.24	69,69,69,69	0
57	MG	DA	3413	1/1	0.66	0.23	48,48,48,48	0
57	MG	CX	3002	1/1	0.67	0.14	70,70,70,70	0
57	MG	AX	3014	1/1	0.67	0.19	72,72,72,72	0
57	MG	DA	3256	1/1	0.67	0.19	62,62,62,62	0
57	MG	DB	3011	1/1	0.69	0.14	72,72,72,72	0
57	MG	DA	3076	1/1	0.69	0.14	58,58,58,58	0
57	MG	DA	3244	1/1	0.69	0.11	71,71,71,71	0
57	MG	BA	3678	1/1	0.70	0.08	65,65,65,65	0
57	MG	DA	3633	1/1	0.71	0.12	58,58,58,58	0
57	MG	DA	3125	1/1	0.71	0.26	70,70,70,70	0
57	MG	BA	3053	1/1	0.72	0.21	54,54,54,54	0
57	MG	BA	3070	1/1	0.72	0.37	59,59,59,59	0
57	MG	BA	3003	1/1	0.72	0.19	60,60,60,60	0
57	MG	DA	3316	1/1	0.72	0.11	45,45,45,45	0
57	MG	CA	3018	1/1	0.72	0.16	69,69,69,69	0
57	MG	BA	3540	1/1	0.73	0.23	37,37,37,37	0
57	MG	AA	3103	1/1	0.73	0.24	73,73,73,73	0
57	MG	BA	3257	1/1	0.73	0.23	53,53,53,53	0
57	MG	DA	3546	1/1	0.73	0.11	71,71,71,71	0
57	MG	DA	3060	1/1	0.74	0.15	64,64,64,64	0
57	MG	BA	3300	1/1	0.74	0.25	57,57,57,57	0
57	MG	AA	3169	1/1	0.74	0.13	62,62,62,62	0
57	MG	DD	303	1/1	0.74	0.62	87,87,87,87	0
57	MG	DA	3616	1/1	0.74	0.11	71,71,71,71	0
57	MG	AA	3206	1/1	0.74	0.19	64,64,64,64	0
57	MG	BA	3641	1/1	0.75	0.21	68,68,68,68	0
57	MG	BB	209	1/1	0.75	0.32	65,65,65,65	0
57	MG	BA	3503	1/1	0.75	0.12	49,49,49,49	0
57	MG	B4	502	1/1	0.75	0.14	71,71,71,71	0
57	MG	BA	3538	1/1	0.75	0.15	40,40,40,40	0
57	MG	DA	3608	1/1	0.75	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3401	1/1	0.75	0.16	35,35,35,35	0
57	MG	BA	3602	1/1	0.76	0.16	53,53,53,53	0
57	MG	BA	3095	1/1	0.76	0.24	51,51,51,51	0
57	MG	CJ	5001	1/1	0.76	0.08	73,73,73,73	0
57	MG	BA	3353	1/1	0.76	0.12	50,50,50,50	0
57	MG	BA	3362	1/1	0.76	0.20	41,41,41,41	0
57	MG	DA	3620	1/1	0.76	0.12	68,68,68,68	0
57	MG	BF	304	1/1	0.76	0.18	45,45,45,45	0
57	MG	DA	3635	1/1	0.76	0.11	38,38,38,38	0
57	MG	DA	3642	1/1	0.76	0.28	54,54,54,54	0
57	MG	BF	308	1/1	0.76	0.20	46,46,46,46	0
57	MG	BA	3225	1/1	0.76	0.16	61,61,61,61	0
57	MG	DB	3008	1/1	0.76	0.20	67,67,67,67	0
57	MG	AA	3013	1/1	0.76	0.17	69,69,69,69	0
57	MG	BA	3704	1/1	0.76	0.14	77,77,77,77	0
57	MG	DA	3531	1/1	0.76	0.18	61,61,61,61	0
57	MG	DA	3252	1/1	0.76	0.08	37,37,37,37	0
57	MG	DA	3383	1/1	0.77	0.21	54,54,54,54	0
57	MG	BA	3615	1/1	0.77	0.21	68,68,68,68	0
57	MG	BA	3733	1/1	0.77	0.11	58,58,58,58	0
57	MG	DA	3205	1/1	0.77	0.10	56,56,56,56	0
57	MG	DA	3262	1/1	0.77	0.10	65,65,65,65	0
57	MG	BA	3560	1/1	0.77	0.14	56,56,56,56	0
57	MG	DA	3234	1/1	0.77	0.21	63,63,63,63	0
57	MG	BB	214	1/1	0.77	0.18	49,49,49,49	0
57	MG	DA	3554	1/1	0.78	0.10	62,62,62,62	0
57	MG	BA	3421	1/1	0.78	0.17	32,32,32,32	0
57	MG	AA	3084	1/1	0.78	0.24	51,51,51,51	0
57	MG	DA	3585	1/1	0.78	0.12	43,43,43,43	0
57	MG	CA	3017	1/1	0.78	0.19	53,53,53,53	0
57	MG	DA	3610	1/1	0.78	0.22	64,64,64,64	0
57	MG	BA	3716	1/1	0.78	0.12	65,65,65,65	0
57	MG	BA	3771	1/1	0.78	0.29	50,50,50,50	0
57	MG	DA	3218	1/1	0.78	0.13	59,59,59,59	0
57	MG	CA	3013	1/1	0.79	0.13	69,69,69,69	0
57	MG	BA	3114	1/1	0.79	0.18	53,53,53,53	0
57	MG	DA	3212	1/1	0.79	0.15	45,45,45,45	0
57	MG	DA	3417	1/1	0.79	0.11	52,52,52,52	0
57	MG	BA	3638	1/1	0.79	0.14	63,63,63,63	0
57	MG	DA	3607	1/1	0.79	0.14	65,65,65,65	0
57	MG	CA	3024	1/1	0.79	0.10	74,74,74,74	0
57	MG	BA	3724	1/1	0.79	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DP	201	1/1	0.79	0.29	70,70,70,70	0
57	MG	AE	202	1/1	0.79	0.12	80,80,80,80	0
57	MG	DA	3335	1/1	0.79	0.16	47,47,47,47	0
59	ZN	D4	501	1/1	0.79	0.07	144,144,144,144	0
57	MG	AA	3069	1/1	0.80	0.19	68,68,68,68	0
57	MG	CA	3152	1/1	0.80	0.20	76,76,76,76	0
57	MG	DA	3222	1/1	0.80	0.14	57,57,57,57	0
57	MG	CA	3166	1/1	0.80	0.14	66,66,66,66	0
57	MG	BA	3757	1/1	0.80	0.20	76,76,76,76	0
57	MG	AA	3160	1/1	0.80	0.21	59,59,59,59	0
57	MG	BA	3781	1/1	0.80	0.20	41,41,41,41	0
57	MG	DA	3025	1/1	0.80	0.16	54,54,54,54	0
57	MG	BA	3020	1/1	0.80	0.22	53,53,53,53	0
57	MG	BA	3052	1/1	0.80	0.16	56,56,56,56	0
57	MG	DA	3078	1/1	0.80	0.19	57,57,57,57	0
57	MG	BA	3728	1/1	0.80	0.33	48,48,48,48	0
57	MG	CA	3064	1/1	0.80	0.17	60,60,60,60	0
57	MG	DA	3340	1/1	0.80	0.18	58,58,58,58	0
57	MG	AX	3011	1/1	0.80	0.20	78,78,78,78	0
57	MG	AA	3091	1/1	0.81	0.14	60,60,60,60	0
57	MG	BA	3693	1/1	0.81	0.19	56,56,56,56	0
57	MG	DA	3321	1/1	0.81	0.08	48,48,48,48	0
57	MG	DA	3589	1/1	0.81	0.07	68,68,68,68	0
57	MG	DA	3082	1/1	0.81	0.14	47,47,47,47	0
57	MG	DA	3118	1/1	0.81	0.15	77,77,77,77	0
57	MG	AW	3001	1/1	0.81	0.11	60,60,60,60	0
57	MG	BA	3715	1/1	0.81	0.14	63,63,63,63	0
57	MG	DA	3402	1/1	0.81	0.10	66,66,66,66	0
57	MG	BA	3172	1/1	0.81	0.19	46,46,46,46	0
57	MG	DA	3408	1/1	0.81	0.08	58,58,58,58	0
57	MG	CA	3146	1/1	0.81	0.19	66,66,66,66	0
57	MG	BB	218	1/1	0.81	0.22	77,77,77,77	0
57	MG	DA	3669	1/1	0.81	0.25	55,55,55,55	0
57	MG	AA	3170	1/1	0.81	0.13	75,75,75,75	0
57	MG	DA	3451	1/1	0.81	0.16	55,55,55,55	0
57	MG	BA	3463	1/1	0.81	0.20	48,48,48,48	0
57	MG	AA	3183	1/1	0.81	0.15	65,65,65,65	0
57	MG	DG	3001	1/1	0.81	0.09	55,55,55,55	0
57	MG	BA	3066	1/1	0.81	0.19	49,49,49,49	0
57	MG	CX	3003	1/1	0.81	0.22	54,54,54,54	0
57	MG	BA	3316	1/1	0.81	0.12	66,66,66,66	0
57	MG	AA	3138	1/1	0.81	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	3107	1/1	0.82	0.20	80,80,80,80	0
57	MG	CA	3109	1/1	0.82	0.13	67,67,67,67	0
57	MG	DA	3333	1/1	0.82	0.13	41,41,41,41	0
57	MG	DA	3582	1/1	0.82	0.07	56,56,56,56	0
57	MG	BA	3242	1/1	0.82	0.21	55,55,55,55	0
57	MG	CA	3149	1/1	0.82	0.14	52,52,52,52	0
57	MG	DA	3342	1/1	0.82	0.11	42,42,42,42	0
57	MG	BA	3273	1/1	0.82	0.22	54,54,54,54	0
57	MG	DA	3394	1/1	0.82	0.18	65,65,65,65	0
57	MG	BA	3473	1/1	0.82	0.19	56,56,56,56	0
57	MG	BA	3695	1/1	0.82	0.18	67,67,67,67	0
57	MG	DA	3628	1/1	0.82	0.24	76,76,76,76	0
57	MG	DA	3630	1/1	0.82	0.19	61,61,61,61	0
57	MG	DA	3406	1/1	0.82	0.11	51,51,51,51	0
57	MG	BA	3317	1/1	0.82	0.18	53,53,53,53	0
57	MG	BA	3760	1/1	0.82	0.19	44,44,44,44	0
57	MG	BA	3761	1/1	0.82	0.16	59,59,59,59	0
57	MG	BA	3707	1/1	0.82	0.24	44,44,44,44	0
57	MG	BA	3709	1/1	0.82	0.20	62,62,62,62	0
57	MG	DA	3487	1/1	0.82	0.21	62,62,62,62	0
57	MG	DA	3513	1/1	0.82	0.16	52,52,52,52	0
57	MG	BA	3418	1/1	0.82	0.17	30,30,30,30	0
57	MG	DA	3276	1/1	0.82	0.12	49,49,49,49	0
57	MG	DA	3308	1/1	0.82	0.15	61,61,61,61	0
57	MG	BA	3335	1/1	0.82	0.23	52,52,52,52	0
57	MG	BA	3342	1/1	0.82	0.10	46,46,46,46	0
57	MG	DA	3553	1/1	0.82	0.10	49,49,49,49	0
57	MG	BA	3587	1/1	0.83	0.17	36,36,36,36	0
57	MG	BA	3594	1/1	0.83	0.12	40,40,40,40	0
57	MG	AA	3002	1/1	0.83	0.15	71,71,71,71	0
57	MG	AA	3017	1/1	0.83	0.18	71,71,71,71	0
57	MG	BA	3434	1/1	0.83	0.13	55,55,55,55	0
57	MG	B5	101	1/1	0.83	0.24	51,51,51,51	0
57	MG	DA	3075	1/1	0.83	0.29	59,59,59,59	0
57	MG	CA	3009	1/1	0.83	0.11	64,64,64,64	0
57	MG	BA	3446	1/1	0.83	0.17	40,40,40,40	0
57	MG	AA	3020	1/1	0.83	0.13	76,76,76,76	0
57	MG	DA	3385	1/1	0.83	0.11	52,52,52,52	0
57	MG	BA	3154	1/1	0.83	0.23	47,47,47,47	0
57	MG	BA	3669	1/1	0.83	0.09	62,62,62,62	0
57	MG	BA	3759	1/1	0.83	0.18	33,33,33,33	0
57	MG	CA	3058	1/1	0.83	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	3127	1/1	0.83	0.16	65,65,65,65	0
57	MG	AA	3189	1/1	0.83	0.12	65,65,65,65	0
57	MG	CA	3087	1/1	0.83	0.19	67,67,67,67	0
57	MG	DA	3422	1/1	0.83	0.08	46,46,46,46	0
57	MG	DA	3446	1/1	0.83	0.11	45,45,45,45	0
57	MG	BA	3769	1/1	0.83	0.18	52,52,52,52	0
57	MG	AA	3023	1/1	0.83	0.13	74,74,74,74	0
57	MG	BA	3372	1/1	0.83	0.16	28,28,28,28	0
57	MG	BA	3788	1/1	0.83	0.15	51,51,51,51	0
57	MG	BA	3802	1/1	0.83	0.47	54,54,54,54	0
57	MG	AA	3139	1/1	0.83	0.14	59,59,59,59	0
57	MG	DA	3268	1/1	0.83	0.17	51,51,51,51	0
57	MG	AA	3008	1/1	0.83	0.27	73,73,73,73	0
57	MG	DA	3544	1/1	0.83	0.12	65,65,65,65	0
57	MG	CA	3066	1/1	0.84	0.14	66,66,66,66	0
57	MG	DA	3071	1/1	0.84	0.13	59,59,59,59	0
57	MG	BA	3129	1/1	0.84	0.28	58,58,58,58	0
57	MG	BA	3404	1/1	0.84	0.13	59,59,59,59	0
57	MG	BA	3480	1/1	0.84	0.20	35,35,35,35	0
57	MG	CA	3098	1/1	0.84	0.09	65,65,65,65	0
57	MG	DA	3088	1/1	0.84	0.18	47,47,47,47	0
57	MG	BA	3764	1/1	0.84	0.17	51,51,51,51	0
57	MG	DA	3122	1/1	0.84	0.11	49,49,49,49	0
57	MG	BA	3253	1/1	0.84	0.23	55,55,55,55	0
57	MG	DA	3147	1/1	0.84	0.15	56,56,56,56	0
57	MG	CA	3116	1/1	0.84	0.22	68,68,68,68	0
57	MG	CA	3140	1/1	0.84	0.15	67,67,67,67	0
57	MG	BA	3512	1/1	0.84	0.18	52,52,52,52	0
57	MG	AA	3025	1/1	0.84	0.24	62,62,62,62	0
57	MG	BA	3018	1/1	0.84	0.20	56,56,56,56	0
57	MG	BA	3794	1/1	0.84	0.26	51,51,51,51	0
57	MG	DA	3414	1/1	0.84	0.13	43,43,43,43	0
57	MG	CA	3021	1/1	0.84	0.14	61,61,61,61	0
57	MG	DA	3421	1/1	0.84	0.13	50,50,50,50	0
57	MG	DA	3247	1/1	0.84	0.09	45,45,45,45	0
57	MG	DA	3430	1/1	0.84	0.11	37,37,37,37	0
57	MG	DA	3646	1/1	0.84	0.14	59,59,59,59	0
57	MG	DA	3431	1/1	0.84	0.23	50,50,50,50	0
57	MG	BA	3179	1/1	0.84	0.17	50,50,50,50	0
57	MG	CV	101	1/1	0.84	0.13	72,72,72,72	0
57	MG	DA	3450	1/1	0.84	0.10	40,40,40,40	0
57	MG	BA	3438	1/1	0.84	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3468	1/1	0.84	0.27	66,66,66,66	0
57	MG	DA	3476	1/1	0.84	0.14	62,62,62,62	0
57	MG	AA	3005	1/1	0.84	0.14	62,62,62,62	0
57	MG	DA	3497	1/1	0.84	0.11	55,55,55,55	0
57	MG	BA	3391	1/1	0.84	0.24	63,63,63,63	0
57	MG	DA	3044	1/1	0.84	0.10	62,62,62,62	0
57	MG	CA	3141	1/1	0.85	0.04	92,92,92,92	0
57	MG	BA	3231	1/1	0.85	0.32	63,63,63,63	0
57	MG	BA	3506	1/1	0.85	0.10	58,58,58,58	0
57	MG	DA	3498	1/1	0.85	0.08	51,51,51,51	0
57	MG	AA	3073	1/1	0.85	0.10	56,56,56,56	0
57	MG	CA	3158	1/1	0.85	0.13	67,67,67,67	0
57	MG	BB	220	1/1	0.85	0.13	57,57,57,57	0
57	MG	AA	3079	1/1	0.85	0.13	68,68,68,68	0
57	MG	AA	3033	1/1	0.85	0.14	59,59,59,59	0
57	MG	B2	3001	1/1	0.85	0.21	56,56,56,56	0
57	MG	BA	3718	1/1	0.85	0.11	71,71,71,71	0
57	MG	BA	3546	1/1	0.85	0.19	40,40,40,40	0
57	MG	AA	3166	1/1	0.85	0.14	69,69,69,69	0
57	MG	BA	3293	1/1	0.85	0.26	50,50,50,50	0
57	MG	CA	3016	1/1	0.85	0.11	57,57,57,57	0
57	MG	DA	3571	1/1	0.85	0.12	56,56,56,56	0
57	MG	DA	3069	1/1	0.85	0.23	57,57,57,57	0
57	MG	BA	3296	1/1	0.85	0.18	53,53,53,53	0
57	MG	DA	3362	1/1	0.85	0.21	44,44,44,44	0
57	MG	AA	3034	1/1	0.85	0.11	47,47,47,47	0
57	MG	BA	3754	1/1	0.85	0.18	48,48,48,48	0
57	MG	BA	3755	1/1	0.85	0.15	55,55,55,55	0
57	MG	BA	3432	1/1	0.85	0.14	58,58,58,58	0
57	MG	CA	3052	1/1	0.85	0.21	72,72,72,72	0
57	MG	BA	3301	1/1	0.85	0.13	60,60,60,60	0
57	MG	BA	3305	1/1	0.85	0.09	62,62,62,62	0
57	MG	DA	3410	1/1	0.85	0.13	53,53,53,53	0
57	MG	BA	3443	1/1	0.85	0.23	37,37,37,37	0
57	MG	DA	3139	1/1	0.85	0.17	53,53,53,53	0
57	MG	DA	3415	1/1	0.85	0.11	68,68,68,68	0
57	MG	AA	3041	1/1	0.85	0.21	46,46,46,46	0
57	MG	DA	3657	1/1	0.85	0.10	63,63,63,63	0
57	MG	DA	3661	1/1	0.85	0.16	62,62,62,62	0
57	MG	DA	3178	1/1	0.85	0.22	50,50,50,50	0
57	MG	DA	3180	1/1	0.85	0.20	42,42,42,42	0
57	MG	DA	3425	1/1	0.85	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3453	1/1	0.85	0.32	45,45,45,45	0
57	MG	BA	3456	1/1	0.85	0.18	49,49,49,49	0
57	MG	DE	303	1/1	0.85	0.12	54,54,54,54	0
57	MG	AA	3047	1/1	0.85	0.17	63,63,63,63	0
57	MG	AA	3184	1/1	0.85	0.12	60,60,60,60	0
57	MG	BA	3681	1/1	0.85	0.08	66,66,66,66	0
57	MG	DU	3002	1/1	0.85	0.40	55,55,55,55	0
57	MG	D0	101	1/1	0.85	0.08	71,71,71,71	0
57	MG	AA	3001	1/1	0.85	0.14	61,61,61,61	0
57	MG	AA	3196	1/1	0.85	0.21	74,74,74,74	0
57	MG	DA	3360	1/1	0.86	0.16	46,46,46,46	0
57	MG	DA	3138	1/1	0.86	0.13	55,55,55,55	0
57	MG	BA	3213	1/1	0.86	0.26	40,40,40,40	0
57	MG	BA	3447	1/1	0.86	0.10	72,72,72,72	0
57	MG	AA	3065	1/1	0.86	0.20	63,63,63,63	0
57	MG	AA	3214	1/1	0.86	0.17	73,73,73,73	0
57	MG	DA	3185	1/1	0.86	0.11	68,68,68,68	0
57	MG	AA	3177	1/1	0.86	0.08	66,66,66,66	0
57	MG	DA	3577	1/1	0.86	0.14	58,58,58,58	0
57	MG	BA	3598	1/1	0.86	0.14	63,63,63,63	0
57	MG	CE	3001	1/1	0.86	0.10	79,79,79,79	0
57	MG	BA	3601	1/1	0.86	0.12	55,55,55,55	0
57	MG	DA	3592	1/1	0.86	0.07	51,51,51,51	0
57	MG	CA	3033	1/1	0.86	0.19	71,71,71,71	0
57	MG	BA	3308	1/1	0.86	0.19	43,43,43,43	0
57	MG	BB	202	1/1	0.86	0.28	59,59,59,59	0
57	MG	BA	3165	1/1	0.86	0.17	45,45,45,45	0
57	MG	BA	3426	1/1	0.86	0.20	37,37,37,37	0
57	MG	DA	3035	1/1	0.86	0.20	52,52,52,52	0
57	MG	BA	3486	1/1	0.86	0.13	57,57,57,57	0
57	MG	AA	3192	1/1	0.86	0.14	71,71,71,71	0
57	MG	DA	3440	1/1	0.86	0.09	61,61,61,61	0
57	MG	DA	3641	1/1	0.86	0.20	69,69,69,69	0
57	MG	DA	3062	1/1	0.86	0.20	63,63,63,63	0
57	MG	CA	3073	1/1	0.86	0.14	57,57,57,57	0
57	MG	AA	3054	1/1	0.86	0.13	53,53,53,53	0
57	MG	DA	3654	1/1	0.86	0.12	56,56,56,56	0
57	MG	DA	3309	1/1	0.86	0.09	51,51,51,51	0
57	MG	DA	3658	1/1	0.86	0.12	62,62,62,62	0
57	MG	DA	3462	1/1	0.86	0.20	42,42,42,42	0
57	MG	DA	3667	1/1	0.86	0.12	50,50,50,50	0
57	MG	DA	3312	1/1	0.86	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BE	305	1/1	0.86	0.17	43,43,43,43	0
57	MG	DA	3484	1/1	0.86	0.12	62,62,62,62	0
57	MG	CA	3097	1/1	0.86	0.15	69,69,69,69	0
57	MG	DB	3012	1/1	0.86	0.33	61,61,61,61	0
57	MG	DA	3495	1/1	0.86	0.11	47,47,47,47	0
57	MG	BA	3274	1/1	0.86	0.14	49,49,49,49	0
57	MG	BA	3530	1/1	0.86	0.22	49,49,49,49	0
57	MG	BA	3284	1/1	0.86	0.27	43,43,43,43	0
57	MG	CA	3115	1/1	0.86	0.09	63,63,63,63	0
57	MG	DA	3523	1/1	0.86	0.10	59,59,59,59	0
57	MG	DA	3528	1/1	0.86	0.15	62,62,62,62	0
57	MG	BA	3680	1/1	0.86	0.11	68,68,68,68	0
57	MG	BA	3180	1/1	0.86	0.17	47,47,47,47	0
57	MG	AA	3038	1/1	0.87	0.33	68,68,68,68	0
57	MG	BX	3002	1/1	0.87	0.19	46,46,46,46	0
57	MG	CA	3168	1/1	0.87	0.11	56,56,56,56	0
57	MG	AA	3197	1/1	0.87	0.26	70,70,70,70	0
57	MG	DA	3521	1/1	0.87	0.13	58,58,58,58	0
57	MG	BA	3583	1/1	0.87	0.21	45,45,45,45	0
57	MG	BA	3584	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	3283	1/1	0.87	0.11	51,51,51,51	0
57	MG	AA	3121	1/1	0.87	0.12	70,70,70,70	0
57	MG	BA	3206	1/1	0.87	0.23	49,49,49,49	0
57	MG	BA	3732	1/1	0.87	0.26	51,51,51,51	0
57	MG	DA	3002	1/1	0.87	0.10	48,48,48,48	0
57	MG	DA	3007	1/1	0.87	0.14	50,50,50,50	0
57	MG	AA	3124	1/1	0.87	0.09	47,47,47,47	0
57	MG	DA	3558	1/1	0.87	0.17	61,61,61,61	0
57	MG	BA	3742	1/1	0.87	0.24	65,65,65,65	0
57	MG	BA	3318	1/1	0.87	0.12	41,41,41,41	0
57	MG	AA	3049	1/1	0.87	0.21	64,64,64,64	0
57	MG	DA	3575	1/1	0.87	0.14	64,64,64,64	0
57	MG	DA	3339	1/1	0.87	0.15	61,61,61,61	0
57	MG	DA	3061	1/1	0.87	0.13	48,48,48,48	0
57	MG	CA	3027	1/1	0.87	0.20	64,64,64,64	0
57	MG	DA	3356	1/1	0.87	0.10	36,36,36,36	0
57	MG	AA	3051	1/1	0.87	0.23	73,73,73,73	0
57	MG	DA	3361	1/1	0.87	0.12	44,44,44,44	0
57	MG	BA	3071	1/1	0.87	0.35	59,59,59,59	0
57	MG	BA	3074	1/1	0.87	0.21	46,46,46,46	0
57	MG	BA	3637	1/1	0.87	0.11	39,39,39,39	0
57	MG	AA	3031	1/1	0.87	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3400	1/1	0.87	0.12	54,54,54,54	0
57	MG	BA	3386	1/1	0.87	0.16	53,53,53,53	0
57	MG	DA	3632	1/1	0.87	0.15	36,36,36,36	0
57	MG	BA	3658	1/1	0.87	0.26	61,61,61,61	0
57	MG	DA	3110	1/1	0.87	0.31	58,58,58,58	0
57	MG	BA	3780	1/1	0.87	0.11	62,62,62,62	0
57	MG	BA	3258	1/1	0.87	0.13	44,44,44,44	0
57	MG	AA	3089	1/1	0.87	0.15	60,60,60,60	0
57	MG	CA	3090	1/1	0.87	0.10	67,67,67,67	0
57	MG	BA	3128	1/1	0.87	0.14	69,69,69,69	0
57	MG	DA	3140	1/1	0.87	0.15	58,58,58,58	0
57	MG	AA	3190	1/1	0.87	0.10	58,58,58,58	0
57	MG	DA	3659	1/1	0.87	0.14	48,48,48,48	0
57	MG	DA	3148	1/1	0.87	0.12	54,54,54,54	0
57	MG	BA	3513	1/1	0.87	0.15	59,59,59,59	0
57	MG	BA	3684	1/1	0.87	0.12	68,68,68,68	0
57	MG	BB	211	1/1	0.87	0.10	51,51,51,51	0
57	MG	DA	3676	1/1	0.87	0.33	67,67,67,67	0
57	MG	DA	3437	1/1	0.87	0.16	52,52,52,52	0
57	MG	BA	3419	1/1	0.87	0.23	37,37,37,37	0
57	MG	CA	3124	1/1	0.87	0.12	59,59,59,59	0
57	MG	CA	3138	1/1	0.87	0.19	80,80,80,80	0
57	MG	DA	3217	1/1	0.87	0.14	38,38,38,38	0
57	MG	DF	3001	1/1	0.87	0.20	44,44,44,44	0
57	MG	BA	3147	1/1	0.87	0.16	45,45,45,45	0
57	MG	BA	3001	1/1	0.87	0.14	53,53,53,53	0
57	MG	DQ	3004	1/1	0.87	0.28	54,54,54,54	0
57	MG	BA	3545	1/1	0.87	0.14	65,65,65,65	0
57	MG	DA	3240	1/1	0.87	0.09	48,48,48,48	0
57	MG	DA	3242	1/1	0.87	0.11	52,52,52,52	0
57	MG	AA	3045	1/1	0.87	0.12	58,58,58,58	0
57	MG	BA	3548	1/1	0.87	0.17	40,40,40,40	0
57	MG	AA	3200	1/1	0.88	0.08	73,73,73,73	0
57	MG	BA	3297	1/1	0.88	0.14	43,43,43,43	0
57	MG	CA	3157	1/1	0.88	0.11	58,58,58,58	0
57	MG	BA	3006	1/1	0.88	0.19	48,48,48,48	0
57	MG	CA	3163	1/1	0.88	0.09	63,63,63,63	0
57	MG	AA	3094	1/1	0.88	0.17	59,59,59,59	0
57	MG	BA	3162	1/1	0.88	0.15	38,38,38,38	0
57	MG	DA	3526	1/1	0.88	0.11	48,48,48,48	0
57	MG	DA	3527	1/1	0.88	0.12	60,60,60,60	0
57	MG	DA	3274	1/1	0.88	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	3026	1/1	0.88	0.13	70,70,70,70	0
57	MG	BA	3030	1/1	0.88	0.18	46,46,46,46	0
57	MG	DA	3288	1/1	0.88	0.14	52,52,52,52	0
57	MG	BA	3673	1/1	0.88	0.17	55,55,55,55	0
57	MG	BA	3471	1/1	0.88	0.27	53,53,53,53	0
57	MG	BA	3679	1/1	0.88	0.12	62,62,62,62	0
57	MG	BA	3033	1/1	0.88	0.29	53,53,53,53	0
57	MG	AA	3145	1/1	0.88	0.12	66,66,66,66	0
57	MG	BA	3333	1/1	0.88	0.20	38,38,38,38	0
57	MG	DA	3323	1/1	0.88	0.11	50,50,50,50	0
57	MG	DA	3567	1/1	0.88	0.27	62,62,62,62	0
57	MG	BA	3502	1/1	0.88	0.12	56,56,56,56	0
57	MG	DA	3572	1/1	0.88	0.06	62,62,62,62	0
57	MG	B7	105	1/1	0.88	0.16	56,56,56,56	0
57	MG	DA	3334	1/1	0.88	0.15	52,52,52,52	0
57	MG	CA	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	DA	3056	1/1	0.88	0.09	51,51,51,51	0
57	MG	BA	3185	1/1	0.88	0.19	57,57,57,57	0
57	MG	DA	3590	1/1	0.88	0.10	51,51,51,51	0
57	MG	DA	3591	1/1	0.88	0.17	55,55,55,55	0
57	MG	BA	3337	1/1	0.88	0.17	58,58,58,58	0
57	MG	DA	3603	1/1	0.88	0.06	41,41,41,41	0
57	MG	DA	3606	1/1	0.88	0.10	71,71,71,71	0
57	MG	AA	3107	1/1	0.88	0.18	64,64,64,64	0
57	MG	BA	3212	1/1	0.88	0.24	54,54,54,54	0
57	MG	DA	3609	1/1	0.88	0.10	46,46,46,46	0
57	MG	BA	3710	1/1	0.88	0.17	57,57,57,57	0
57	MG	DA	3614	1/1	0.88	0.07	65,65,65,65	0
57	MG	BA	3514	1/1	0.88	0.23	48,48,48,48	0
57	MG	DA	3618	1/1	0.88	0.12	53,53,53,53	0
57	MG	DA	3367	1/1	0.88	0.14	61,61,61,61	0
57	MG	DA	3380	1/1	0.88	0.07	55,55,55,55	0
57	MG	BA	3526	1/1	0.88	0.17	44,44,44,44	0
57	MG	BA	3057	1/1	0.88	0.20	34,34,34,34	0
57	MG	DA	3388	1/1	0.88	0.15	53,53,53,53	0
57	MG	BA	3532	1/1	0.88	0.15	52,52,52,52	0
57	MG	DA	3636	1/1	0.88	0.32	63,63,63,63	0
57	MG	CA	3039	1/1	0.88	0.11	68,68,68,68	0
57	MG	DA	3092	1/1	0.88	0.18	45,45,45,45	0
57	MG	DA	3093	1/1	0.88	0.09	62,62,62,62	0
57	MG	AA	3046	1/1	0.88	0.22	55,55,55,55	0
57	MG	AX	3002	1/1	0.88	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AX	3010	1/1	0.88	0.21	59,59,59,59	0
57	MG	BA	3072	1/1	0.88	0.14	47,47,47,47	0
57	MG	AA	3072	1/1	0.88	0.12	66,66,66,66	0
57	MG	BA	3740	1/1	0.88	0.16	28,28,28,28	0
57	MG	BA	3409	1/1	0.88	0.16	30,30,30,30	0
57	MG	BA	3566	1/1	0.88	0.21	67,67,67,67	0
57	MG	AA	3019	1/1	0.88	0.11	66,66,66,66	0
57	MG	BA	3578	1/1	0.88	0.09	46,46,46,46	0
57	MG	DB	3002	1/1	0.88	0.17	65,65,65,65	0
57	MG	DB	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3266	1/1	0.88	0.19	39,39,39,39	0
57	MG	BA	3267	1/1	0.88	0.19	65,65,65,65	0
57	MG	AA	3128	1/1	0.88	0.08	57,57,57,57	0
57	MG	DA	3208	1/1	0.88	0.36	58,58,58,58	0
57	MG	BA	3117	1/1	0.88	0.20	59,59,59,59	0
57	MG	BA	3430	1/1	0.88	0.16	37,37,37,37	0
57	MG	DA	3216	1/1	0.88	0.22	56,56,56,56	0
57	MG	BA	3275	1/1	0.88	0.17	58,58,58,58	0
57	MG	BA	3122	1/1	0.88	0.15	41,41,41,41	0
57	MG	BA	3002	1/1	0.88	0.10	50,50,50,50	0
57	MG	DA	3469	1/1	0.88	0.28	44,44,44,44	0
57	MG	BA	3442	1/1	0.88	0.17	44,44,44,44	0
57	MG	BA	3619	1/1	0.88	0.20	58,58,58,58	0
57	MG	BA	3624	1/1	0.88	0.10	68,68,68,68	0
57	MG	BA	3397	1/1	0.89	0.15	30,30,30,30	0
57	MG	BA	3499	1/1	0.89	0.10	58,58,58,58	0
57	MG	DA	3470	1/1	0.89	0.19	45,45,45,45	0
57	MG	CA	3076	1/1	0.89	0.14	57,57,57,57	0
57	MG	DA	3481	1/1	0.89	0.41	55,55,55,55	0
57	MG	DA	3206	1/1	0.89	0.13	50,50,50,50	0
57	MG	CA	3081	1/1	0.89	0.09	46,46,46,46	0
57	MG	DA	3492	1/1	0.89	0.12	55,55,55,55	0
57	MG	BA	3399	1/1	0.89	0.20	45,45,45,45	0
57	MG	AA	3108	1/1	0.89	0.28	67,67,67,67	0
57	MG	BA	3640	1/1	0.89	0.17	53,53,53,53	0
57	MG	BA	3402	1/1	0.89	0.14	40,40,40,40	0
57	MG	BA	3092	1/1	0.89	0.16	37,37,37,37	0
57	MG	BA	3298	1/1	0.89	0.16	51,51,51,51	0
57	MG	DA	3223	1/1	0.89	0.15	50,50,50,50	0
57	MG	BA	3790	1/1	0.89	0.18	34,34,34,34	0
57	MG	BA	3793	1/1	0.89	0.13	40,40,40,40	0
57	MG	BA	3023	1/1	0.89	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3106	1/1	0.89	0.22	42,42,42,42	0
57	MG	CA	3128	1/1	0.89	0.15	65,65,65,65	0
57	MG	DA	3248	1/1	0.89	0.12	56,56,56,56	0
57	MG	BA	3810	1/1	0.89	0.18	41,41,41,41	0
57	MG	BA	3109	1/1	0.89	0.18	51,51,51,51	0
57	MG	AA	3042	1/1	0.89	0.09	57,57,57,57	0
57	MG	BA	3314	1/1	0.89	0.13	58,58,58,58	0
57	MG	BA	3315	1/1	0.89	0.19	31,31,31,31	0
57	MG	BA	3431	1/1	0.89	0.17	59,59,59,59	0
57	MG	DA	3564	1/1	0.89	0.16	61,61,61,61	0
57	MG	DA	3275	1/1	0.89	0.17	42,42,42,42	0
57	MG	CA	3156	1/1	0.89	0.10	73,73,73,73	0
57	MG	BA	3032	1/1	0.89	0.20	47,47,47,47	0
57	MG	AA	3209	1/1	0.89	0.08	59,59,59,59	0
57	MG	CA	3159	1/1	0.89	0.18	70,70,70,70	0
57	MG	BE	301	1/1	0.89	0.14	35,35,35,35	0
57	MG	DA	3311	1/1	0.89	0.17	54,54,54,54	0
57	MG	BA	3697	1/1	0.89	0.17	61,61,61,61	0
57	MG	DA	3313	1/1	0.89	0.16	47,47,47,47	0
57	MG	BA	3703	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3125	1/1	0.89	0.17	47,47,47,47	0
57	MG	BQ	3005	1/1	0.89	0.13	49,49,49,49	0
57	MG	DA	3593	1/1	0.89	0.11	40,40,40,40	0
57	MG	BU	201	1/1	0.89	0.15	43,43,43,43	0
57	MG	DA	3605	1/1	0.89	0.12	58,58,58,58	0
57	MG	BV	203	1/1	0.89	0.19	38,38,38,38	0
57	MG	DA	3332	1/1	0.89	0.11	53,53,53,53	0
57	MG	BA	3324	1/1	0.89	0.17	45,45,45,45	0
57	MG	BZ	3001	1/1	0.89	0.29	55,55,55,55	0
57	MG	AA	3210	1/1	0.89	0.27	59,59,59,59	0
57	MG	BA	3573	1/1	0.89	0.16	51,51,51,51	0
57	MG	BA	3444	1/1	0.89	0.21	29,29,29,29	0
57	MG	BA	3445	1/1	0.89	0.30	63,63,63,63	0
57	MG	DA	3355	1/1	0.89	0.12	58,58,58,58	0
57	MG	DA	3621	1/1	0.89	0.08	44,44,44,44	0
57	MG	DA	3626	1/1	0.89	0.07	67,67,67,67	0
57	MG	AA	3102	1/1	0.89	0.25	59,59,59,59	0
57	MG	CA	3004	1/1	0.89	0.25	66,66,66,66	0
57	MG	BA	3131	1/1	0.89	0.11	58,58,58,58	0
57	MG	BA	3590	1/1	0.89	0.16	50,50,50,50	0
57	MG	AA	3176	1/1	0.89	0.10	67,67,67,67	0
57	MG	DA	3371	1/1	0.89	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3638	1/1	0.89	0.10	51,51,51,51	0
57	MG	DA	3066	1/1	0.89	0.10	42,42,42,42	0
57	MG	BA	3596	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3058	1/1	0.89	0.15	49,49,49,49	0
57	MG	CA	3020	1/1	0.89	0.11	56,56,56,56	0
57	MG	BA	3361	1/1	0.89	0.13	49,49,49,49	0
57	MG	DA	3077	1/1	0.89	0.23	61,61,61,61	0
57	MG	CA	3022	1/1	0.89	0.20	78,78,78,78	0
57	MG	AM	201	1/1	0.89	0.16	51,51,51,51	0
57	MG	BA	3741	1/1	0.89	0.74	64,64,64,64	0
57	MG	DA	3090	1/1	0.89	0.10	52,52,52,52	0
57	MG	AA	3064	1/1	0.89	0.24	60,60,60,60	0
57	MG	CA	3036	1/1	0.89	0.14	66,66,66,66	0
57	MG	DA	3095	1/1	0.89	0.15	58,58,58,58	0
57	MG	DA	3098	1/1	0.89	0.17	53,53,53,53	0
57	MG	DA	3106	1/1	0.89	0.13	52,52,52,52	0
57	MG	DA	3420	1/1	0.89	0.24	60,60,60,60	0
57	MG	BA	3745	1/1	0.89	0.08	75,75,75,75	0
57	MG	CA	3041	1/1	0.89	0.13	59,59,59,59	0
57	MG	CA	3044	1/1	0.89	0.23	62,62,62,62	0
57	MG	DA	3124	1/1	0.89	0.15	57,57,57,57	0
57	MG	BA	3749	1/1	0.89	0.12	56,56,56,56	0
57	MG	BA	3008	1/1	0.89	0.17	47,47,47,47	0
57	MG	BA	3618	1/1	0.89	0.14	65,65,65,65	0
57	MG	DP	202	1/1	0.89	0.11	53,53,53,53	0
57	MG	DA	3444	1/1	0.89	0.06	44,44,44,44	0
57	MG	CA	3061	1/1	0.89	0.28	66,66,66,66	0
57	MG	CA	3062	1/1	0.89	0.17	64,64,64,64	0
57	MG	DX	101	1/1	0.89	0.12	51,51,51,51	0
57	MG	AA	3093	1/1	0.89	0.12	66,66,66,66	0
57	MG	DA	3151	1/1	0.89	0.09	55,55,55,55	0
57	MG	BA	3622	1/1	0.89	0.19	48,48,48,48	0
57	MG	CA	3002	1/1	0.90	0.12	63,63,63,63	0
57	MG	BA	3599	1/1	0.90	0.21	43,43,43,43	0
57	MG	AA	3143	1/1	0.90	0.08	60,60,60,60	0
57	MG	DA	3245	1/1	0.90	0.12	54,54,54,54	0
57	MG	CA	3006	1/1	0.90	0.14	64,64,64,64	0
57	MG	AA	3211	1/1	0.90	0.12	47,47,47,47	0
57	MG	DA	3499	1/1	0.90	0.10	53,53,53,53	0
57	MG	DA	3502	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3612	1/1	0.90	0.14	21,21,21,21	0
57	MG	BA	3485	1/1	0.90	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3192	1/1	0.90	0.28	46,46,46,46	0
57	MG	BA	3195	1/1	0.90	0.11	46,46,46,46	0
57	MG	DA	3524	1/1	0.90	0.17	61,61,61,61	0
57	MG	BA	3501	1/1	0.90	0.23	71,71,71,71	0
57	MG	DA	3270	1/1	0.90	0.10	46,46,46,46	0
57	MG	DA	3271	1/1	0.90	0.15	48,48,48,48	0
57	MG	DA	3018	1/1	0.90	0.20	62,62,62,62	0
57	MG	BA	3199	1/1	0.90	0.15	46,46,46,46	0
57	MG	DA	3033	1/1	0.90	0.10	42,42,42,42	0
57	MG	DA	3280	1/1	0.90	0.16	33,33,33,33	0
57	MG	BA	3623	1/1	0.90	0.26	55,55,55,55	0
57	MG	DA	3547	1/1	0.90	0.14	54,54,54,54	0
57	MG	BA	3411	1/1	0.90	0.19	33,33,33,33	0
57	MG	DA	3301	1/1	0.90	0.19	52,52,52,52	0
57	MG	DA	3556	1/1	0.90	0.11	67,67,67,67	0
57	MG	DA	3051	1/1	0.90	0.11	48,48,48,48	0
57	MG	CA	3026	1/1	0.90	0.20	63,63,63,63	0
57	MG	BA	3634	1/1	0.90	0.14	62,62,62,62	0
57	MG	BA	3104	1/1	0.90	0.13	42,42,42,42	0
57	MG	BA	3312	1/1	0.90	0.18	32,32,32,32	0
57	MG	DA	3314	1/1	0.90	0.12	43,43,43,43	0
57	MG	CA	3038	1/1	0.90	0.14	58,58,58,58	0
57	MG	AA	3100	1/1	0.90	0.12	65,65,65,65	0
57	MG	DA	3070	1/1	0.90	0.13	58,58,58,58	0
57	MG	AA	3185	1/1	0.90	0.12	82,82,82,82	0
57	MG	DA	3328	1/1	0.90	0.08	47,47,47,47	0
57	MG	AA	3187	1/1	0.90	0.13	62,62,62,62	0
57	MG	BA	3648	1/1	0.90	0.11	65,65,65,65	0
57	MG	BA	3429	1/1	0.90	0.10	65,65,65,65	0
57	MG	CA	3054	1/1	0.90	0.30	69,69,69,69	0
57	MG	CA	3057	1/1	0.90	0.18	76,76,76,76	0
57	MG	DA	3337	1/1	0.90	0.13	41,41,41,41	0
57	MG	BA	3659	1/1	0.90	0.19	61,61,61,61	0
57	MG	BA	3664	1/1	0.90	0.16	55,55,55,55	0
57	MG	BA	3666	1/1	0.90	0.19	50,50,50,50	0
57	MG	AA	3146	1/1	0.90	0.13	66,66,66,66	0
57	MG	AA	3059	1/1	0.90	0.12	78,78,78,78	0
57	MG	BA	3047	1/1	0.90	0.22	60,60,60,60	0
57	MG	DA	3103	1/1	0.90	0.10	58,58,58,58	0
57	MG	DA	3615	1/1	0.90	0.09	65,65,65,65	0
57	MG	BA	3541	1/1	0.90	0.16	38,38,38,38	0
57	MG	BA	3811	1/1	0.90	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	3036	1/1	0.90	0.17	61,61,61,61	0
57	MG	DA	3378	1/1	0.90	0.13	57,57,57,57	0
57	MG	DA	3119	1/1	0.90	0.22	39,39,39,39	0
57	MG	AA	3194	1/1	0.90	0.11	56,56,56,56	0
57	MG	BB	210	1/1	0.90	0.07	61,61,61,61	0
57	MG	AA	3057	1/1	0.90	0.22	64,64,64,64	0
57	MG	DA	3126	1/1	0.90	0.08	55,55,55,55	0
57	MG	DA	3129	1/1	0.90	0.12	46,46,46,46	0
57	MG	DA	3401	1/1	0.90	0.10	38,38,38,38	0
57	MG	DA	3132	1/1	0.90	0.23	52,52,52,52	0
57	MG	DA	3133	1/1	0.90	0.22	50,50,50,50	0
57	MG	BA	3550	1/1	0.90	0.19	36,36,36,36	0
57	MG	BA	3686	1/1	0.90	0.25	60,60,60,60	0
57	MG	AA	3135	1/1	0.90	0.24	65,65,65,65	0
57	MG	DA	3141	1/1	0.90	0.27	61,61,61,61	0
57	MG	DA	3146	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3351	1/1	0.90	0.17	30,30,30,30	0
57	MG	BD	309	1/1	0.90	0.32	57,57,57,57	0
57	MG	AX	3016	1/1	0.90	0.10	56,56,56,56	0
57	MG	DA	3666	1/1	0.90	0.14	35,35,35,35	0
57	MG	BA	3700	1/1	0.90	0.16	61,61,61,61	0
57	MG	BA	3702	1/1	0.90	0.27	51,51,51,51	0
57	MG	DA	3424	1/1	0.90	0.09	61,61,61,61	0
57	MG	CA	3130	1/1	0.90	0.09	57,57,57,57	0
57	MG	DA	3677	1/1	0.90	0.47	52,52,52,52	0
57	MG	DB	3001	1/1	0.90	0.17	64,64,64,64	0
57	MG	AA	3058	1/1	0.90	0.28	59,59,59,59	0
57	MG	BN	3004	1/1	0.90	0.12	60,60,60,60	0
57	MG	DB	3004	1/1	0.90	0.15	55,55,55,55	0
57	MG	AA	3204	1/1	0.90	0.13	53,53,53,53	0
57	MG	DA	3209	1/1	0.90	0.24	53,53,53,53	0
57	MG	BA	3581	1/1	0.90	0.19	30,30,30,30	0
57	MG	BA	3276	1/1	0.90	0.31	54,54,54,54	0
57	MG	DA	3214	1/1	0.90	0.24	59,59,59,59	0
57	MG	DA	3215	1/1	0.90	0.13	59,59,59,59	0
57	MG	AA	3117	1/1	0.90	0.12	79,79,79,79	0
57	MG	DA	3452	1/1	0.90	0.16	51,51,51,51	0
57	MG	BA	3461	1/1	0.90	0.10	62,62,62,62	0
57	MG	DA	3463	1/1	0.90	0.14	55,55,55,55	0
57	MG	DA	3465	1/1	0.90	0.12	46,46,46,46	0
57	MG	BA	3177	1/1	0.90	0.19	46,46,46,46	0
57	MG	DA	3221	1/1	0.90	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3465	1/1	0.90	0.18	43,43,43,43	0
57	MG	BA	3394	1/1	0.90	0.18	40,40,40,40	0
59	ZN	DY	501	1/1	0.90	0.15	96,96,96,96	0
57	MG	AA	3142	1/1	0.90	0.11	41,41,41,41	0
57	MG	DA	3170	1/1	0.91	0.12	53,53,53,53	0
57	MG	AX	3003	1/1	0.91	0.13	71,71,71,71	0
57	MG	CA	3091	1/1	0.91	0.12	55,55,55,55	0
57	MG	BA	3366	1/1	0.91	0.12	57,57,57,57	0
57	MG	BA	3495	1/1	0.91	0.13	37,37,37,37	0
57	MG	CA	3100	1/1	0.91	0.09	52,52,52,52	0
57	MG	BA	3255	1/1	0.91	0.15	47,47,47,47	0
57	MG	BB	206	1/1	0.91	0.30	47,47,47,47	0
57	MG	CA	3111	1/1	0.91	0.16	64,64,64,64	0
57	MG	BA	3650	1/1	0.91	0.12	52,52,52,52	0
57	MG	BA	3654	1/1	0.91	0.20	57,57,57,57	0
57	MG	DA	3494	1/1	0.91	0.12	47,47,47,47	0
57	MG	CA	3118	1/1	0.91	0.19	68,68,68,68	0
57	MG	AX	3007	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3126	1/1	0.91	0.16	54,54,54,54	0
57	MG	CA	3129	1/1	0.91	0.09	43,43,43,43	0
57	MG	AA	3080	1/1	0.91	0.21	58,58,58,58	0
57	MG	BA	3396	1/1	0.91	0.15	50,50,50,50	0
57	MG	BA	3668	1/1	0.91	0.17	53,53,53,53	0
57	MG	BD	302	1/1	0.91	0.27	50,50,50,50	0
57	MG	DA	3236	1/1	0.91	0.26	47,47,47,47	0
57	MG	DA	3239	1/1	0.91	0.24	56,56,56,56	0
57	MG	CA	3144	1/1	0.91	0.19	71,71,71,71	0
57	MG	BA	3507	1/1	0.91	0.20	49,49,49,49	0
57	MG	DA	3243	1/1	0.91	0.12	55,55,55,55	0
57	MG	BA	3508	1/1	0.91	0.20	51,51,51,51	0
57	MG	CA	3150	1/1	0.91	0.21	56,56,56,56	0
57	MG	AA	3003	1/1	0.91	0.30	72,72,72,72	0
57	MG	DA	3538	1/1	0.91	0.11	58,58,58,58	0
57	MG	CA	3153	1/1	0.91	0.16	70,70,70,70	0
57	MG	BA	3269	1/1	0.91	0.16	53,53,53,53	0
57	MG	BA	3400	1/1	0.91	0.21	33,33,33,33	0
57	MG	DA	3550	1/1	0.91	0.13	57,57,57,57	0
57	MG	BN	3002	1/1	0.91	0.16	39,39,39,39	0
57	MG	AA	3131	1/1	0.91	0.15	71,71,71,71	0
57	MG	CA	3160	1/1	0.91	0.17	62,62,62,62	0
57	MG	BO	201	1/1	0.91	0.19	50,50,50,50	0
57	MG	BO	202	1/1	0.91	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3143	1/1	0.91	0.26	45,45,45,45	0
57	MG	BA	3683	1/1	0.91	0.15	73,73,73,73	0
57	MG	AA	3133	1/1	0.91	0.16	56,56,56,56	0
57	MG	DA	3279	1/1	0.91	0.12	56,56,56,56	0
57	MG	BA	3405	1/1	0.91	0.19	63,63,63,63	0
57	MG	BA	3150	1/1	0.91	0.17	55,55,55,55	0
57	MG	CW	3001	1/1	0.91	0.22	67,67,67,67	0
57	MG	B1	101	1/1	0.91	0.50	51,51,51,51	0
57	MG	AA	3188	1/1	0.91	0.08	69,69,69,69	0
57	MG	DA	3588	1/1	0.91	0.30	65,65,65,65	0
57	MG	BA	3413	1/1	0.91	0.13	47,47,47,47	0
57	MG	DA	3004	1/1	0.91	0.17	40,40,40,40	0
57	MG	BA	3285	1/1	0.91	0.27	50,50,50,50	0
57	MG	DA	3011	1/1	0.91	0.08	48,48,48,48	0
57	MG	B7	104	1/1	0.91	0.27	48,48,48,48	0
57	MG	BA	3061	1/1	0.91	0.23	29,29,29,29	0
57	MG	DA	3604	1/1	0.91	0.18	59,59,59,59	0
57	MG	DA	3317	1/1	0.91	0.12	44,44,44,44	0
57	MG	BA	3164	1/1	0.91	0.21	48,48,48,48	0
57	MG	BA	3423	1/1	0.91	0.18	44,44,44,44	0
57	MG	DA	3038	1/1	0.91	0.16	47,47,47,47	0
57	MG	BA	3561	1/1	0.91	0.12	45,45,45,45	0
57	MG	DA	3049	1/1	0.91	0.27	52,52,52,52	0
57	MG	BA	3562	1/1	0.91	0.14	37,37,37,37	0
57	MG	CA	3007	1/1	0.91	0.13	57,57,57,57	0
57	MG	AA	3162	1/1	0.91	0.07	66,66,66,66	0
57	MG	CA	3011	1/1	0.91	0.23	61,61,61,61	0
57	MG	CA	3012	1/1	0.91	0.21	60,60,60,60	0
57	MG	AA	3066	1/1	0.91	0.31	60,60,60,60	0
57	MG	DA	3622	1/1	0.91	0.21	61,61,61,61	0
57	MG	BA	3005	1/1	0.91	0.16	30,30,30,30	0
57	MG	BA	3575	1/1	0.91	0.12	48,48,48,48	0
57	MG	AA	3028	1/1	0.91	0.22	76,76,76,76	0
57	MG	BA	3303	1/1	0.91	0.17	36,36,36,36	0
57	MG	BA	3304	1/1	0.91	0.15	67,67,67,67	0
57	MG	BA	3433	1/1	0.91	0.20	32,32,32,32	0
57	MG	BA	3073	1/1	0.91	0.22	61,61,61,61	0
57	MG	BA	3007	1/1	0.91	0.19	55,55,55,55	0
57	MG	DA	3085	1/1	0.91	0.08	53,53,53,53	0
57	MG	AA	3030	1/1	0.91	0.18	60,60,60,60	0
57	MG	DA	3643	1/1	0.91	0.13	61,61,61,61	0
57	MG	CA	3028	1/1	0.91	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AN	502	1/1	0.91	0.29	63,63,63,63	0
57	MG	DA	3653	1/1	0.91	0.14	52,52,52,52	0
57	MG	BA	3019	1/1	0.91	0.15	42,42,42,42	0
57	MG	AA	3063	1/1	0.91	0.10	35,35,35,35	0
57	MG	DA	3097	1/1	0.91	0.21	33,33,33,33	0
57	MG	BA	3746	1/1	0.91	0.11	51,51,51,51	0
57	MG	BA	3210	1/1	0.91	0.33	49,49,49,49	0
57	MG	BA	3750	1/1	0.91	0.17	27,27,27,27	0
57	MG	CA	3046	1/1	0.91	0.09	69,69,69,69	0
57	MG	DA	3405	1/1	0.91	0.16	46,46,46,46	0
57	MG	DA	3116	1/1	0.91	0.48	52,52,52,52	0
57	MG	DA	3407	1/1	0.91	0.04	66,66,66,66	0
57	MG	AA	3021	1/1	0.91	0.14	63,63,63,63	0
57	MG	BA	3606	1/1	0.91	0.14	61,61,61,61	0
57	MG	DA	3120	1/1	0.91	0.13	49,49,49,49	0
57	MG	BA	3321	1/1	0.91	0.24	55,55,55,55	0
57	MG	CA	3055	1/1	0.91	0.09	69,69,69,69	0
57	MG	BA	3024	1/1	0.91	0.19	49,49,49,49	0
57	MG	AA	3198	1/1	0.91	0.13	61,61,61,61	0
57	MG	BA	3226	1/1	0.91	0.27	47,47,47,47	0
57	MG	DA	3130	1/1	0.91	0.18	52,52,52,52	0
57	MG	DD	309	1/1	0.91	0.20	59,59,59,59	0
57	MG	BA	3227	1/1	0.91	0.24	57,57,57,57	0
57	MG	BA	3621	1/1	0.91	0.17	53,53,53,53	0
57	MG	DA	3429	1/1	0.91	0.14	41,41,41,41	0
57	MG	DA	3134	1/1	0.91	0.21	41,41,41,41	0
57	MG	BA	3466	1/1	0.91	0.17	49,49,49,49	0
57	MG	BA	3229	1/1	0.91	0.22	54,54,54,54	0
57	MG	BA	3120	1/1	0.91	0.21	55,55,55,55	0
57	MG	CA	3075	1/1	0.91	0.18	59,59,59,59	0
57	MG	BA	3631	1/1	0.91	0.18	42,42,42,42	0
57	MG	BA	3121	1/1	0.91	0.21	64,64,64,64	0
57	MG	BA	3478	1/1	0.91	0.19	58,58,58,58	0
57	MG	BA	3252	1/1	0.91	0.41	60,60,60,60	0
57	MG	DA	3165	1/1	0.91	0.24	57,57,57,57	0
57	MG	DA	3423	1/1	0.92	0.12	49,49,49,49	0
57	MG	AA	3115	1/1	0.92	0.09	79,79,79,79	0
57	MG	BA	3779	1/1	0.92	0.29	66,66,66,66	0
57	MG	BA	3051	1/1	0.92	0.19	43,43,43,43	0
57	MG	CA	3074	1/1	0.92	0.23	64,64,64,64	0
57	MG	BA	3239	1/1	0.92	0.34	48,48,48,48	0
57	MG	DA	3135	1/1	0.92	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3137	1/1	0.92	0.23	54,54,54,54	0
57	MG	BA	3346	1/1	0.92	0.10	27,27,27,27	0
57	MG	BA	3628	1/1	0.92	0.25	49,49,49,49	0
57	MG	BA	3347	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3240	1/1	0.92	0.40	47,47,47,47	0
57	MG	BA	3797	1/1	0.92	0.17	53,53,53,53	0
57	MG	BA	3799	1/1	0.92	0.06	49,49,49,49	0
57	MG	DA	3456	1/1	0.92	0.07	50,50,50,50	0
57	MG	CA	3095	1/1	0.92	0.14	64,64,64,64	0
57	MG	BA	3127	1/1	0.92	0.29	57,57,57,57	0
57	MG	DA	3153	1/1	0.92	0.19	47,47,47,47	0
57	MG	DA	3162	1/1	0.92	0.36	50,50,50,50	0
57	MG	DA	3164	1/1	0.92	0.12	51,51,51,51	0
57	MG	BA	3477	1/1	0.92	0.18	61,61,61,61	0
57	MG	DA	3473	1/1	0.92	0.12	50,50,50,50	0
57	MG	BA	3357	1/1	0.92	0.23	25,25,25,25	0
57	MG	DA	3478	1/1	0.92	0.12	59,59,59,59	0
57	MG	DA	3173	1/1	0.92	0.12	53,53,53,53	0
57	MG	BA	3812	1/1	0.92	0.28	47,47,47,47	0
57	MG	AA	3161	1/1	0.92	0.23	65,65,65,65	0
57	MG	AY	3003	1/1	0.92	0.30	53,53,53,53	0
57	MG	DA	3194	1/1	0.92	0.10	56,56,56,56	0
57	MG	CA	3112	1/1	0.92	0.15	69,69,69,69	0
57	MG	AA	3022	1/1	0.92	0.10	71,71,71,71	0
57	MG	BA	3493	1/1	0.92	0.16	58,58,58,58	0
57	MG	BA	3651	1/1	0.92	0.19	45,45,45,45	0
57	MG	CA	3120	1/1	0.92	0.18	64,64,64,64	0
57	MG	DA	3503	1/1	0.92	0.14	52,52,52,52	0
57	MG	DA	3505	1/1	0.92	0.08	56,56,56,56	0
57	MG	BA	3652	1/1	0.92	0.15	67,67,67,67	0
57	MG	BA	3369	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3134	1/1	0.92	0.17	48,48,48,48	0
57	MG	BB	219	1/1	0.92	0.11	67,67,67,67	0
57	MG	CA	3135	1/1	0.92	0.15	63,63,63,63	0
57	MG	BA	3385	1/1	0.92	0.16	59,59,59,59	0
57	MG	DA	3219	1/1	0.92	0.17	53,53,53,53	0
57	MG	BA	3662	1/1	0.92	0.10	61,61,61,61	0
57	MG	BA	3136	1/1	0.92	0.14	30,30,30,30	0
57	MG	BA	3387	1/1	0.92	0.15	54,54,54,54	0
57	MG	BA	3388	1/1	0.92	0.19	48,48,48,48	0
57	MG	BE	307	1/1	0.92	0.15	62,62,62,62	0
57	MG	DA	3543	1/1	0.92	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BF	302	1/1	0.92	0.18	46,46,46,46	0
57	MG	BA	3138	1/1	0.92	0.34	42,42,42,42	0
57	MG	AA	3163	1/1	0.92	0.18	56,56,56,56	0
57	MG	BG	202	1/1	0.92	0.21	41,41,41,41	0
57	MG	BA	3671	1/1	0.92	0.16	63,63,63,63	0
57	MG	BA	3145	1/1	0.92	0.10	44,44,44,44	0
57	MG	BA	3675	1/1	0.92	0.19	67,67,67,67	0
57	MG	BA	3271	1/1	0.92	0.17	58,58,58,58	0
57	MG	DA	3250	1/1	0.92	0.18	69,69,69,69	0
57	MG	DA	3251	1/1	0.92	0.17	62,62,62,62	0
57	MG	AA	3119	1/1	0.92	0.12	51,51,51,51	0
57	MG	BA	3515	1/1	0.92	0.12	53,53,53,53	0
57	MG	AA	3191	1/1	0.92	0.21	47,47,47,47	0
57	MG	BX	3001	1/1	0.92	0.82	48,48,48,48	0
57	MG	DA	3263	1/1	0.92	0.13	41,41,41,41	0
57	MG	DA	3576	1/1	0.92	0.09	53,53,53,53	0
57	MG	DA	3267	1/1	0.92	0.16	49,49,49,49	0
57	MG	BA	3151	1/1	0.92	0.26	52,52,52,52	0
57	MG	BX	3003	1/1	0.92	0.17	35,35,35,35	0
57	MG	DA	3586	1/1	0.92	0.16	60,60,60,60	0
57	MG	BY	502	1/1	0.92	0.25	40,40,40,40	0
57	MG	DA	3273	1/1	0.92	0.11	47,47,47,47	0
57	MG	AA	3037	1/1	0.92	0.22	55,55,55,55	0
57	MG	B0	102	1/1	0.92	0.22	48,48,48,48	0
57	MG	BA	3535	1/1	0.92	0.19	31,31,31,31	0
57	MG	DA	3001	1/1	0.92	0.17	60,60,60,60	0
57	MG	DA	3595	1/1	0.92	0.17	59,59,59,59	0
57	MG	BA	3403	1/1	0.92	0.08	54,54,54,54	0
57	MG	AA	3122	1/1	0.92	0.11	56,56,56,56	0
57	MG	AA	3171	1/1	0.92	0.10	51,51,51,51	0
57	MG	B6	102	1/1	0.92	0.11	68,68,68,68	0
57	MG	BA	3542	1/1	0.92	0.18	45,45,45,45	0
57	MG	BA	3407	1/1	0.92	0.15	47,47,47,47	0
57	MG	BA	3290	1/1	0.92	0.28	40,40,40,40	0
57	MG	BA	3292	1/1	0.92	0.15	48,48,48,48	0
57	MG	BA	3412	1/1	0.92	0.23	40,40,40,40	0
57	MG	BA	3708	1/1	0.92	0.21	50,50,50,50	0
57	MG	DA	3047	1/1	0.92	0.15	49,49,49,49	0
57	MG	DA	3048	1/1	0.92	0.06	53,53,53,53	0
57	MG	BA	3554	1/1	0.92	0.13	51,51,51,51	0
57	MG	DA	3050	1/1	0.92	0.17	59,59,59,59	0
57	MG	CA	3008	1/1	0.92	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3325	1/1	0.92	0.12	35,35,35,35	0
57	MG	DA	3327	1/1	0.92	0.12	57,57,57,57	0
57	MG	BA	3016	1/1	0.92	0.13	38,38,38,38	0
57	MG	BA	3714	1/1	0.92	0.11	57,57,57,57	0
57	MG	BA	3017	1/1	0.92	0.25	48,48,48,48	0
57	MG	AA	3070	1/1	0.92	0.18	52,52,52,52	0
57	MG	DA	3063	1/1	0.92	0.22	54,54,54,54	0
57	MG	DA	3637	1/1	0.92	0.59	58,58,58,58	0
57	MG	CA	3014	1/1	0.92	0.21	58,58,58,58	0
57	MG	BA	3717	1/1	0.92	0.16	50,50,50,50	0
57	MG	AA	3061	1/1	0.92	0.34	55,55,55,55	0
57	MG	BA	3098	1/1	0.92	0.23	40,40,40,40	0
57	MG	BA	3722	1/1	0.92	0.19	47,47,47,47	0
57	MG	DA	3354	1/1	0.92	0.19	44,44,44,44	0
57	MG	BA	3424	1/1	0.92	0.25	39,39,39,39	0
57	MG	BA	3182	1/1	0.92	0.14	55,55,55,55	0
57	MG	BA	3099	1/1	0.92	0.22	41,41,41,41	0
57	MG	DA	3079	1/1	0.92	0.17	55,55,55,55	0
57	MG	BA	3100	1/1	0.92	0.17	39,39,39,39	0
57	MG	DA	3083	1/1	0.92	0.18	40,40,40,40	0
57	MG	BA	3101	1/1	0.92	0.19	53,53,53,53	0
57	MG	BA	3734	1/1	0.92	0.16	52,52,52,52	0
57	MG	DA	3668	1/1	0.92	0.39	60,60,60,60	0
57	MG	BA	3307	1/1	0.92	0.17	29,29,29,29	0
57	MG	DA	3382	1/1	0.92	0.07	48,48,48,48	0
57	MG	DA	3091	1/1	0.92	0.10	48,48,48,48	0
57	MG	AA	3097	1/1	0.92	0.34	56,56,56,56	0
57	MG	BA	3310	1/1	0.92	0.24	58,58,58,58	0
57	MG	DA	3391	1/1	0.92	0.09	45,45,45,45	0
57	MG	DA	3392	1/1	0.92	0.19	70,70,70,70	0
57	MG	BA	3203	1/1	0.92	0.24	40,40,40,40	0
57	MG	DA	3398	1/1	0.92	0.14	45,45,45,45	0
57	MG	BA	3022	1/1	0.92	0.19	60,60,60,60	0
57	MG	BA	3207	1/1	0.92	0.24	54,54,54,54	0
57	MG	DA	3100	1/1	0.92	0.16	43,43,43,43	0
57	MG	DD	304	1/1	0.92	0.38	52,52,52,52	0
57	MG	AA	3201	1/1	0.92	0.13	52,52,52,52	0
57	MG	AX	3008	1/1	0.92	0.19	70,70,70,70	0
57	MG	AX	3009	1/1	0.92	0.18	64,64,64,64	0
57	MG	DA	3112	1/1	0.92	0.16	59,59,59,59	0
57	MG	AA	3202	1/1	0.92	0.14	57,57,57,57	0
57	MG	DA	3409	1/1	0.92	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3322	1/1	0.92	0.17	52,52,52,52	0
57	MG	AA	3109	1/1	0.92	0.14	62,62,62,62	0
57	MG	BA	3455	1/1	0.92	0.16	64,64,64,64	0
57	MG	DV	3003	1/1	0.92	0.10	65,65,65,65	0
57	MG	CA	3059	1/1	0.92	0.25	72,72,72,72	0
57	MG	BA	3043	1/1	0.92	0.15	48,48,48,48	0
57	MG	D3	3001	1/1	0.92	0.20	57,57,57,57	0
57	MG	BA	3767	1/1	0.92	0.12	73,73,73,73	0
57	MG	BA	3459	1/1	0.92	0.19	48,48,48,48	0
57	MG	DA	3128	1/1	0.92	0.15	58,58,58,58	0
57	MG	CA	3078	1/1	0.93	0.14	44,44,44,44	0
57	MG	BA	3341	1/1	0.93	0.12	51,51,51,51	0
57	MG	DA	3131	1/1	0.93	0.21	46,46,46,46	0
57	MG	CA	3082	1/1	0.93	0.15	79,79,79,79	0
57	MG	DA	3426	1/1	0.93	0.22	49,49,49,49	0
57	MG	CA	3086	1/1	0.93	0.13	64,64,64,64	0
57	MG	BA	3119	1/1	0.93	0.13	45,45,45,45	0
57	MG	BA	3800	1/1	0.93	0.23	38,38,38,38	0
57	MG	DA	3432	1/1	0.93	0.12	37,37,37,37	0
57	MG	BA	3228	1/1	0.93	0.25	59,59,59,59	0
57	MG	DA	3438	1/1	0.93	0.20	47,47,47,47	0
57	MG	BA	3807	1/1	0.93	0.17	47,47,47,47	0
57	MG	AA	3101	1/1	0.93	0.16	43,43,43,43	0
57	MG	BA	3639	1/1	0.93	0.46	48,48,48,48	0
57	MG	DA	3447	1/1	0.93	0.15	58,58,58,58	0
57	MG	AE	203	1/1	0.93	0.18	63,63,63,63	0
57	MG	BB	201	1/1	0.93	0.17	55,55,55,55	0
57	MG	CA	3102	1/1	0.93	0.08	68,68,68,68	0
57	MG	AA	3178	1/1	0.93	0.15	59,59,59,59	0
57	MG	DA	3149	1/1	0.93	0.06	56,56,56,56	0
57	MG	BA	3642	1/1	0.93	0.12	48,48,48,48	0
57	MG	DA	3152	1/1	0.93	0.20	51,51,51,51	0
57	MG	BA	3646	1/1	0.93	0.17	42,42,42,42	0
57	MG	BA	3355	1/1	0.93	0.17	61,61,61,61	0
57	MG	DA	3163	1/1	0.93	0.15	49,49,49,49	0
57	MG	CA	3114	1/1	0.93	0.04	57,57,57,57	0
57	MG	AA	3181	1/1	0.93	0.16	51,51,51,51	0
57	MG	AN	503	1/1	0.93	0.15	54,54,54,54	0
57	MG	CA	3117	1/1	0.93	0.10	71,71,71,71	0
57	MG	BA	3250	1/1	0.93	0.68	42,42,42,42	0
57	MG	DA	3482	1/1	0.93	0.10	50,50,50,50	0
57	MG	AA	3136	1/1	0.93	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3656	1/1	0.93	0.27	53,53,53,53	0
57	MG	BA	3035	1/1	0.93	0.26	39,39,39,39	0
57	MG	DA	3201	1/1	0.93	0.14	61,61,61,61	0
57	MG	AA	3076	1/1	0.93	0.26	77,77,77,77	0
57	MG	AA	3078	1/1	0.93	0.27	66,66,66,66	0
57	MG	BA	3505	1/1	0.93	0.12	55,55,55,55	0
57	MG	AA	3140	1/1	0.93	0.15	53,53,53,53	0
57	MG	DA	3211	1/1	0.93	0.14	48,48,48,48	0
57	MG	BA	3261	1/1	0.93	0.11	61,61,61,61	0
57	MG	BE	308	1/1	0.93	0.17	40,40,40,40	0
57	MG	CA	3142	1/1	0.93	0.13	69,69,69,69	0
57	MG	DA	3514	1/1	0.93	0.13	42,42,42,42	0
57	MG	DA	3517	1/1	0.93	0.05	51,51,51,51	0
57	MG	BA	3265	1/1	0.93	0.21	54,54,54,54	0
57	MG	AA	3141	1/1	0.93	0.23	61,61,61,61	0
57	MG	AA	3056	1/1	0.93	0.13	61,61,61,61	0
57	MG	BA	3055	1/1	0.93	0.21	45,45,45,45	0
57	MG	AA	3029	1/1	0.93	0.22	53,53,53,53	0
57	MG	BA	3519	1/1	0.93	0.08	55,55,55,55	0
57	MG	BN	3006	1/1	0.93	0.20	49,49,49,49	0
57	MG	BA	3524	1/1	0.93	0.13	42,42,42,42	0
57	MG	DA	3227	1/1	0.93	0.28	41,41,41,41	0
57	MG	AA	3007	1/1	0.93	0.13	57,57,57,57	0
57	MG	DA	3536	1/1	0.93	0.11	48,48,48,48	0
57	MG	BP	202	1/1	0.93	0.21	36,36,36,36	0
57	MG	DA	3540	1/1	0.93	0.17	42,42,42,42	0
57	MG	DA	3237	1/1	0.93	0.14	56,56,56,56	0
57	MG	BA	3149	1/1	0.93	0.18	40,40,40,40	0
57	MG	DA	3545	1/1	0.93	0.13	35,35,35,35	0
57	MG	BA	3531	1/1	0.93	0.21	26,26,26,26	0
57	MG	CA	3164	1/1	0.93	0.16	60,60,60,60	0
57	MG	DA	3549	1/1	0.93	0.10	57,57,57,57	0
57	MG	CA	3165	1/1	0.93	0.11	45,45,45,45	0
57	MG	DA	3551	1/1	0.93	0.08	55,55,55,55	0
57	MG	BU	202	1/1	0.93	0.29	40,40,40,40	0
57	MG	AA	3085	1/1	0.93	0.18	48,48,48,48	0
57	MG	DA	3246	1/1	0.93	0.14	43,43,43,43	0
57	MG	DA	3557	1/1	0.93	0.15	51,51,51,51	0
57	MG	CA	3170	1/1	0.93	0.18	58,58,58,58	0
57	MG	BV	204	1/1	0.93	0.21	49,49,49,49	0
57	MG	BA	3533	1/1	0.93	0.10	59,59,59,59	0
57	MG	BA	3688	1/1	0.93	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3690	1/1	0.93	0.18	58,58,58,58	0
57	MG	DA	3255	1/1	0.93	0.09	51,51,51,51	0
57	MG	AA	3193	1/1	0.93	0.08	72,72,72,72	0
57	MG	BA	3537	1/1	0.93	0.16	45,45,45,45	0
57	MG	BA	3277	1/1	0.93	0.65	47,47,47,47	0
57	MG	BA	3282	1/1	0.93	0.16	39,39,39,39	0
57	MG	DA	3578	1/1	0.93	0.18	59,59,59,59	0
57	MG	AA	3149	1/1	0.93	0.10	46,46,46,46	0
57	MG	BA	3406	1/1	0.93	0.10	50,50,50,50	0
57	MG	DA	3006	1/1	0.93	0.10	38,38,38,38	0
57	MG	BA	3161	1/1	0.93	0.17	52,52,52,52	0
57	MG	DA	3009	1/1	0.93	0.15	48,48,48,48	0
57	MG	BA	3706	1/1	0.93	0.11	53,53,53,53	0
57	MG	DA	3013	1/1	0.93	0.09	40,40,40,40	0
57	MG	DA	3017	1/1	0.93	0.06	55,55,55,55	0
57	MG	B7	102	1/1	0.93	0.16	47,47,47,47	0
57	MG	AA	3152	1/1	0.93	0.10	62,62,62,62	0
57	MG	DA	3029	1/1	0.93	0.35	49,49,49,49	0
57	MG	DA	3284	1/1	0.93	0.12	47,47,47,47	0
57	MG	DA	3032	1/1	0.93	0.15	48,48,48,48	0
57	MG	DA	3291	1/1	0.93	0.20	44,44,44,44	0
57	MG	BA	3291	1/1	0.93	0.21	33,33,33,33	0
57	MG	B9	502	1/1	0.93	0.19	48,48,48,48	0
57	MG	DA	3036	1/1	0.93	0.14	48,48,48,48	0
57	MG	AA	3088	1/1	0.93	0.27	65,65,65,65	0
57	MG	DA	3041	1/1	0.93	0.09	38,38,38,38	0
57	MG	AA	3155	1/1	0.93	0.24	48,48,48,48	0
57	MG	DA	3045	1/1	0.93	0.29	51,51,51,51	0
57	MG	DA	3617	1/1	0.93	0.07	56,56,56,56	0
57	MG	BA	3713	1/1	0.93	0.18	33,33,33,33	0
57	MG	BA	3555	1/1	0.93	0.14	29,29,29,29	0
57	MG	BA	3295	1/1	0.93	0.19	38,38,38,38	0
57	MG	AA	3067	1/1	0.93	0.26	57,57,57,57	0
57	MG	DA	3625	1/1	0.93	0.07	69,69,69,69	0
57	MG	BA	3173	1/1	0.93	0.15	48,48,48,48	0
57	MG	DA	3627	1/1	0.93	0.17	63,63,63,63	0
57	MG	BA	3075	1/1	0.93	0.24	45,45,45,45	0
57	MG	BA	3077	1/1	0.93	0.17	49,49,49,49	0
57	MG	DA	3631	1/1	0.93	0.12	57,57,57,57	0
57	MG	BA	3078	1/1	0.93	0.24	51,51,51,51	0
57	MG	BA	3302	1/1	0.93	0.12	69,69,69,69	0
57	MG	BA	3576	1/1	0.93	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3064	1/1	0.93	0.20	49,49,49,49	0
57	MG	DA	3065	1/1	0.93	0.18	43,43,43,43	0
57	MG	BA	3079	1/1	0.93	0.19	39,39,39,39	0
57	MG	BA	3580	1/1	0.93	0.13	55,55,55,55	0
57	MG	AA	3027	1/1	0.93	0.15	50,50,50,50	0
57	MG	BA	3186	1/1	0.93	0.45	45,45,45,45	0
57	MG	DA	3074	1/1	0.93	0.13	37,37,37,37	0
57	MG	DA	3650	1/1	0.93	0.12	67,67,67,67	0
57	MG	DA	3351	1/1	0.93	0.12	48,48,48,48	0
57	MG	DA	3652	1/1	0.93	0.39	67,67,67,67	0
57	MG	BA	3190	1/1	0.93	0.20	52,52,52,52	0
57	MG	BA	3585	1/1	0.93	0.09	46,46,46,46	0
57	MG	AA	3060	1/1	0.93	0.27	46,46,46,46	0
57	MG	DA	3358	1/1	0.93	0.14	45,45,45,45	0
57	MG	AA	3071	1/1	0.93	0.22	53,53,53,53	0
57	MG	AA	3095	1/1	0.93	0.29	60,60,60,60	0
57	MG	BA	3595	1/1	0.93	0.09	51,51,51,51	0
57	MG	BA	3439	1/1	0.93	0.13	33,33,33,33	0
57	MG	BA	3200	1/1	0.93	0.15	67,67,67,67	0
57	MG	BA	3201	1/1	0.93	0.20	62,62,62,62	0
57	MG	DA	3670	1/1	0.93	0.42	60,60,60,60	0
57	MG	DA	3672	1/1	0.93	0.16	71,71,71,71	0
57	MG	CA	3040	1/1	0.93	0.11	51,51,51,51	0
57	MG	DA	3675	1/1	0.93	0.13	52,52,52,52	0
57	MG	DA	3381	1/1	0.93	0.17	56,56,56,56	0
57	MG	BA	3014	1/1	0.93	0.29	42,42,42,42	0
57	MG	BA	3758	1/1	0.93	0.11	45,45,45,45	0
57	MG	AA	3096	1/1	0.93	0.22	63,63,63,63	0
57	MG	BA	3604	1/1	0.93	0.15	36,36,36,36	0
57	MG	AA	3130	1/1	0.93	0.08	56,56,56,56	0
57	MG	DB	3005	1/1	0.93	0.08	59,59,59,59	0
57	MG	BA	3319	1/1	0.93	0.19	46,46,46,46	0
57	MG	BA	3765	1/1	0.93	0.22	48,48,48,48	0
57	MG	DA	3396	1/1	0.93	0.10	40,40,40,40	0
57	MG	DA	3397	1/1	0.93	0.09	57,57,57,57	0
57	MG	BA	3320	1/1	0.93	0.22	48,48,48,48	0
57	MG	BA	3768	1/1	0.93	0.12	47,47,47,47	0
57	MG	DA	3107	1/1	0.93	0.13	51,51,51,51	0
57	MG	DA	3108	1/1	0.93	0.07	52,52,52,52	0
57	MG	AA	3012	1/1	0.93	0.16	46,46,46,46	0
57	MG	CA	3060	1/1	0.93	0.08	65,65,65,65	0
57	MG	AA	3055	1/1	0.93	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3773	1/1	0.93	0.25	52,52,52,52	0
57	MG	BA	3457	1/1	0.93	0.19	32,32,32,32	0
57	MG	AE	201	1/1	0.93	0.15	59,59,59,59	0
57	MG	DV	3001	1/1	0.93	0.23	70,70,70,70	0
57	MG	DA	3121	1/1	0.93	0.07	44,44,44,44	0
57	MG	DW	3003	1/1	0.93	0.09	72,72,72,72	0
57	MG	BA	3328	1/1	0.93	0.27	40,40,40,40	0
57	MG	BA	3223	1/1	0.93	0.13	41,41,41,41	0
57	MG	BA	3464	1/1	0.93	0.14	45,45,45,45	0
57	MG	BA	3021	1/1	0.93	0.19	49,49,49,49	0
57	MG	DA	3127	1/1	0.93	0.15	35,35,35,35	0
57	MG	BA	3118	1/1	0.93	0.17	48,48,48,48	0
57	MG	DA	3434	1/1	0.94	0.11	39,39,39,39	0
57	MG	BQ	3003	1/1	0.94	0.27	49,49,49,49	0
57	MG	BA	3063	1/1	0.94	0.15	59,59,59,59	0
57	MG	BR	201	1/1	0.94	0.26	57,57,57,57	0
57	MG	BA	3340	1/1	0.94	0.14	39,39,39,39	0
57	MG	DA	3172	1/1	0.94	0.09	62,62,62,62	0
57	MG	CA	3145	1/1	0.94	0.14	66,66,66,66	0
57	MG	BA	3183	1/1	0.94	0.18	42,42,42,42	0
57	MG	DA	3179	1/1	0.94	0.12	52,52,52,52	0
57	MG	BU	205	1/1	0.94	0.24	47,47,47,47	0
57	MG	BU	208	1/1	0.94	0.21	40,40,40,40	0
57	MG	DA	3188	1/1	0.94	0.19	48,48,48,48	0
57	MG	DA	3458	1/1	0.94	0.05	52,52,52,52	0
57	MG	BA	3268	1/1	0.94	0.22	55,55,55,55	0
57	MG	DA	3195	1/1	0.94	0.09	43,43,43,43	0
57	MG	DA	3200	1/1	0.94	0.09	66,66,66,66	0
57	MG	BA	3344	1/1	0.94	0.12	66,66,66,66	0
57	MG	DA	3202	1/1	0.94	0.11	57,57,57,57	0
57	MG	DA	3203	1/1	0.94	0.57	50,50,50,50	0
57	MG	DA	3472	1/1	0.94	0.16	44,44,44,44	0
57	MG	BA	3064	1/1	0.94	0.13	43,43,43,43	0
57	MG	BA	3448	1/1	0.94	0.24	32,32,32,32	0
57	MG	BA	3452	1/1	0.94	0.16	55,55,55,55	0
57	MG	DA	3479	1/1	0.94	0.17	43,43,43,43	0
57	MG	BA	3065	1/1	0.94	0.19	60,60,60,60	0
57	MG	DA	3210	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3350	1/1	0.94	0.20	28,28,28,28	0
57	MG	CA	3161	1/1	0.94	0.09	56,56,56,56	0
57	MG	DA	3490	1/1	0.94	0.13	47,47,47,47	0
57	MG	BA	3189	1/1	0.94	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3352	1/1	0.94	0.22	53,53,53,53	0
57	MG	AA	3083	1/1	0.94	0.31	57,57,57,57	0
57	MG	AA	3199	1/1	0.94	0.15	73,73,73,73	0
57	MG	AA	3016	1/1	0.94	0.09	63,63,63,63	0
57	MG	BA	3196	1/1	0.94	0.25	38,38,38,38	0
57	MG	BA	3279	1/1	0.94	0.24	43,43,43,43	0
57	MG	CF	3001	1/1	0.94	0.12	46,46,46,46	0
57	MG	BA	3365	1/1	0.94	0.13	62,62,62,62	0
57	MG	DA	3511	1/1	0.94	0.16	49,49,49,49	0
57	MG	AX	3004	1/1	0.94	0.15	64,64,64,64	0
57	MG	BA	3738	1/1	0.94	0.15	43,43,43,43	0
57	MG	DA	3516	1/1	0.94	0.07	67,67,67,67	0
57	MG	DA	3229	1/1	0.94	0.22	50,50,50,50	0
57	MG	DA	3230	1/1	0.94	0.22	73,73,73,73	0
57	MG	DA	3232	1/1	0.94	0.13	62,62,62,62	0
57	MG	BA	3739	1/1	0.94	0.22	40,40,40,40	0
57	MG	DA	3235	1/1	0.94	0.20	45,45,45,45	0
57	MG	AA	3132	1/1	0.94	0.19	55,55,55,55	0
57	MG	AA	3111	1/1	0.94	0.09	79,79,79,79	0
57	MG	DA	3238	1/1	0.94	0.27	44,44,44,44	0
57	MG	BA	3610	1/1	0.94	0.09	61,61,61,61	0
57	MG	BA	3743	1/1	0.94	0.17	44,44,44,44	0
57	MG	BA	3376	1/1	0.94	0.16	48,48,48,48	0
57	MG	DA	3533	1/1	0.94	0.11	43,43,43,43	0
57	MG	BA	3377	1/1	0.94	0.14	44,44,44,44	0
57	MG	CA	3010	1/1	0.94	0.17	56,56,56,56	0
57	MG	BA	3747	1/1	0.94	0.20	52,52,52,52	0
57	MG	BA	3748	1/1	0.94	0.15	29,29,29,29	0
57	MG	BA	3289	1/1	0.94	0.21	56,56,56,56	0
57	MG	AA	3009	1/1	0.94	0.18	57,57,57,57	0
57	MG	DA	3249	1/1	0.94	0.14	45,45,45,45	0
57	MG	BA	3204	1/1	0.94	0.23	36,36,36,36	0
57	MG	DA	3024	1/1	0.94	0.21	59,59,59,59	0
57	MG	AA	3159	1/1	0.94	0.12	66,66,66,66	0
57	MG	DA	3254	1/1	0.94	0.07	52,52,52,52	0
57	MG	BA	3389	1/1	0.94	0.13	55,55,55,55	0
57	MG	AA	3098	1/1	0.94	0.18	55,55,55,55	0
57	MG	BA	3294	1/1	0.94	0.23	61,61,61,61	0
57	MG	DA	3260	1/1	0.94	0.09	55,55,55,55	0
57	MG	AA	3075	1/1	0.94	0.11	49,49,49,49	0
57	MG	BA	3084	1/1	0.94	0.22	38,38,38,38	0
57	MG	DA	3264	1/1	0.94	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3037	1/1	0.94	0.16	43,43,43,43	0
57	MG	CA	3025	1/1	0.94	0.14	51,51,51,51	0
57	MG	DA	3039	1/1	0.94	0.10	43,43,43,43	0
57	MG	BA	3633	1/1	0.94	0.12	49,49,49,49	0
57	MG	DA	3573	1/1	0.94	0.12	43,43,43,43	0
57	MG	DA	3043	1/1	0.94	0.15	38,38,38,38	0
57	MG	BA	3504	1/1	0.94	0.13	56,56,56,56	0
57	MG	AA	3068	1/1	0.94	0.14	69,69,69,69	0
57	MG	CA	3030	1/1	0.94	0.22	57,57,57,57	0
57	MG	BA	3217	1/1	0.94	0.16	37,37,37,37	0
57	MG	DA	3584	1/1	0.94	0.18	53,53,53,53	0
57	MG	CA	3035	1/1	0.94	0.09	59,59,59,59	0
57	MG	BA	3219	1/1	0.94	0.17	36,36,36,36	0
57	MG	DA	3587	1/1	0.94	0.12	56,56,56,56	0
57	MG	CA	3037	1/1	0.94	0.14	73,73,73,73	0
57	MG	DA	3053	1/1	0.94	0.10	47,47,47,47	0
57	MG	DA	3054	1/1	0.94	0.23	48,48,48,48	0
57	MG	DA	3300	1/1	0.94	0.20	45,45,45,45	0
57	MG	BA	3770	1/1	0.94	0.16	45,45,45,45	0
57	MG	DA	3302	1/1	0.94	0.28	70,70,70,70	0
57	MG	DA	3594	1/1	0.94	0.31	54,54,54,54	0
57	MG	BA	3220	1/1	0.94	0.22	29,29,29,29	0
57	MG	BA	3509	1/1	0.94	0.21	31,31,31,31	0
57	MG	BA	3777	1/1	0.94	0.17	40,40,40,40	0
57	MG	BA	3511	1/1	0.94	0.14	30,30,30,30	0
57	MG	AY	3002	1/1	0.94	0.24	56,56,56,56	0
57	MG	BA	3096	1/1	0.94	0.23	54,54,54,54	0
57	MG	BA	3785	1/1	0.94	0.23	59,59,59,59	0
57	MG	DA	3067	1/1	0.94	0.26	57,57,57,57	0
57	MG	CA	3053	1/1	0.94	0.15	41,41,41,41	0
57	MG	DA	3612	1/1	0.94	0.09	62,62,62,62	0
57	MG	AA	3032	1/1	0.94	0.19	67,67,67,67	0
57	MG	BA	3649	1/1	0.94	0.11	40,40,40,40	0
57	MG	DA	3324	1/1	0.94	0.11	33,33,33,33	0
57	MG	AA	3123	1/1	0.94	0.26	51,51,51,51	0
57	MG	BA	3516	1/1	0.94	0.19	52,52,52,52	0
57	MG	BA	3306	1/1	0.94	0.17	37,37,37,37	0
57	MG	BA	3520	1/1	0.94	0.16	61,61,61,61	0
57	MG	DA	3331	1/1	0.94	0.17	37,37,37,37	0
57	MG	DA	3623	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3624	1/1	0.94	0.19	56,56,56,56	0
57	MG	BA	3655	1/1	0.94	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3801	1/1	0.94	0.31	50,50,50,50	0
57	MG	BA	3522	1/1	0.94	0.09	52,52,52,52	0
57	MG	BA	3803	1/1	0.94	0.23	44,44,44,44	0
57	MG	DA	3336	1/1	0.94	0.19	40,40,40,40	0
57	MG	CA	3068	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3805	1/1	0.94	0.12	44,44,44,44	0
57	MG	BA	3523	1/1	0.94	0.11	48,48,48,48	0
57	MG	DA	3634	1/1	0.94	0.14	60,60,60,60	0
57	MG	BA	3809	1/1	0.94	0.13	63,63,63,63	0
57	MG	BA	3155	1/1	0.94	0.27	44,44,44,44	0
57	MG	BA	3157	1/1	0.94	0.24	45,45,45,45	0
57	MG	CA	3077	1/1	0.94	0.08	66,66,66,66	0
57	MG	BA	3663	1/1	0.94	0.19	41,41,41,41	0
57	MG	CA	3079	1/1	0.94	0.21	66,66,66,66	0
57	MG	AA	3052	1/1	0.94	0.29	65,65,65,65	0
57	MG	DA	3102	1/1	0.94	0.19	40,40,40,40	0
57	MG	BA	3236	1/1	0.94	0.20	49,49,49,49	0
57	MG	DA	3104	1/1	0.94	0.29	53,53,53,53	0
57	MG	DA	3368	1/1	0.94	0.24	50,50,50,50	0
57	MG	CA	3083	1/1	0.94	0.10	79,79,79,79	0
57	MG	BA	3415	1/1	0.94	0.16	28,28,28,28	0
57	MG	DA	3655	1/1	0.94	0.11	64,64,64,64	0
57	MG	DA	3656	1/1	0.94	0.13	58,58,58,58	0
57	MG	DA	3379	1/1	0.94	0.14	63,63,63,63	0
57	MG	BA	3417	1/1	0.94	0.24	38,38,38,38	0
57	MG	BA	3237	1/1	0.94	0.15	45,45,45,45	0
57	MG	DA	3660	1/1	0.94	0.09	61,61,61,61	0
57	MG	BA	3536	1/1	0.94	0.27	49,49,49,49	0
57	MG	DA	3662	1/1	0.94	0.13	62,62,62,62	0
57	MG	DA	3114	1/1	0.94	0.15	55,55,55,55	0
57	MG	BA	3672	1/1	0.94	0.20	43,43,43,43	0
57	MG	CA	3094	1/1	0.94	0.11	70,70,70,70	0
57	MG	AA	3104	1/1	0.94	0.28	59,59,59,59	0
57	MG	CA	3096	1/1	0.94	0.10	44,44,44,44	0
57	MG	AA	3014	1/1	0.94	0.21	32,32,32,32	0
57	MG	AA	3172	1/1	0.94	0.10	72,72,72,72	0
57	MG	BA	3243	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3166	1/1	0.94	0.14	38,38,38,38	0
57	MG	BA	3543	1/1	0.94	0.23	37,37,37,37	0
57	MG	CA	3108	1/1	0.94	0.31	68,68,68,68	0
57	MG	BA	3682	1/1	0.94	0.19	53,53,53,53	0
57	MG	CA	3110	1/1	0.94	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BE	303	1/1	0.94	0.20	51,51,51,51	0
57	MG	BA	3170	1/1	0.94	0.16	38,38,38,38	0
57	MG	BA	3054	1/1	0.94	0.28	36,36,36,36	0
57	MG	DB	3009	1/1	0.94	0.18	59,59,59,59	0
57	MG	BA	3685	1/1	0.94	0.19	53,53,53,53	0
57	MG	AA	3174	1/1	0.94	0.10	50,50,50,50	0
57	MG	DB	3013	1/1	0.94	0.17	64,64,64,64	0
57	MG	DD	302	1/1	0.94	0.15	42,42,42,42	0
57	MG	BA	3323	1/1	0.94	0.20	30,30,30,30	0
57	MG	DA	3411	1/1	0.94	0.22	53,53,53,53	0
57	MG	DD	306	1/1	0.94	0.28	39,39,39,39	0
57	MG	BA	3176	1/1	0.94	0.17	45,45,45,45	0
57	MG	CA	3119	1/1	0.94	0.16	64,64,64,64	0
57	MG	AA	3175	1/1	0.94	0.18	63,63,63,63	0
57	MG	CA	3122	1/1	0.94	0.21	64,64,64,64	0
57	MG	DA	3419	1/1	0.94	0.11	32,32,32,32	0
57	MG	BA	3559	1/1	0.94	0.08	47,47,47,47	0
57	MG	DQ	3003	1/1	0.94	0.15	51,51,51,51	0
57	MG	CA	3125	1/1	0.94	0.08	63,63,63,63	0
57	MG	CA	3126	1/1	0.94	0.11	67,67,67,67	0
57	MG	BA	3329	1/1	0.94	0.19	60,60,60,60	0
57	MG	BA	3436	1/1	0.94	0.14	40,40,40,40	0
57	MG	BA	3009	1/1	0.94	0.17	28,28,28,28	0
57	MG	BA	3564	1/1	0.94	0.16	44,44,44,44	0
57	MG	DA	3427	1/1	0.94	0.14	45,45,45,45	0
57	MG	DA	3428	1/1	0.94	0.18	37,37,37,37	0
57	MG	AW	3003	1/1	0.94	0.13	72,72,72,72	0
57	MG	DA	3154	1/1	0.94	0.17	48,48,48,48	0
57	MG	DA	3158	1/1	0.94	0.16	60,60,60,60	0
57	MG	CA	3139	1/1	0.94	0.14	62,62,62,62	0
60	K	AX	3001	1/1	0.94	0.12	65,65,65,65	0
57	MG	BA	3383	1/1	0.95	0.12	53,53,53,53	0
57	MG	AA	3010	1/1	0.95	0.17	52,52,52,52	0
57	MG	B3	3001	1/1	0.95	0.12	34,34,34,34	0
57	MG	BA	3205	1/1	0.95	0.27	50,50,50,50	0
57	MG	BA	3482	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3600	1/1	0.95	0.31	44,44,44,44	0
57	MG	DA	3207	1/1	0.95	0.30	63,63,63,63	0
57	MG	BA	3484	1/1	0.95	0.13	54,54,54,54	0
57	MG	BA	3133	1/1	0.95	0.19	45,45,45,45	0
57	MG	AA	3156	1/1	0.95	0.26	63,63,63,63	0
57	MG	DA	3467	1/1	0.95	0.25	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3209	1/1	0.95	0.24	54,54,54,54	0
57	MG	CA	3169	1/1	0.95	0.24	51,51,51,51	0
57	MG	CA	3001	1/1	0.95	0.10	75,75,75,75	0
57	MG	CD	301	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3608	1/1	0.95	0.31	62,62,62,62	0
57	MG	DA	3474	1/1	0.95	0.14	51,51,51,51	0
57	MG	DA	3475	1/1	0.95	0.16	51,51,51,51	0
57	MG	AA	3157	1/1	0.95	0.17	45,45,45,45	0
57	MG	DA	3477	1/1	0.95	0.09	43,43,43,43	0
57	MG	BA	3496	1/1	0.95	0.17	41,41,41,41	0
57	MG	CK	3001	1/1	0.95	0.17	45,45,45,45	0
57	MG	AA	3179	1/1	0.95	0.13	69,69,69,69	0
57	MG	BA	3500	1/1	0.95	0.14	56,56,56,56	0
57	MG	DA	3483	1/1	0.95	0.32	55,55,55,55	0
57	MG	BA	3617	1/1	0.95	0.16	51,51,51,51	0
57	MG	DA	3485	1/1	0.95	0.12	52,52,52,52	0
57	MG	DA	3486	1/1	0.95	0.09	47,47,47,47	0
57	MG	BA	3395	1/1	0.95	0.17	38,38,38,38	0
57	MG	DA	3488	1/1	0.95	0.07	41,41,41,41	0
57	MG	DA	3224	1/1	0.95	0.17	49,49,49,49	0
57	MG	DA	3225	1/1	0.95	0.07	49,49,49,49	0
57	MG	DA	3226	1/1	0.95	0.38	45,45,45,45	0
57	MG	AA	3050	1/1	0.95	0.15	33,33,33,33	0
57	MG	DA	3496	1/1	0.95	0.07	53,53,53,53	0
57	MG	CX	3004	1/1	0.95	0.18	63,63,63,63	0
57	MG	BA	3751	1/1	0.95	0.17	26,26,26,26	0
57	MG	BA	3620	1/1	0.95	0.15	40,40,40,40	0
57	MG	DA	3501	1/1	0.95	0.15	37,37,37,37	0
57	MG	BA	3215	1/1	0.95	0.27	36,36,36,36	0
57	MG	BA	3398	1/1	0.95	0.21	32,32,32,32	0
57	MG	CA	3015	1/1	0.95	0.22	56,56,56,56	0
57	MG	DA	3507	1/1	0.95	0.14	43,43,43,43	0
57	MG	DA	3510	1/1	0.95	0.25	49,49,49,49	0
57	MG	AA	3116	1/1	0.95	0.11	55,55,55,55	0
57	MG	BA	3218	1/1	0.95	0.20	47,47,47,47	0
57	MG	BA	3626	1/1	0.95	0.25	44,44,44,44	0
57	MG	DA	3015	1/1	0.95	0.20	52,52,52,52	0
57	MG	CA	3019	1/1	0.95	0.10	65,65,65,65	0
57	MG	BA	3146	1/1	0.95	0.17	40,40,40,40	0
57	MG	DA	3519	1/1	0.95	0.18	63,63,63,63	0
57	MG	DA	3023	1/1	0.95	0.30	40,40,40,40	0
57	MG	DA	3522	1/1	0.95	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	3205	1/1	0.95	0.22	51,51,51,51	0
57	MG	BA	3632	1/1	0.95	0.07	50,50,50,50	0
57	MG	AA	3129	1/1	0.95	0.11	47,47,47,47	0
57	MG	DA	3030	1/1	0.95	0.14	39,39,39,39	0
57	MG	BA	3510	1/1	0.95	0.17	46,46,46,46	0
57	MG	BA	3635	1/1	0.95	0.13	58,58,58,58	0
57	MG	BA	3026	1/1	0.95	0.15	41,41,41,41	0
57	MG	BA	3081	1/1	0.95	0.21	46,46,46,46	0
57	MG	CA	3029	1/1	0.95	0.17	63,63,63,63	0
57	MG	BA	3027	1/1	0.95	0.11	26,26,26,26	0
57	MG	CA	3031	1/1	0.95	0.10	68,68,68,68	0
57	MG	DA	3539	1/1	0.95	0.12	53,53,53,53	0
57	MG	CA	3032	1/1	0.95	0.24	62,62,62,62	0
57	MG	DA	3541	1/1	0.95	0.14	44,44,44,44	0
57	MG	BA	3775	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3087	1/1	0.95	0.24	42,42,42,42	0
57	MG	BA	3156	1/1	0.95	0.29	41,41,41,41	0
57	MG	BA	3090	1/1	0.95	0.31	53,53,53,53	0
57	MG	AA	3035	1/1	0.95	0.21	56,56,56,56	0
57	MG	DA	3548	1/1	0.95	0.06	60,60,60,60	0
57	MG	BA	3782	1/1	0.95	0.16	65,65,65,65	0
57	MG	BA	3783	1/1	0.95	0.12	56,56,56,56	0
57	MG	BA	3031	1/1	0.95	0.19	52,52,52,52	0
57	MG	DA	3272	1/1	0.95	0.10	41,41,41,41	0
57	MG	CA	3042	1/1	0.95	0.11	59,59,59,59	0
57	MG	BA	3647	1/1	0.95	0.09	56,56,56,56	0
57	MG	BA	3163	1/1	0.95	0.14	55,55,55,55	0
57	MG	AA	3118	1/1	0.95	0.17	47,47,47,47	0
57	MG	DA	3562	1/1	0.95	0.12	64,64,64,64	0
57	MG	DA	3277	1/1	0.95	0.11	55,55,55,55	0
57	MG	AX	3015	1/1	0.95	0.21	42,42,42,42	0
57	MG	DA	3565	1/1	0.95	0.08	59,59,59,59	0
57	MG	BA	3795	1/1	0.95	0.15	35,35,35,35	0
57	MG	BA	3796	1/1	0.95	0.25	45,45,45,45	0
57	MG	DA	3568	1/1	0.95	0.08	52,52,52,52	0
57	MG	DA	3570	1/1	0.95	0.13	31,31,31,31	0
57	MG	AA	3165	1/1	0.95	0.20	54,54,54,54	0
57	MG	DA	3286	1/1	0.95	0.14	42,42,42,42	0
57	MG	DA	3287	1/1	0.95	0.10	41,41,41,41	0
57	MG	BA	3798	1/1	0.95	0.20	28,28,28,28	0
57	MG	DA	3290	1/1	0.95	0.15	59,59,59,59	0
57	MG	BA	3527	1/1	0.95	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3295	1/1	0.95	0.21	44,44,44,44	0
57	MG	DA	3581	1/1	0.95	0.22	57,57,57,57	0
57	MG	BA	3246	1/1	0.95	0.35	39,39,39,39	0
57	MG	DA	3583	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3249	1/1	0.95	0.13	49,49,49,49	0
57	MG	AY	3001	1/1	0.95	0.39	65,65,65,65	0
57	MG	DA	3303	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3304	1/1	0.95	0.06	48,48,48,48	0
57	MG	BA	3171	1/1	0.95	0.25	31,31,31,31	0
57	MG	DA	3073	1/1	0.95	0.09	42,42,42,42	0
57	MG	CA	3063	1/1	0.95	0.23	58,58,58,58	0
57	MG	BA	3325	1/1	0.95	0.15	48,48,48,48	0
57	MG	BA	3661	1/1	0.95	0.09	44,44,44,44	0
57	MG	BA	3808	1/1	0.95	0.16	42,42,42,42	0
57	MG	AA	3213	1/1	0.95	0.23	54,54,54,54	0
57	MG	AA	3144	1/1	0.95	0.14	46,46,46,46	0
57	MG	DA	3598	1/1	0.95	0.08	61,61,61,61	0
57	MG	DA	3600	1/1	0.95	0.35	70,70,70,70	0
57	MG	DA	3602	1/1	0.95	0.10	65,65,65,65	0
57	MG	DA	3318	1/1	0.95	0.14	40,40,40,40	0
57	MG	DA	3080	1/1	0.95	0.10	55,55,55,55	0
57	MG	BA	3175	1/1	0.95	0.20	20,20,20,20	0
57	MG	BA	3539	1/1	0.95	0.20	52,52,52,52	0
57	MG	BA	3667	1/1	0.95	0.15	61,61,61,61	0
57	MG	DA	3087	1/1	0.95	0.18	58,58,58,58	0
57	MG	AA	3167	1/1	0.95	0.10	57,57,57,57	0
57	MG	AA	3106	1/1	0.95	0.10	57,57,57,57	0
57	MG	DA	3611	1/1	0.95	0.14	48,48,48,48	0
57	MG	BA	3262	1/1	0.95	0.14	41,41,41,41	0
57	MG	CA	3080	1/1	0.95	0.09	49,49,49,49	0
57	MG	BA	3178	1/1	0.95	0.13	46,46,46,46	0
57	MG	BA	3110	1/1	0.95	0.17	41,41,41,41	0
57	MG	AA	3081	1/1	0.95	0.11	48,48,48,48	0
57	MG	BA	3440	1/1	0.95	0.12	42,42,42,42	0
57	MG	AF	3001	1/1	0.95	0.26	44,44,44,44	0
57	MG	BA	3551	1/1	0.95	0.19	36,36,36,36	0
57	MG	BA	3552	1/1	0.95	0.26	29,29,29,29	0
57	MG	BD	301	1/1	0.95	0.23	40,40,40,40	0
57	MG	CA	3092	1/1	0.95	0.10	50,50,50,50	0
57	MG	DA	3343	1/1	0.95	0.16	50,50,50,50	0
57	MG	DA	3348	1/1	0.95	0.10	34,34,34,34	0
57	MG	BA	3056	1/1	0.95	0.21	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BD	304	1/1	0.95	0.22	32,32,32,32	0
57	MG	DA	3629	1/1	0.95	0.27	62,62,62,62	0
57	MG	BA	3348	1/1	0.95	0.18	36,36,36,36	0
57	MG	BA	3557	1/1	0.95	0.16	33,33,33,33	0
57	MG	DA	3113	1/1	0.95	0.19	60,60,60,60	0
57	MG	DA	3359	1/1	0.95	0.13	47,47,47,47	0
57	MG	AA	3134	1/1	0.95	0.14	66,66,66,66	0
57	MG	AA	3150	1/1	0.95	0.20	57,57,57,57	0
57	MG	DA	3117	1/1	0.95	0.20	52,52,52,52	0
57	MG	DA	3364	1/1	0.95	0.07	40,40,40,40	0
57	MG	CA	3101	1/1	0.95	0.11	49,49,49,49	0
57	MG	DA	3640	1/1	0.95	0.19	43,43,43,43	0
57	MG	BE	306	1/1	0.95	0.20	26,26,26,26	0
57	MG	CA	3104	1/1	0.95	0.12	68,68,68,68	0
57	MG	DA	3372	1/1	0.95	0.08	56,56,56,56	0
57	MG	DA	3645	1/1	0.95	0.07	45,45,45,45	0
57	MG	DA	3375	1/1	0.95	0.16	39,39,39,39	0
57	MG	DA	3649	1/1	0.95	0.05	58,58,58,58	0
57	MG	DA	3376	1/1	0.95	0.16	61,61,61,61	0
57	MG	DA	3377	1/1	0.95	0.10	38,38,38,38	0
57	MG	CA	3106	1/1	0.95	0.07	56,56,56,56	0
57	MG	AA	3195	1/1	0.95	0.12	57,57,57,57	0
57	MG	BA	3687	1/1	0.95	0.21	22,22,22,22	0
57	MG	BA	3062	1/1	0.95	0.27	42,42,42,42	0
57	MG	BA	3451	1/1	0.95	0.16	31,31,31,31	0
57	MG	BA	3354	1/1	0.95	0.10	48,48,48,48	0
57	MG	BA	3567	1/1	0.95	0.15	34,34,34,34	0
57	MG	DA	3386	1/1	0.95	0.11	35,35,35,35	0
57	MG	CA	3113	1/1	0.95	0.11	67,67,67,67	0
57	MG	DA	3389	1/1	0.95	0.14	46,46,46,46	0
57	MG	BA	3123	1/1	0.95	0.22	32,32,32,32	0
57	MG	BA	3570	1/1	0.95	0.16	42,42,42,42	0
57	MG	BA	3571	1/1	0.95	0.18	58,58,58,58	0
57	MG	BA	3194	1/1	0.95	0.18	47,47,47,47	0
57	MG	BA	3359	1/1	0.95	0.30	62,62,62,62	0
57	MG	BP	201	1/1	0.95	0.28	41,41,41,41	0
57	MG	DA	3136	1/1	0.95	0.14	52,52,52,52	0
57	MG	AA	3039	1/1	0.95	0.15	56,56,56,56	0
57	MG	DA	3674	1/1	0.95	0.15	37,37,37,37	0
57	MG	CA	3121	1/1	0.95	0.14	63,63,63,63	0
57	MG	BP	205	1/1	0.95	0.18	65,65,65,65	0
57	MG	BQ	3001	1/1	0.95	0.22	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3577	1/1	0.95	0.19	51,51,51,51	0
57	MG	BQ	3004	1/1	0.95	0.27	42,42,42,42	0
57	MG	CA	3127	1/1	0.95	0.18	62,62,62,62	0
57	MG	AW	3002	1/1	0.95	0.22	53,53,53,53	0
57	MG	BA	3579	1/1	0.95	0.17	49,49,49,49	0
57	MG	DB	3006	1/1	0.95	0.14	57,57,57,57	0
57	MG	BA	3283	1/1	0.95	0.20	35,35,35,35	0
57	MG	CA	3132	1/1	0.95	0.13	66,66,66,66	0
57	MG	BA	3712	1/1	0.95	0.18	53,53,53,53	0
57	MG	CA	3136	1/1	0.95	0.14	72,72,72,72	0
57	MG	BU	204	1/1	0.95	0.16	35,35,35,35	0
57	MG	DA	3418	1/1	0.95	0.11	52,52,52,52	0
57	MG	BA	3015	1/1	0.95	0.16	32,32,32,32	0
57	MG	BU	207	1/1	0.95	0.17	38,38,38,38	0
57	MG	AA	3015	1/1	0.95	0.15	65,65,65,65	0
57	MG	BA	3288	1/1	0.95	0.20	56,56,56,56	0
57	MG	DA	3167	1/1	0.95	0.13	41,41,41,41	0
57	MG	DE	304	1/1	0.95	0.15	43,43,43,43	0
57	MG	BA	3373	1/1	0.95	0.17	48,48,48,48	0
57	MG	BW	201	1/1	0.95	0.31	44,44,44,44	0
57	MG	DO	5001	1/1	0.95	0.13	59,59,59,59	0
57	MG	BA	3068	1/1	0.95	0.18	43,43,43,43	0
57	MG	DA	3174	1/1	0.95	0.13	44,44,44,44	0
57	MG	DQ	3002	1/1	0.95	0.10	51,51,51,51	0
57	MG	BA	3130	1/1	0.95	0.08	44,44,44,44	0
57	MG	BA	3592	1/1	0.95	0.20	28,28,28,28	0
57	MG	CA	3151	1/1	0.95	0.27	59,59,59,59	0
57	MG	DA	3181	1/1	0.95	0.13	50,50,50,50	0
57	MG	DA	3183	1/1	0.95	0.15	38,38,38,38	0
57	MG	DA	3433	1/1	0.95	0.18	46,46,46,46	0
57	MG	BA	3593	1/1	0.95	0.22	38,38,38,38	0
57	MG	DA	3186	1/1	0.95	0.15	54,54,54,54	0
57	MG	DY	502	1/1	0.95	0.13	50,50,50,50	0
57	MG	BA	3723	1/1	0.95	0.07	47,47,47,47	0
57	MG	DA	3439	1/1	0.95	0.23	42,42,42,42	0
57	MG	CA	3154	1/1	0.95	0.17	56,56,56,56	0
59	ZN	B4	501	1/1	0.95	0.15	89,89,89,89	0
57	MG	DA	3441	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3381	1/1	0.95	0.16	46,46,46,46	0
57	MG	DA	3196	1/1	0.95	0.22	49,49,49,49	0
57	MG	DA	3068	1/1	0.96	0.10	58,58,58,58	0
57	MG	BE	304	1/1	0.96	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3224	1/1	0.96	0.22	65,65,65,65	0
57	MG	BA	3088	1/1	0.96	0.35	48,48,48,48	0
57	MG	AA	3044	1/1	0.96	0.25	60,60,60,60	0
57	MG	DA	3269	1/1	0.96	0.06	49,49,49,49	0
57	MG	BA	3603	1/1	0.96	0.13	53,53,53,53	0
57	MG	BA	3091	1/1	0.96	0.40	56,56,56,56	0
57	MG	BF	303	1/1	0.96	0.54	49,49,49,49	0
57	MG	DA	3504	1/1	0.96	0.07	47,47,47,47	0
57	MG	BA	3711	1/1	0.96	0.19	54,54,54,54	0
57	MG	BA	3356	1/1	0.96	0.16	37,37,37,37	0
57	MG	DA	3509	1/1	0.96	0.12	59,59,59,59	0
57	MG	BA	3059	1/1	0.96	0.21	26,26,26,26	0
57	MG	BG	203	1/1	0.96	0.16	42,42,42,42	0
57	MG	DA	3081	1/1	0.96	0.28	55,55,55,55	0
57	MG	BN	3001	1/1	0.96	0.31	53,53,53,53	0
57	MG	DA	3515	1/1	0.96	0.15	45,45,45,45	0
57	MG	CA	3093	1/1	0.96	0.10	55,55,55,55	0
57	MG	DA	3282	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3084	1/1	0.96	0.08	39,39,39,39	0
57	MG	BA	3517	1/1	0.96	0.14	45,45,45,45	0
57	MG	DA	3520	1/1	0.96	0.11	57,57,57,57	0
57	MG	BA	3132	1/1	0.96	0.14	40,40,40,40	0
57	MG	BA	3613	1/1	0.96	0.41	42,42,42,42	0
57	MG	BA	3614	1/1	0.96	0.11	63,63,63,63	0
57	MG	BA	3094	1/1	0.96	0.21	36,36,36,36	0
57	MG	BA	3720	1/1	0.96	0.14	65,65,65,65	0
57	MG	DA	3293	1/1	0.96	0.14	54,54,54,54	0
57	MG	BA	3437	1/1	0.96	0.14	36,36,36,36	0
57	MG	DA	3296	1/1	0.96	0.12	28,28,28,28	0
57	MG	DA	3298	1/1	0.96	0.16	59,59,59,59	0
57	MG	DA	3299	1/1	0.96	0.20	55,55,55,55	0
57	MG	BP	204	1/1	0.96	0.06	46,46,46,46	0
57	MG	AA	3180	1/1	0.96	0.10	73,73,73,73	0
57	MG	DA	3537	1/1	0.96	0.08	44,44,44,44	0
57	MG	AA	3212	1/1	0.96	0.13	42,42,42,42	0
57	MG	BQ	3002	1/1	0.96	0.23	43,43,43,43	0
57	MG	DA	3101	1/1	0.96	0.16	49,49,49,49	0
57	MG	DA	3306	1/1	0.96	0.13	55,55,55,55	0
57	MG	BA	3525	1/1	0.96	0.17	34,34,34,34	0
57	MG	BA	3727	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3238	1/1	0.96	0.24	62,62,62,62	0
57	MG	BA	3729	1/1	0.96	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3441	1/1	0.96	0.13	35,35,35,35	0
57	MG	BA	3528	1/1	0.96	0.18	56,56,56,56	0
57	MG	DA	3109	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3529	1/1	0.96	0.20	56,56,56,56	0
57	MG	DA	3111	1/1	0.96	0.19	61,61,61,61	0
57	MG	DA	3319	1/1	0.96	0.12	41,41,41,41	0
57	MG	BA	3184	1/1	0.96	0.32	43,43,43,43	0
57	MG	BA	3370	1/1	0.96	0.20	39,39,39,39	0
57	MG	BA	3627	1/1	0.96	0.17	56,56,56,56	0
57	MG	BV	202	1/1	0.96	0.17	50,50,50,50	0
57	MG	DA	3559	1/1	0.96	0.12	43,43,43,43	0
57	MG	AA	3087	1/1	0.96	0.11	41,41,41,41	0
57	MG	BA	3629	1/1	0.96	0.16	43,43,43,43	0
57	MG	BV	205	1/1	0.96	0.09	38,38,38,38	0
57	MG	BA	3140	1/1	0.96	0.14	47,47,47,47	0
57	MG	BW	202	1/1	0.96	0.22	54,54,54,54	0
57	MG	BW	203	1/1	0.96	0.20	44,44,44,44	0
57	MG	DA	3123	1/1	0.96	0.20	56,56,56,56	0
57	MG	DA	3569	1/1	0.96	0.23	49,49,49,49	0
57	MG	BW	204	1/1	0.96	0.22	42,42,42,42	0
57	MG	BA	3375	1/1	0.96	0.13	68,68,68,68	0
57	MG	AA	3006	1/1	0.96	0.12	52,52,52,52	0
57	MG	BA	3244	1/1	0.96	0.22	53,53,53,53	0
57	MG	DA	3574	1/1	0.96	0.11	53,53,53,53	0
57	MG	AA	3011	1/1	0.96	0.34	57,57,57,57	0
57	MG	BA	3382	1/1	0.96	0.09	63,63,63,63	0
57	MG	DA	3341	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3248	1/1	0.96	0.30	42,42,42,42	0
57	MG	DA	3580	1/1	0.96	0.16	36,36,36,36	0
57	MG	B0	103	1/1	0.96	0.08	53,53,53,53	0
57	MG	DA	3346	1/1	0.96	0.12	48,48,48,48	0
57	MG	BA	3191	1/1	0.96	0.18	43,43,43,43	0
57	MG	DA	3350	1/1	0.96	0.12	51,51,51,51	0
57	MG	AA	3074	1/1	0.96	0.09	50,50,50,50	0
57	MG	DA	3353	1/1	0.96	0.16	42,42,42,42	0
57	MG	BA	3753	1/1	0.96	0.15	33,33,33,33	0
57	MG	B3	3002	1/1	0.96	0.12	66,66,66,66	0
57	MG	BA	3251	1/1	0.96	0.19	44,44,44,44	0
57	MG	CA	3143	1/1	0.96	0.10	64,64,64,64	0
57	MG	AA	3043	1/1	0.96	0.23	51,51,51,51	0
57	MG	BA	3460	1/1	0.96	0.10	62,62,62,62	0
57	MG	BA	3644	1/1	0.96	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3645	1/1	0.96	0.20	33,33,33,33	0
57	MG	DA	3145	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3596	1/1	0.96	0.10	56,56,56,56	0
57	MG	DA	3597	1/1	0.96	0.06	51,51,51,51	0
57	MG	DA	3365	1/1	0.96	0.08	36,36,36,36	0
57	MG	DA	3366	1/1	0.96	0.14	42,42,42,42	0
57	MG	BA	3547	1/1	0.96	0.23	39,39,39,39	0
57	MG	BA	3034	1/1	0.96	0.25	56,56,56,56	0
57	MG	BA	3763	1/1	0.96	0.19	24,24,24,24	0
57	MG	BA	3462	1/1	0.96	0.19	36,36,36,36	0
57	MG	DA	3374	1/1	0.96	0.16	56,56,56,56	0
57	MG	DA	3150	1/1	0.96	0.08	56,56,56,56	0
57	MG	BA	3107	1/1	0.96	0.16	53,53,53,53	0
57	MG	BA	3256	1/1	0.96	0.15	40,40,40,40	0
57	MG	CA	3005	1/1	0.96	0.15	62,62,62,62	0
57	MG	BA	3197	1/1	0.96	0.30	41,41,41,41	0
57	MG	DA	3156	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3108	1/1	0.96	0.32	44,44,44,44	0
57	MG	DA	3159	1/1	0.96	0.15	58,58,58,58	0
57	MG	DA	3160	1/1	0.96	0.10	56,56,56,56	0
57	MG	BA	3468	1/1	0.96	0.17	62,62,62,62	0
57	MG	BA	3469	1/1	0.96	0.15	49,49,49,49	0
57	MG	DA	3619	1/1	0.96	0.11	69,69,69,69	0
57	MG	DA	3387	1/1	0.96	0.10	42,42,42,42	0
57	MG	CA	3162	1/1	0.96	0.10	66,66,66,66	0
57	MG	BA	3153	1/1	0.96	0.31	47,47,47,47	0
57	MG	BA	3657	1/1	0.96	0.26	47,47,47,47	0
57	MG	DA	3169	1/1	0.96	0.24	47,47,47,47	0
57	MG	BA	3012	1/1	0.96	0.20	39,39,39,39	0
57	MG	DA	3395	1/1	0.96	0.12	47,47,47,47	0
57	MG	BA	3778	1/1	0.96	0.16	48,48,48,48	0
57	MG	BA	3264	1/1	0.96	0.22	58,58,58,58	0
57	MG	BA	3660	1/1	0.96	0.11	61,61,61,61	0
57	MG	DA	3176	1/1	0.96	0.19	41,41,41,41	0
57	MG	BA	3041	1/1	0.96	0.24	40,40,40,40	0
57	MG	BA	3112	1/1	0.96	0.23	30,30,30,30	0
57	MG	AA	3173	1/1	0.96	0.15	54,54,54,54	0
57	MG	BA	3160	1/1	0.96	0.32	55,55,55,55	0
57	MG	BA	3665	1/1	0.96	0.16	49,49,49,49	0
57	MG	AX	3012	1/1	0.96	0.17	59,59,59,59	0
57	MG	BA	3208	1/1	0.96	0.16	44,44,44,44	0
57	MG	CA	3023	1/1	0.96	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3639	1/1	0.96	0.48	59,59,59,59	0
57	MG	DA	3193	1/1	0.96	0.13	57,57,57,57	0
57	MG	BA	3572	1/1	0.96	0.16	61,61,61,61	0
57	MG	BA	3272	1/1	0.96	0.61	48,48,48,48	0
57	MG	BA	3574	1/1	0.96	0.19	66,66,66,66	0
57	MG	DA	3199	1/1	0.96	0.11	47,47,47,47	0
57	MG	DA	3416	1/1	0.96	0.12	50,50,50,50	0
57	MG	DA	3648	1/1	0.96	0.14	57,57,57,57	0
57	MG	BA	3488	1/1	0.96	0.19	60,60,60,60	0
57	MG	BA	3491	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3492	1/1	0.96	0.13	46,46,46,46	0
57	MG	AX	3013	1/1	0.96	0.13	58,58,58,58	0
57	MG	DA	3204	1/1	0.96	0.31	46,46,46,46	0
57	MG	BA	3676	1/1	0.96	0.21	33,33,33,33	0
57	MG	BA	3494	1/1	0.96	0.09	49,49,49,49	0
57	MG	BA	3408	1/1	0.96	0.20	36,36,36,36	0
57	MG	BA	3804	1/1	0.96	0.42	53,53,53,53	0
57	MG	DA	3012	1/1	0.96	0.12	33,33,33,33	0
57	MG	BA	3336	1/1	0.96	0.15	64,64,64,64	0
57	MG	DA	3014	1/1	0.96	0.21	46,46,46,46	0
57	MG	BA	3806	1/1	0.96	0.16	30,30,30,30	0
57	MG	BA	3582	1/1	0.96	0.16	74,74,74,74	0
57	MG	DA	3663	1/1	0.96	0.13	60,60,60,60	0
57	MG	BA	3076	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3022	1/1	0.96	0.27	51,51,51,51	0
57	MG	BA	3211	1/1	0.96	0.15	55,55,55,55	0
57	MG	AA	3110	1/1	0.96	0.13	48,48,48,48	0
57	MG	BA	3586	1/1	0.96	0.09	53,53,53,53	0
57	MG	BA	3414	1/1	0.96	0.18	41,41,41,41	0
57	MG	DA	3220	1/1	0.96	0.16	46,46,46,46	0
57	MG	CA	3045	1/1	0.96	0.24	54,54,54,54	0
57	MG	BA	3589	1/1	0.96	0.21	27,27,27,27	0
57	MG	DA	3443	1/1	0.96	0.10	54,54,54,54	0
57	MG	CA	3048	1/1	0.96	0.12	67,67,67,67	0
57	MG	DA	3445	1/1	0.96	0.10	32,32,32,32	0
57	MG	CA	3049	1/1	0.96	0.20	63,63,63,63	0
57	MG	AA	3203	1/1	0.96	0.13	59,59,59,59	0
57	MG	BB	205	1/1	0.96	0.20	60,60,60,60	0
57	MG	BA	3689	1/1	0.96	0.17	42,42,42,42	0
57	MG	BB	207	1/1	0.96	0.22	54,54,54,54	0
57	MG	DB	3007	1/1	0.96	0.20	58,58,58,58	0
57	MG	DA	3040	1/1	0.96	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3454	1/1	0.96	0.16	56,56,56,56	0
57	MG	BA	3591	1/1	0.96	0.17	35,35,35,35	0
57	MG	DA	3457	1/1	0.96	0.07	54,54,54,54	0
57	MG	DA	3233	1/1	0.96	0.19	53,53,53,53	0
57	MG	DD	301	1/1	0.96	0.15	47,47,47,47	0
57	MG	DA	3461	1/1	0.96	0.11	62,62,62,62	0
57	MG	CA	3056	1/1	0.96	0.10	64,64,64,64	0
57	MG	BA	3691	1/1	0.96	0.16	55,55,55,55	0
57	MG	DA	3464	1/1	0.96	0.10	46,46,46,46	0
57	MG	BA	3692	1/1	0.96	0.15	40,40,40,40	0
57	MG	DE	302	1/1	0.96	0.17	33,33,33,33	0
57	MG	BB	213	1/1	0.96	0.19	60,60,60,60	0
57	MG	AA	3048	1/1	0.96	0.22	57,57,57,57	0
57	MG	BA	3694	1/1	0.96	0.10	51,51,51,51	0
57	MG	BB	216	1/1	0.96	0.23	51,51,51,51	0
57	MG	DA	3241	1/1	0.96	0.13	45,45,45,45	0
57	MG	BA	3169	1/1	0.96	0.17	45,45,45,45	0
57	MG	DA	3052	1/1	0.96	0.13	61,61,61,61	0
57	MG	BA	3696	1/1	0.96	0.14	33,33,33,33	0
57	MG	AA	3113	1/1	0.96	0.12	58,58,58,58	0
57	MG	DA	3055	1/1	0.96	0.17	49,49,49,49	0
57	MG	CA	3067	1/1	0.96	0.31	61,61,61,61	0
57	MG	DA	3057	1/1	0.96	0.20	42,42,42,42	0
57	MG	DA	3059	1/1	0.96	0.26	43,43,43,43	0
57	MG	BA	3699	1/1	0.96	0.23	35,35,35,35	0
57	MG	DW	3002	1/1	0.96	0.15	45,45,45,45	0
57	MG	CA	3069	1/1	0.96	0.12	60,60,60,60	0
57	MG	BA	3083	1/1	0.96	0.15	56,56,56,56	0
57	MG	DA	3253	1/1	0.96	0.13	45,45,45,45	0
57	MG	BA	3701	1/1	0.96	0.15	43,43,43,43	0
57	MG	BD	308	1/1	0.96	0.23	46,46,46,46	0
57	MG	BA	3349	1/1	0.96	0.09	56,56,56,56	0
57	MG	DA	3489	1/1	0.96	0.13	51,51,51,51	0
57	MG	AA	3114	1/1	0.96	0.17	59,59,59,59	0
57	MG	AA	3151	1/1	0.96	0.14	45,45,45,45	0
57	MG	DA	3493	1/1	0.96	0.30	66,66,66,66	0
57	MG	DA	3086	1/1	0.97	0.09	43,43,43,43	0
57	MG	BA	3611	1/1	0.97	0.17	46,46,46,46	0
57	MG	DA	3278	1/1	0.97	0.06	43,43,43,43	0
57	MG	BN	3005	1/1	0.97	0.17	36,36,36,36	0
57	MG	DA	3089	1/1	0.97	0.39	52,52,52,52	0
57	MG	BA	3111	1/1	0.97	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3506	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3393	1/1	0.97	0.18	51,51,51,51	0
57	MG	AA	3207	1/1	0.97	0.09	65,65,65,65	0
57	MG	BA	3725	1/1	0.97	0.14	44,44,44,44	0
57	MG	BA	3113	1/1	0.97	0.25	53,53,53,53	0
57	MG	DA	3096	1/1	0.97	0.23	42,42,42,42	0
57	MG	BA	3168	1/1	0.97	0.17	47,47,47,47	0
57	MG	BA	3004	1/1	0.97	0.19	33,33,33,33	0
57	MG	DA	3099	1/1	0.97	0.17	32,32,32,32	0
57	MG	BA	3115	1/1	0.97	0.24	59,59,59,59	0
57	MG	BA	3731	1/1	0.97	0.30	37,37,37,37	0
57	MG	BA	3232	1/1	0.97	0.20	52,52,52,52	0
57	MG	BA	3116	1/1	0.97	0.28	50,50,50,50	0
57	MG	AA	3208	1/1	0.97	0.17	60,60,60,60	0
57	MG	DA	3105	1/1	0.97	0.19	48,48,48,48	0
57	MG	BA	3309	1/1	0.97	0.18	41,41,41,41	0
57	MG	AA	3147	1/1	0.97	0.10	70,70,70,70	0
57	MG	BA	3311	1/1	0.97	0.27	48,48,48,48	0
57	MG	DA	3305	1/1	0.97	0.20	50,50,50,50	0
57	MG	AA	3148	1/1	0.97	0.22	57,57,57,57	0
57	MG	DA	3529	1/1	0.97	0.08	38,38,38,38	0
57	MG	DA	3307	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3036	1/1	0.97	0.17	40,40,40,40	0
57	MG	AX	3005	1/1	0.97	0.14	47,47,47,47	0
57	MG	DA	3310	1/1	0.97	0.13	38,38,38,38	0
57	MG	BA	3042	1/1	0.97	0.20	43,43,43,43	0
57	MG	BA	3630	1/1	0.97	0.14	58,58,58,58	0
57	MG	AX	3006	1/1	0.97	0.10	65,65,65,65	0
57	MG	CA	3123	1/1	0.97	0.14	58,58,58,58	0
57	MG	BA	3410	1/1	0.97	0.16	27,27,27,27	0
57	MG	BA	3518	1/1	0.97	0.20	44,44,44,44	0
57	MG	DA	3542	1/1	0.97	0.17	24,24,24,24	0
57	MG	BA	3245	1/1	0.97	0.23	34,34,34,34	0
57	MG	BA	3046	1/1	0.97	0.28	41,41,41,41	0
57	MG	BA	3752	1/1	0.97	0.19	32,32,32,32	0
57	MG	BA	3181	1/1	0.97	0.25	43,43,43,43	0
57	MG	DA	3322	1/1	0.97	0.19	51,51,51,51	0
57	MG	BA	3082	1/1	0.97	0.22	39,39,39,39	0
57	MG	CA	3131	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3011	1/1	0.97	0.19	35,35,35,35	0
57	MG	DA	3326	1/1	0.97	0.16	43,43,43,43	0
57	MG	DA	3552	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	3134	1/1	0.97	0.16	69,69,69,69	0
57	MG	BA	3756	1/1	0.97	0.20	48,48,48,48	0
57	MG	BA	3048	1/1	0.97	0.13	47,47,47,47	0
57	MG	CA	3137	1/1	0.97	0.16	56,56,56,56	0
57	MG	BA	3086	1/1	0.97	0.21	22,22,22,22	0
57	MG	AA	3120	1/1	0.97	0.19	45,45,45,45	0
57	MG	DA	3561	1/1	0.97	0.04	57,57,57,57	0
57	MG	BA	3420	1/1	0.97	0.16	40,40,40,40	0
57	MG	BA	3643	1/1	0.97	0.13	46,46,46,46	0
57	MG	BA	3326	1/1	0.97	0.19	20,20,20,20	0
57	MG	BA	3254	1/1	0.97	0.22	25,25,25,25	0
57	MG	DA	3338	1/1	0.97	0.15	61,61,61,61	0
57	MG	BA	3188	1/1	0.97	0.30	49,49,49,49	0
57	MG	BA	3766	1/1	0.97	0.15	28,28,28,28	0
57	MG	BA	3425	1/1	0.97	0.15	40,40,40,40	0
57	MG	CA	3147	1/1	0.97	0.12	64,64,64,64	0
57	MG	BA	3330	1/1	0.97	0.23	37,37,37,37	0
57	MG	DA	3345	1/1	0.97	0.09	44,44,44,44	0
57	MG	B7	101	1/1	0.97	0.24	39,39,39,39	0
57	MG	DA	3142	1/1	0.97	0.13	47,47,47,47	0
57	MG	DA	3349	1/1	0.97	0.07	52,52,52,52	0
57	MG	DA	3143	1/1	0.97	0.18	38,38,38,38	0
57	MG	BA	3331	1/1	0.97	0.17	49,49,49,49	0
57	MG	DA	3352	1/1	0.97	0.19	63,63,63,63	0
57	MG	DA	3579	1/1	0.97	0.10	48,48,48,48	0
57	MG	B7	103	1/1	0.97	0.16	42,42,42,42	0
57	MG	BA	3428	1/1	0.97	0.19	46,46,46,46	0
57	MG	AA	3099	1/1	0.97	0.20	51,51,51,51	0
57	MG	CA	3155	1/1	0.97	0.12	53,53,53,53	0
57	MG	B8	101	1/1	0.97	0.21	44,44,44,44	0
57	MG	BA	3334	1/1	0.97	0.14	37,37,37,37	0
57	MG	BA	3774	1/1	0.97	0.07	46,46,46,46	0
57	MG	BA	3653	1/1	0.97	0.21	39,39,39,39	0
57	MG	BA	3776	1/1	0.97	0.20	43,43,43,43	0
57	MG	DA	3155	1/1	0.97	0.25	48,48,48,48	0
57	MG	BA	3089	1/1	0.97	0.17	19,19,19,19	0
57	MG	AA	3164	1/1	0.97	0.10	61,61,61,61	0
57	MG	BA	3260	1/1	0.97	0.30	39,39,39,39	0
57	MG	BA	3338	1/1	0.97	0.13	40,40,40,40	0
57	MG	DA	3369	1/1	0.97	0.15	28,28,28,28	0
57	MG	DA	3370	1/1	0.97	0.14	51,51,51,51	0
57	MG	BA	3435	1/1	0.97	0.27	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	3018	1/1	0.97	0.24	56,56,56,56	0
57	MG	DA	3373	1/1	0.97	0.15	44,44,44,44	0
57	MG	DA	3599	1/1	0.97	0.20	36,36,36,36	0
57	MG	CA	3167	1/1	0.97	0.17	60,60,60,60	0
57	MG	DA	3601	1/1	0.97	0.10	44,44,44,44	0
57	MG	BA	3193	1/1	0.97	0.20	48,48,48,48	0
57	MG	DA	3166	1/1	0.97	0.11	55,55,55,55	0
57	MG	BA	3784	1/1	0.97	0.21	33,33,33,33	0
57	MG	DA	3168	1/1	0.97	0.29	45,45,45,45	0
57	MG	BA	3263	1/1	0.97	0.34	49,49,49,49	0
57	MG	BA	3786	1/1	0.97	0.13	35,35,35,35	0
57	MG	DA	3171	1/1	0.97	0.12	31,31,31,31	0
57	MG	BA	3787	1/1	0.97	0.23	45,45,45,45	0
57	MG	BA	3343	1/1	0.97	0.15	53,53,53,53	0
57	MG	DA	3384	1/1	0.97	0.10	49,49,49,49	0
57	MG	BA	3789	1/1	0.97	0.18	12,12,12,12	0
57	MG	DA	3613	1/1	0.97	0.15	54,54,54,54	0
57	MG	DA	3175	1/1	0.97	0.12	41,41,41,41	0
57	MG	BA	3549	1/1	0.97	0.29	39,39,39,39	0
57	MG	AA	3105	1/1	0.97	0.32	69,69,69,69	0
57	MG	BA	3345	1/1	0.97	0.14	38,38,38,38	0
57	MG	DA	3390	1/1	0.97	0.11	43,43,43,43	0
57	MG	BA	3137	1/1	0.97	0.24	39,39,39,39	0
57	MG	BA	3553	1/1	0.97	0.10	59,59,59,59	0
57	MG	DA	3182	1/1	0.97	0.24	51,51,51,51	0
57	MG	BA	3093	1/1	0.97	0.26	56,56,56,56	0
57	MG	DA	3184	1/1	0.97	0.16	47,47,47,47	0
57	MG	BA	3139	1/1	0.97	0.33	40,40,40,40	0
57	MG	AA	3182	1/1	0.97	0.14	49,49,49,49	0
57	MG	DA	3187	1/1	0.97	0.11	42,42,42,42	0
57	MG	AA	3024	1/1	0.97	0.12	54,54,54,54	0
57	MG	DA	3189	1/1	0.97	0.20	41,41,41,41	0
57	MG	DA	3191	1/1	0.97	0.17	37,37,37,37	0
57	MG	DA	3192	1/1	0.97	0.10	60,60,60,60	0
57	MG	BA	3270	1/1	0.97	0.17	48,48,48,48	0
57	MG	BA	3144	1/1	0.97	0.19	41,41,41,41	0
57	MG	BA	3674	1/1	0.97	0.15	63,63,63,63	0
57	MG	BA	3202	1/1	0.97	0.19	60,60,60,60	0
57	MG	AA	3154	1/1	0.97	0.11	69,69,69,69	0
57	MG	BA	3677	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3565	1/1	0.97	0.17	40,40,40,40	0
57	MG	BA	3097	1/1	0.97	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	3034	1/1	0.97	0.14	59,59,59,59	0
57	MG	DA	3016	1/1	0.97	0.34	50,50,50,50	0
57	MG	AK	3001	1/1	0.97	0.18	44,44,44,44	0
57	MG	AA	3125	1/1	0.97	0.24	37,37,37,37	0
57	MG	DA	3019	1/1	0.97	0.29	37,37,37,37	0
57	MG	DA	3644	1/1	0.97	0.08	55,55,55,55	0
57	MG	DA	3020	1/1	0.97	0.16	55,55,55,55	0
57	MG	BA	3358	1/1	0.97	0.21	49,49,49,49	0
57	MG	DA	3647	1/1	0.97	0.11	54,54,54,54	0
57	MG	AA	3186	1/1	0.97	0.12	42,42,42,42	0
57	MG	BA	3360	1/1	0.97	0.16	41,41,41,41	0
57	MG	AA	3112	1/1	0.97	0.17	63,63,63,63	0
57	MG	DA	3028	1/1	0.97	0.36	52,52,52,52	0
57	MG	BB	203	1/1	0.97	0.24	43,43,43,43	0
57	MG	BB	204	1/1	0.97	0.18	41,41,41,41	0
57	MG	BA	3280	1/1	0.97	0.14	37,37,37,37	0
57	MG	BA	3363	1/1	0.97	0.15	22,22,22,22	0
57	MG	BA	3152	1/1	0.97	0.30	43,43,43,43	0
57	MG	BB	208	1/1	0.97	0.14	45,45,45,45	0
57	MG	BA	3102	1/1	0.97	0.19	44,44,44,44	0
57	MG	CA	3050	1/1	0.97	0.20	61,61,61,61	0
57	MG	BA	3368	1/1	0.97	0.20	40,40,40,40	0
57	MG	DA	3435	1/1	0.97	0.15	50,50,50,50	0
57	MG	DA	3436	1/1	0.97	0.12	54,54,54,54	0
57	MG	BA	3103	1/1	0.97	0.17	38,38,38,38	0
57	MG	DA	3664	1/1	0.97	0.39	48,48,48,48	0
57	MG	BB	212	1/1	0.97	0.13	55,55,55,55	0
57	MG	DA	3042	1/1	0.97	0.17	38,38,38,38	0
57	MG	AA	3092	1/1	0.97	0.14	63,63,63,63	0
57	MG	BA	3371	1/1	0.97	0.14	35,35,35,35	0
57	MG	DA	3228	1/1	0.97	0.30	38,38,38,38	0
57	MG	BA	3286	1/1	0.97	0.21	34,34,34,34	0
57	MG	DA	3046	1/1	0.97	0.16	47,47,47,47	0
57	MG	DA	3231	1/1	0.97	0.09	62,62,62,62	0
57	MG	BA	3105	1/1	0.97	0.18	37,37,37,37	0
57	MG	BA	3474	1/1	0.97	0.18	55,55,55,55	0
57	MG	DA	3449	1/1	0.97	0.10	54,54,54,54	0
57	MG	BA	3475	1/1	0.97	0.13	42,42,42,42	0
57	MG	BA	3698	1/1	0.97	0.22	31,31,31,31	0
57	MG	BA	3476	1/1	0.97	0.15	55,55,55,55	0
57	MG	BA	3214	1/1	0.97	0.17	41,41,41,41	0
57	MG	DA	3455	1/1	0.97	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BD	303	1/1	0.97	0.14	39,39,39,39	0
57	MG	AA	3158	1/1	0.97	0.14	45,45,45,45	0
57	MG	BD	305	1/1	0.97	0.16	35,35,35,35	0
57	MG	DA	3460	1/1	0.97	0.13	41,41,41,41	0
57	MG	DB	3010	1/1	0.97	0.17	57,57,57,57	0
57	MG	BD	306	1/1	0.97	0.25	38,38,38,38	0
57	MG	BA	3479	1/1	0.97	0.07	50,50,50,50	0
57	MG	DA	3058	1/1	0.97	0.14	29,29,29,29	0
57	MG	BA	3158	1/1	0.97	0.20	41,41,41,41	0
57	MG	BA	3481	1/1	0.97	0.18	41,41,41,41	0
57	MG	DA	3466	1/1	0.97	0.11	41,41,41,41	0
57	MG	CA	3071	1/1	0.97	0.15	68,68,68,68	0
57	MG	CA	3072	1/1	0.97	0.17	54,54,54,54	0
57	MG	DD	307	1/1	0.97	0.32	43,43,43,43	0
57	MG	BE	302	1/1	0.97	0.23	39,39,39,39	0
57	MG	BA	3379	1/1	0.97	0.18	31,31,31,31	0
57	MG	BA	3483	1/1	0.97	0.15	28,28,28,28	0
57	MG	BA	3380	1/1	0.97	0.10	48,48,48,48	0
57	MG	BA	3159	1/1	0.97	0.25	50,50,50,50	0
57	MG	DF	3003	1/1	0.97	0.40	43,43,43,43	0
57	MG	BA	3028	1/1	0.97	0.22	51,51,51,51	0
57	MG	BA	3067	1/1	0.97	0.15	41,41,41,41	0
57	MG	BF	301	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3489	1/1	0.97	0.07	59,59,59,59	0
57	MG	DA	3257	1/1	0.97	0.18	50,50,50,50	0
57	MG	DA	3072	1/1	0.97	0.14	47,47,47,47	0
57	MG	BA	3490	1/1	0.97	0.10	54,54,54,54	0
57	MG	DA	3261	1/1	0.97	0.12	49,49,49,49	0
57	MG	BA	3221	1/1	0.97	0.17	37,37,37,37	0
57	MG	CA	3084	1/1	0.97	0.13	60,60,60,60	0
57	MG	DV	3002	1/1	0.97	0.30	49,49,49,49	0
57	MG	BF	306	1/1	0.97	0.28	31,31,31,31	0
57	MG	DW	3001	1/1	0.97	0.40	54,54,54,54	0
57	MG	DA	3265	1/1	0.97	0.12	30,30,30,30	0
57	MG	DA	3266	1/1	0.97	0.09	57,57,57,57	0
57	MG	DW	3004	1/1	0.97	0.22	52,52,52,52	0
57	MG	BF	307	1/1	0.97	0.24	37,37,37,37	0
57	MG	BA	3222	1/1	0.97	0.18	37,37,37,37	0
57	MG	BF	309	1/1	0.97	0.15	53,53,53,53	0
57	MG	BG	201	1/1	0.97	0.20	58,58,58,58	0
57	MG	BA	3029	1/1	0.97	0.48	37,37,37,37	0
57	MG	AA	3137	1/1	0.97	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3299	1/1	0.97	0.16	25,25,25,25	0
57	MG	BA	3390	1/1	0.97	0.26	38,38,38,38	0
59	ZN	D9	501	1/1	0.97	0.12	68,68,68,68	0
57	MG	BN	3003	1/1	0.97	0.19	48,48,48,48	0
60	K	CX	3001	1/1	0.97	0.19	82,82,82,82	0
57	MG	BA	3332	1/1	0.98	0.18	38,38,38,38	0
57	MG	BA	3040	1/1	0.98	0.36	35,35,35,35	0
57	MG	DA	3471	1/1	0.98	0.23	50,50,50,50	0
57	MG	BA	3588	1/1	0.98	0.23	31,31,31,31	0
57	MG	AA	3040	1/1	0.98	0.11	60,60,60,60	0
57	MG	DA	3034	1/1	0.98	0.18	38,38,38,38	0
57	MG	BA	3141	1/1	0.98	0.28	42,42,42,42	0
57	MG	BA	3791	1/1	0.98	0.18	28,28,28,28	0
57	MG	BA	3792	1/1	0.98	0.14	54,54,54,54	0
57	MG	DA	3357	1/1	0.98	0.07	50,50,50,50	0
57	MG	BA	3719	1/1	0.98	0.18	53,53,53,53	0
57	MG	BA	3259	1/1	0.98	0.21	25,25,25,25	0
57	MG	BA	3167	1/1	0.98	0.12	41,41,41,41	0
57	MG	BP	203	1/1	0.98	0.15	33,33,33,33	0
57	MG	BA	3142	1/1	0.98	0.17	49,49,49,49	0
57	MG	DA	3363	1/1	0.98	0.16	29,29,29,29	0
57	MG	BA	3534	1/1	0.98	0.21	44,44,44,44	0
57	MG	BA	3339	1/1	0.98	0.21	23,23,23,23	0
57	MG	BA	3060	1/1	0.98	0.20	30,30,30,30	0
57	MG	DA	3144	1/1	0.98	0.11	38,38,38,38	0
57	MG	BA	3080	1/1	0.98	0.17	60,60,60,60	0
57	MG	DA	3491	1/1	0.98	0.16	51,51,51,51	0
57	MG	AA	3168	1/1	0.98	0.11	59,59,59,59	0
57	MG	BA	3230	1/1	0.98	0.20	53,53,53,53	0
57	MG	AA	3053	1/1	0.98	0.20	61,61,61,61	0
57	MG	BR	202	1/1	0.98	0.14	31,31,31,31	0
57	MG	CA	3043	1/1	0.98	0.11	47,47,47,47	0
57	MG	CA	3133	1/1	0.98	0.21	59,59,59,59	0
57	MG	BA	3487	1/1	0.98	0.14	50,50,50,50	0
57	MG	DA	3258	1/1	0.98	0.14	48,48,48,48	0
57	MG	DA	3500	1/1	0.98	0.10	49,49,49,49	0
57	MG	BA	3044	1/1	0.98	0.22	20,20,20,20	0
57	MG	BU	203	1/1	0.98	0.21	47,47,47,47	0
57	MG	CA	3047	1/1	0.98	0.14	53,53,53,53	0
57	MG	BA	3234	1/1	0.98	0.15	38,38,38,38	0
57	MG	DA	3157	1/1	0.98	0.11	47,47,47,47	0
57	MG	BA	3605	1/1	0.98	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3735	1/1	0.98	0.43	57,57,57,57	0
57	MG	DA	3508	1/1	0.98	0.10	44,44,44,44	0
57	MG	BA	3736	1/1	0.98	0.16	42,42,42,42	0
57	MG	DA	3161	1/1	0.98	0.19	38,38,38,38	0
57	MG	BV	201	1/1	0.98	0.31	33,33,33,33	0
57	MG	DA	3512	1/1	0.98	0.09	47,47,47,47	0
57	MG	BA	3737	1/1	0.98	0.29	43,43,43,43	0
57	MG	BA	3544	1/1	0.98	0.22	44,44,44,44	0
57	MG	BA	3607	1/1	0.98	0.24	38,38,38,38	0
57	MG	BA	3235	1/1	0.98	0.16	42,42,42,42	0
57	MG	BA	3609	1/1	0.98	0.11	39,39,39,39	0
57	MG	CA	3148	1/1	0.98	0.11	70,70,70,70	0
57	MG	DA	3393	1/1	0.98	0.10	50,50,50,50	0
57	MG	BA	3174	1/1	0.98	0.18	37,37,37,37	0
57	MG	BA	3148	1/1	0.98	0.33	44,44,44,44	0
57	MG	BA	3744	1/1	0.98	0.14	39,39,39,39	0
57	MG	BA	3124	1/1	0.98	0.21	19,19,19,19	0
57	MG	AA	3086	1/1	0.98	0.07	57,57,57,57	0
57	MG	DA	3525	1/1	0.98	0.13	59,59,59,59	0
57	MG	DA	3399	1/1	0.98	0.13	59,59,59,59	0
57	MG	BA	3085	1/1	0.98	0.27	35,35,35,35	0
57	MG	DA	3281	1/1	0.98	0.16	53,53,53,53	0
57	MG	BA	3241	1/1	0.98	0.19	36,36,36,36	0
57	MG	CA	3065	1/1	0.98	0.17	49,49,49,49	0
57	MG	DA	3404	1/1	0.98	0.12	48,48,48,48	0
57	MG	DA	3177	1/1	0.98	0.15	42,42,42,42	0
57	MG	BA	3497	1/1	0.98	0.14	28,28,28,28	0
57	MG	DA	3534	1/1	0.98	0.15	55,55,55,55	0
57	MG	DA	3665	1/1	0.98	0.14	42,42,42,42	0
57	MG	B0	101	1/1	0.98	0.17	36,36,36,36	0
57	MG	BA	3498	1/1	0.98	0.18	36,36,36,36	0
57	MG	DA	3289	1/1	0.98	0.10	53,53,53,53	0
57	MG	BA	3313	1/1	0.98	0.07	53,53,53,53	0
57	MG	AA	3077	1/1	0.98	0.25	56,56,56,56	0
57	MG	DA	3412	1/1	0.98	0.20	50,50,50,50	0
57	MG	DA	3292	1/1	0.98	0.17	30,30,30,30	0
57	MG	BA	3556	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3294	1/1	0.98	0.16	43,43,43,43	0
57	MG	AA	3082	1/1	0.98	0.13	46,46,46,46	0
57	MG	BA	3558	1/1	0.98	0.14	32,32,32,32	0
57	MG	BB	217	1/1	0.98	0.18	29,29,29,29	0
57	MG	BA	3449	1/1	0.98	0.21	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	B6	101	1/1	0.98	0.17	48,48,48,48	0
57	MG	BA	3450	1/1	0.98	0.13	48,48,48,48	0
57	MG	DA	3190	1/1	0.98	0.20	54,54,54,54	0
57	MG	BA	3625	1/1	0.98	0.18	39,39,39,39	0
57	MG	BA	3278	1/1	0.98	0.18	34,34,34,34	0
57	MG	BA	3049	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3555	1/1	0.98	0.29	53,53,53,53	0
57	MG	BA	3563	1/1	0.98	0.17	36,36,36,36	0
57	MG	BA	3762	1/1	0.98	0.20	46,46,46,46	0
57	MG	BA	3050	1/1	0.98	0.20	38,38,38,38	0
57	MG	DA	3197	1/1	0.98	0.14	55,55,55,55	0
57	MG	DA	3198	1/1	0.98	0.13	40,40,40,40	0
57	MG	DA	3094	1/1	0.98	0.22	50,50,50,50	0
57	MG	BA	3454	1/1	0.98	0.23	27,27,27,27	0
57	MG	CA	3085	1/1	0.98	0.13	54,54,54,54	0
57	MG	DD	305	1/1	0.98	0.12	36,36,36,36	0
57	MG	BA	3281	1/1	0.98	0.28	60,60,60,60	0
57	MG	BA	3010	1/1	0.98	0.16	39,39,39,39	0
57	MG	DD	308	1/1	0.98	0.29	48,48,48,48	0
57	MG	BA	3247	1/1	0.98	0.16	25,25,25,25	0
57	MG	DE	301	1/1	0.98	0.40	46,46,46,46	0
57	MG	CA	3089	1/1	0.98	0.12	47,47,47,47	0
57	MG	AA	3062	1/1	0.98	0.28	51,51,51,51	0
57	MG	BA	3364	1/1	0.98	0.27	60,60,60,60	0
57	MG	AA	3090	1/1	0.98	0.21	66,66,66,66	0
57	MG	DF	3002	1/1	0.98	0.18	48,48,48,48	0
57	MG	DA	3003	1/1	0.98	0.15	27,27,27,27	0
57	MG	DA	3442	1/1	0.98	0.12	39,39,39,39	0
57	MG	DN	5001	1/1	0.98	0.11	66,66,66,66	0
57	MG	AA	3126	1/1	0.98	0.09	49,49,49,49	0
57	MG	BA	3772	1/1	0.98	0.19	33,33,33,33	0
57	MG	BA	3367	1/1	0.98	0.25	29,29,29,29	0
57	MG	DQ	3001	1/1	0.98	0.13	47,47,47,47	0
57	MG	DA	3008	1/1	0.98	0.09	36,36,36,36	0
57	MG	BA	3287	1/1	0.98	0.14	42,42,42,42	0
57	MG	DA	3010	1/1	0.98	0.17	47,47,47,47	0
57	MG	BA	3416	1/1	0.98	0.21	21,21,21,21	0
57	MG	DU	3001	1/1	0.98	0.32	55,55,55,55	0
57	MG	DA	3330	1/1	0.98	0.11	45,45,45,45	0
57	MG	BA	3187	1/1	0.98	0.25	29,29,29,29	0
57	MG	CA	3099	1/1	0.98	0.15	44,44,44,44	0
57	MG	DA	3453	1/1	0.98	0.22	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3705	1/1	0.98	0.11	62,62,62,62	0
57	MG	DA	3115	1/1	0.98	0.24	40,40,40,40	0
57	MG	BA	3467	1/1	0.98	0.23	50,50,50,50	0
57	MG	BF	305	1/1	0.98	0.09	49,49,49,49	0
57	MG	CA	3103	1/1	0.98	0.13	46,46,46,46	0
57	MG	DA	3459	1/1	0.98	0.19	47,47,47,47	0
57	MG	BA	3327	1/1	0.98	0.18	38,38,38,38	0
57	MG	CA	3105	1/1	0.98	0.18	52,52,52,52	0
57	MG	BA	3521	1/1	0.98	0.20	39,39,39,39	0
58	SF4	AD	501	8/8	0.98	0.16	62,68,73,86	0
58	SF4	CD	302	8/8	0.98	0.16	60,68,83,86	0
59	ZN	AN	501	1/1	0.98	0.19	69,69,69,69	0
59	ZN	BY	501	1/1	0.98	0.15	58,58,58,58	0
57	MG	DA	3021	1/1	0.98	0.09	31,31,31,31	0
59	ZN	B6	103	1/1	0.98	0.24	49,49,49,49	0
59	ZN	CN	501	1/1	0.98	0.08	93,93,93,93	0
57	MG	BA	3135	1/1	0.98	0.20	43,43,43,43	0
57	MG	BA	3025	1/1	0.98	0.16	27,27,27,27	0
57	MG	BA	3038	1/1	0.98	0.25	35,35,35,35	0
57	MG	BA	3472	1/1	0.98	0.16	20,20,20,20	0
57	MG	BA	3039	1/1	0.98	0.20	32,32,32,32	0
57	MG	BU	206	1/1	0.99	0.40	35,35,35,35	0
57	MG	DA	3026	1/1	0.99	0.56	59,59,59,59	0
57	MG	DA	3027	1/1	0.99	0.57	51,51,51,51	0
57	MG	BD	307	1/1	0.99	0.21	40,40,40,40	0
57	MG	BA	3384	1/1	0.99	0.19	41,41,41,41	0
57	MG	BA	3216	1/1	0.99	0.23	37,37,37,37	0
57	MG	DA	3031	1/1	0.99	0.43	43,43,43,43	0
57	MG	BA	3569	1/1	0.99	0.19	49,49,49,49	0
57	MG	DA	3285	1/1	0.99	0.13	32,32,32,32	0
57	MG	BA	3045	1/1	0.99	0.21	36,36,36,36	0
57	MG	BA	3597	1/1	0.99	0.21	25,25,25,25	0
57	MG	BA	3378	1/1	0.99	0.12	28,28,28,28	0
57	MG	BA	3233	1/1	0.99	0.30	56,56,56,56	0
57	MG	BA	3726	1/1	0.99	0.19	63,63,63,63	0
57	MG	BA	3013	1/1	0.99	0.14	32,32,32,32	0
57	MG	DA	3315	1/1	0.99	0.08	42,42,42,42	0
57	MG	BA	3198	1/1	0.99	0.24	37,37,37,37	0
57	MG	BA	3374	1/1	0.99	0.17	40,40,40,40	0
57	MG	BA	3422	1/1	0.99	0.24	33,33,33,33	0
57	MG	DA	3671	1/1	0.99	0.13	74,74,74,74	0
57	MG	BA	3392	1/1	0.99	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3344	1/1	0.99	0.16	31,31,31,31	0
57	MG	BA	3069	1/1	0.99	0.27	22,22,22,22	0
57	MG	DA	3297	1/1	0.99	0.11	39,39,39,39	0
59	ZN	B5	102	1/1	0.99	0.22	48,48,48,48	0
57	MG	DA	3347	1/1	0.99	0.20	27,27,27,27	0
59	ZN	B9	501	1/1	0.99	0.18	38,38,38,38	0
57	MG	DF	3004	1/1	0.99	0.38	44,44,44,44	0
57	MG	DA	3560	1/1	0.99	0.07	40,40,40,40	0
57	MG	DA	3005	1/1	0.99	0.22	57,57,57,57	0
59	ZN	D5	501	1/1	0.99	0.20	58,58,58,58	0
59	ZN	D6	501	1/1	0.99	0.17	71,71,71,71	0
57	MG	BA	3458	1/1	0.99	0.18	18,18,18,18	0
57	MG	DA	3480	1/1	0.99	0.10	40,40,40,40	0
57	MG	DA	3535	1/1	0.99	0.18	56,56,56,56	0
57	MG	BA	3037	1/1	1.00	0.24	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.