wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 11:25 PM EST

PDB ID	:	1VY4
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in the pre-attack state of peptide bond formation containing acylated tRNA-substrates in the A and P sites.
Authors	:	Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on	:	2014-05-13
Resolution	:	2.60 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:

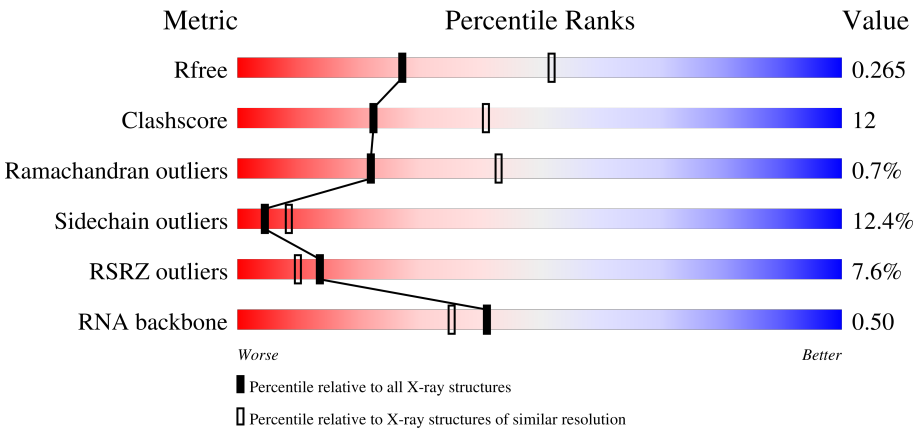
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	.% 49% 38% 11% • •
1	CA	1521	4% 43% 40% 14% • •
2	AB	256	11% 45% 37% 8% • 10%
2	CB	256	33% 36% 44% 10% • 10%

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Mol	Chain	Length	Quality of chain
3	AC	239	10% 51% 32% • 14%
3	CC	239	31% 47% 32% 7% 14%
4	AD	209	18% 65% 28% 6%
4	CD	209	12% 58% 35% 7%
5	AE	162	7% 66% 23% • 9%
5	CE	162	13% 52% 35% 5% 9%
6	AF	101	% 70% 23% 6% •
6	CF	101	3% 72% 25% • •
7	AG	156	6% 72% 21% 6% • •
7	CG	156	30% 71% 22% 7% •
8	AH	138	% 60% 35% • •
8	CH	138	25% 52% 41% 6% •
9	AI	128	15% 55% 37% 8% •
9	CI	128	65% 44% 45% 10% •
10	AJ	105	12% 57% 31% • 8%
10	CJ	105	41% 38% 48% 6% 9%
11	AK	129	8% 62% 22% 5% 12%
11	CK	129	10% 57% 29% • 12%
12	AL	132	% 61% 30% • 8%
12	CL	132	17% 55% 35% • 8%
13	AM	126	6% 57% 32% 9% •
13	CM	126	40% 35% 49% 12% • •
14	AN	61	13% 48% 44% 7% •
14	CN	61	69% 39% 46% 13% •
15	AO	89	6% 65% 31% • •

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Mol	Chain	Length	Quality of chain
15	CO	89	7% 62% 31% 6%
16	AP	88	25% 53% 33% 7% 7%
16	CP	88	3% 59% 28% 6% 7%
17	AQ	105	8% 65% 26% 6%
17	CQ	105	20% 66% 26% 6%
18	AR	88	10% 50% 25% 23%
18	CR	88	13% 41% 32% 5% 23%
19	AS	93	2% 44% 41% 5% 10%
19	CS	93	41% 42% 38% 10% 11%
20	AT	106	5% 54% 29% 8% 9%
20	CT	106	8% 53% 30% 8% 9%
21	AU	27	19% 44% 33% 7% 15%
21	CU	27	56% 37% 41% 7% 15%
22	AV	24	21% 29% 17% 8% 46%
22	CV	24	29% 29% 8% 12% 50%
23	AW	76	13% 28% 43% 25%
23	CW	76	62% 18% 43% 26% 7% 5%
24	AX	77	52% 30% 13%
24	CX	77	3% 32% 38% 27%
25	AY	76	11% 13% 37% 38% 9%
25	CY	76	36% 13% 32% 38% 13%
26	BA	2915	% 63% 26% 7%
26	DA	2915	2% 52% 34% 9%
27	BB	121	71% 23% 5%
27	DB	121	2% 29% 50% 19%

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Mol	Chain	Length	Quality of chain
28	BD	276	%, 79%, 17%
28	DD	276	3%, 71%, 25%
29	BE	206	76%, 19%
29	DE	206	70%, 21%, 7%
30	BF	210	69%, 24%
30	DF	210	3%, 56%, 35%, 6%
31	BG	182	2%, 66%, 30%
31	DG	182	32%, 43%, 48%, 8%
32	BH	180	%, 64%, 30%
32	DH	180	40%, 55%, 36%, 6%
33	BI	148	%, 60%, 28%, 10%
33	DI	148	%, 68%, 24%, 6%
34	BN	140	76%, 19%
34	DN	140	9%, 67%, 31%
35	BO	122	69%, 28%
35	DO	122	2%, 66%, 27%, 7%
36	BP	150	69%, 25%, 6%
36	DP	150	4%, 61%, 33%, 5%
37	BQ	141	%, 74%, 23%
37	DQ	141	19%, 61%, 35%
38	BR	118	69%, 25%, 7%
38	DR	118	5%, 64%, 31%, 6%
39	BS	112	71%, 22%, 5%
39	DS	112	26%, 54%, 38%, 6%
40	BT	146	66%, 22%, 10%

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Mol	Chain	Length	Quality of chain
40	DT	146	%, 57%, 31%, 10%
41	BU	118	76%, 21%
41	DU	118	4%, 64%, 33%
42	BV	101	72%, 23%, 5%
42	DV	101	4%, 63%, 29%, 7%
43	BW	113	79%, 18%
43	DW	113	4%, 78%, 19%
44	BX	96	75%, 20%
44	DX	96	10%, 64%, 30%, 5%
45	BY	110	%, 63%, 31%
45	DY	110	11%, 60%, 34%
46	BZ	206	15%, 51%, 28%, 17%
46	DZ	206	33%, 41%, 38%, 5%, 16%
47	B0	85	7%, 84%, 11%
47	D0	85	12%, 67%, 26%, 5%
48	B1	98	2%, 73%, 22%
48	D1	98	5%, 74%, 19%
49	B2	72	68%, 28%
49	D2	72	%, 65%, 29%
50	B3	60	83%, 12%
50	D3	60	13%, 63%, 33%
51	B4	71	6%, 54%, 28%, 14%
51	D4	71	38%, 48%, 41%, 8%
52	B5	60	2%, 68%, 25%, 5%
52	D5	60	2%, 70%, 27%

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Mol	Chain	Length	Quality of chain
53	B6	54	65% 26% 7%
53	D6	54	6% 65% 28% 6%
54	B7	49	6% 73% 22%
54	D7	49	10% 69% 27%
55	B8	65	71% 26%
55	D8	65	2% 65% 31%
56	B9	37	3% 73% 27%
56	D9	37	11% 57% 43%

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	PSU	CY	39	-	-	X	-
25	5MU	CY	54	-	-	-	X
25	PSU	CY	55	-	-	-	X
57	MG	BA	3710	-	-	-	X
57	MG	DA	3024	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3624	-	-	-	X
57	MG	DA	3657	-	-	-	X
57	MG	DQ	3003	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 297127 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	1497	32185	14324	5968	10396	1497	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	1544	970	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	1678	1052	333	286	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	812	514	146	149	3	0	0	0
6	CF	100	820	518	147	152	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	986	626	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	833	519	156	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	966	598	200	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	84	661	423	122	114	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	731	449	156	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	1599	722	287	515	73	2	0	0	0
23	CW	72	1552	697	280	502	72	1	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	1635	731	296	530	76	2	0	0	0
24	CX	76	1635	731	296	530	76	2	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	2142	1352	426	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	1073	688	188	196	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	1139	709	231	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	517	331	102	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	216	216	216	0	0
57	AB	1	1	1	0	0
57	AE	1	1	1	0	0
57	AF	1	1	1	0	0
57	AK	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	AL	2	2	2	0	0
57	AM	2	2	2	0	0
57	AN	2	2	2	0	0
57	AT	1	1	1	0	0
57	AU	1	1	1	0	0
57	AW	2	2	2	0	0
57	AX	15	15	15	0	0
57	AY	3	3	3	0	0
57	BA	814	814	814	0	0
57	BB	23	23	23	0	0
57	BD	10	10	10	0	0
57	BE	6	6	6	0	0
57	BF	11	11	11	0	0
57	BG	2	2	2	0	0
57	BH	1	1	1	0	0
57	BN	3	3	3	0	0
57	BO	1	1	1	0	0
57	BP	2	2	2	0	0
57	BQ	2	2	2	0	0
57	BR	2	2	2	0	0
57	BU	4	4	4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	BV	5	5	5	0	0
57	BW	4	4	4	0	0
57	BX	1	1	1	0	0
57	BY	1	1	1	0	0
57	BZ	2	2	2	0	0
57	B0	2	2	2	0	0
57	B2	1	1	1	0	0
57	B4	1	1	1	0	0
57	B5	3	3	3	0	0
57	B6	2	2	2	0	0
57	B7	5	5	5	0	0
57	B8	2	2	2	0	0
57	B9	1	1	1	0	0
57	CA	169	169	169	0	0
57	CD	1	1	1	0	0
57	CE	2	2	2	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	CW	1	1	1	0	0

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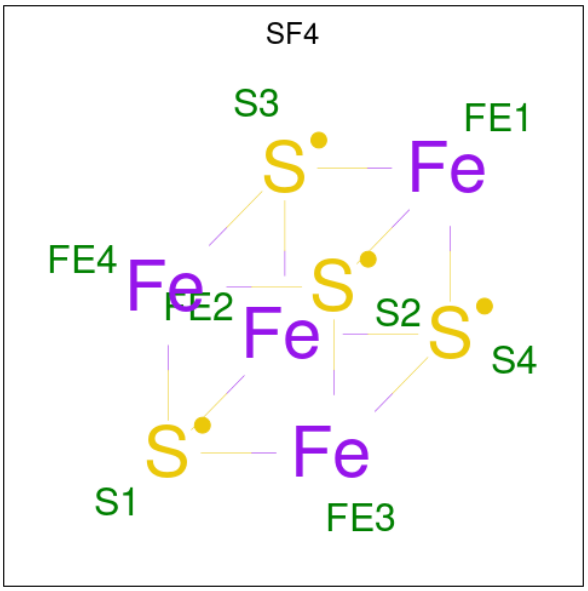
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	CX	2	2	2	0	0
57	DA	664	664	664	0	0
57	DB	13	13	13	0	0
57	DD	4	4	4	0	0
57	DE	7	7	7	0	0
57	DF	5	5	5	0	0
57	DG	1	1	1	0	0
57	DN	1	1	1	0	0
57	DO	2	2	2	0	0
57	DP	2	2	2	0	0
57	DQ	3	3	3	0	0
57	DR	1	1	1	0	0
57	DU	1	1	1	0	0
57	DV	1	1	1	0	0
57	DW	1	1	1	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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	210	Total O 210 210	0	0
61	AD	1	Total O 1 1	0	0
61	AE	2	Total O 2 2	0	0
61	AJ	1	Total O 1 1	0	0
61	AL	2	Total O 2 2	0	0
61	AM	2	Total O 2 2	0	0
61	AV	2	Total O 2 2	0	0
61	AW	4	Total O 4 4	0	0
61	AX	4	Total O 4 4	0	0
61	AY	1	Total O 1 1	0	0
61	BA	1405	Total O 1406 1406	0	1
61	BB	37	Total O 37 37	0	0
61	BD	15	Total O 15 15	0	0
61	BE	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BF	11	Total O 11 11	0	0
61	BG	3	Total O 3 3	0	0
61	BH	1	Total O 1 1	0	0
61	BI	1	Total O 1 1	0	0
61	BN	1	Total O 1 1	0	0
61	BO	2	Total O 2 2	0	0
61	BP	13	Total O 13 13	0	0
61	BQ	4	Total O 4 4	0	0
61	BR	2	Total O 2 2	0	0
61	BS	2	Total O 2 2	0	0
61	BT	2	Total O 2 2	0	0
61	BU	4	Total O 4 4	0	0
61	BV	2	Total O 2 2	0	0
61	BW	3	Total O 3 3	0	0
61	BX	3	Total O 3 3	0	0
61	BZ	1	Total O 1 1	0	0
61	B0	6	Total O 6 6	0	0
61	B1	2	Total O 2 2	0	0
61	B3	2	Total O 2 2	0	0
61	B5	4	Total O 4 4	0	0
61	B6	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	B7	3	Total O 3 3	0	0
61	B8	13	Total O 13 13	0	0
61	B9	1	Total O 1 1	0	0
61	CA	156	Total O 156 156	0	0
61	CE	2	Total O 2 2	0	0
61	CH	1	Total O 1 1	0	0
61	CJ	1	Total O 1 1	0	0
61	CK	1	Total O 1 1	0	0
61	CL	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CW	2	Total O 2 2	0	0
61	CX	2	Total O 2 2	0	0
61	CY	1	Total O 1 1	0	0
61	DA	989	Total O 989 989	0	0
61	DB	9	Total O 9 9	0	0
61	DD	18	Total O 18 18	0	0
61	DE	5	Total O 5 5	0	0
61	DF	4	Total O 4 4	0	0
61	DN	2	Total O 2 2	0	0
61	DP	12	Total O 12 12	0	0
61	DQ	1	Total O 1 1	0	0

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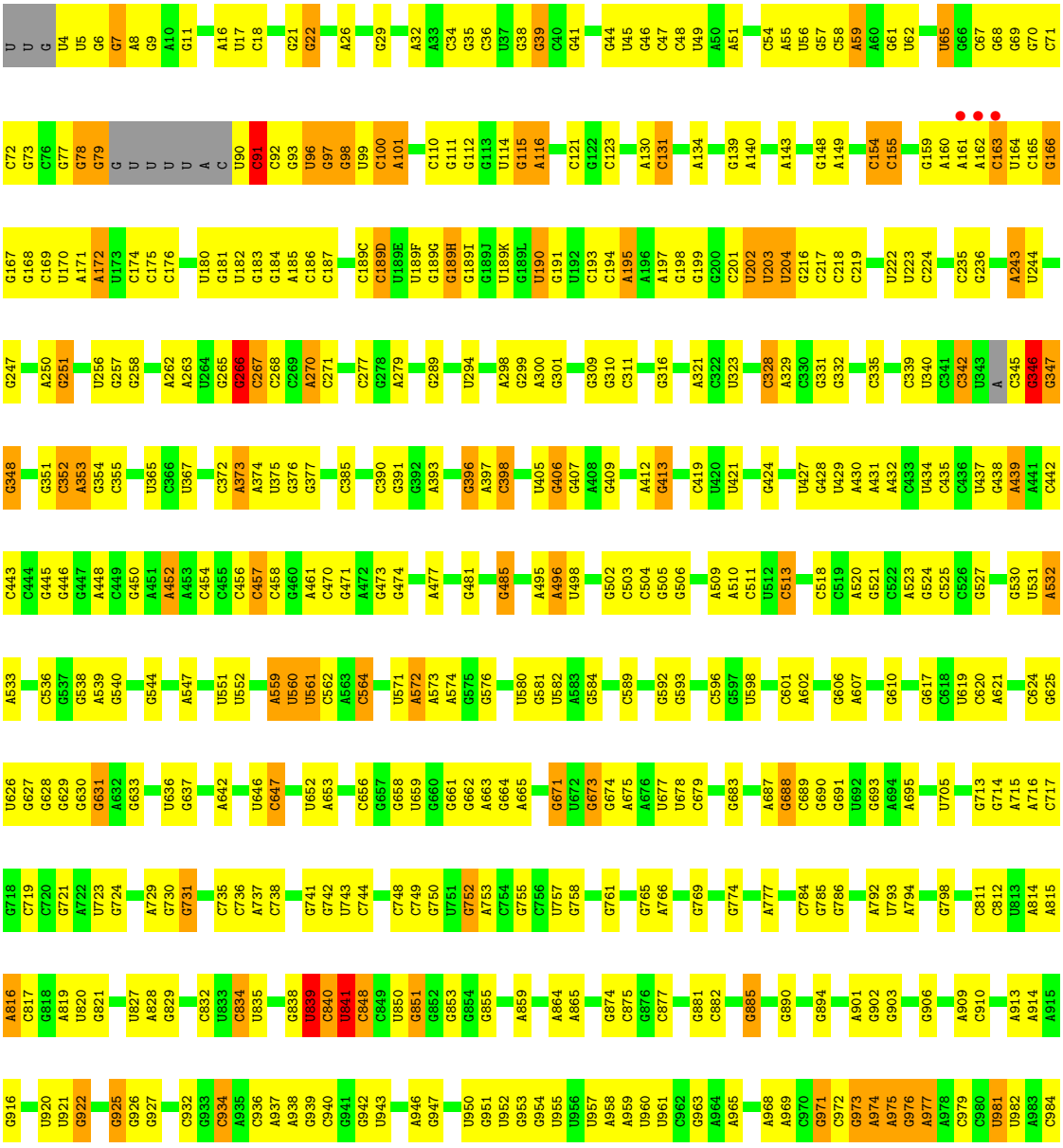
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DT	4	Total O 4 4	0	0
61	DU	1	Total O 1 1	0	0
61	DV	1	Total O 1 1	0	0
61	DW	1	Total O 1 1	0	0
61	DX	2	Total O 2 2	0	0
61	DY	1	Total O 1 1	0	0
61	D0	4	Total O 4 4	0	0
61	D1	1	Total O 1 1	0	0
61	D3	2	Total O 2 2	0	0
61	D5	1	Total O 1 1	0	0
61	D6	1	Total O 1 1	0	0
61	D8	3	Total O 3 3	0	0

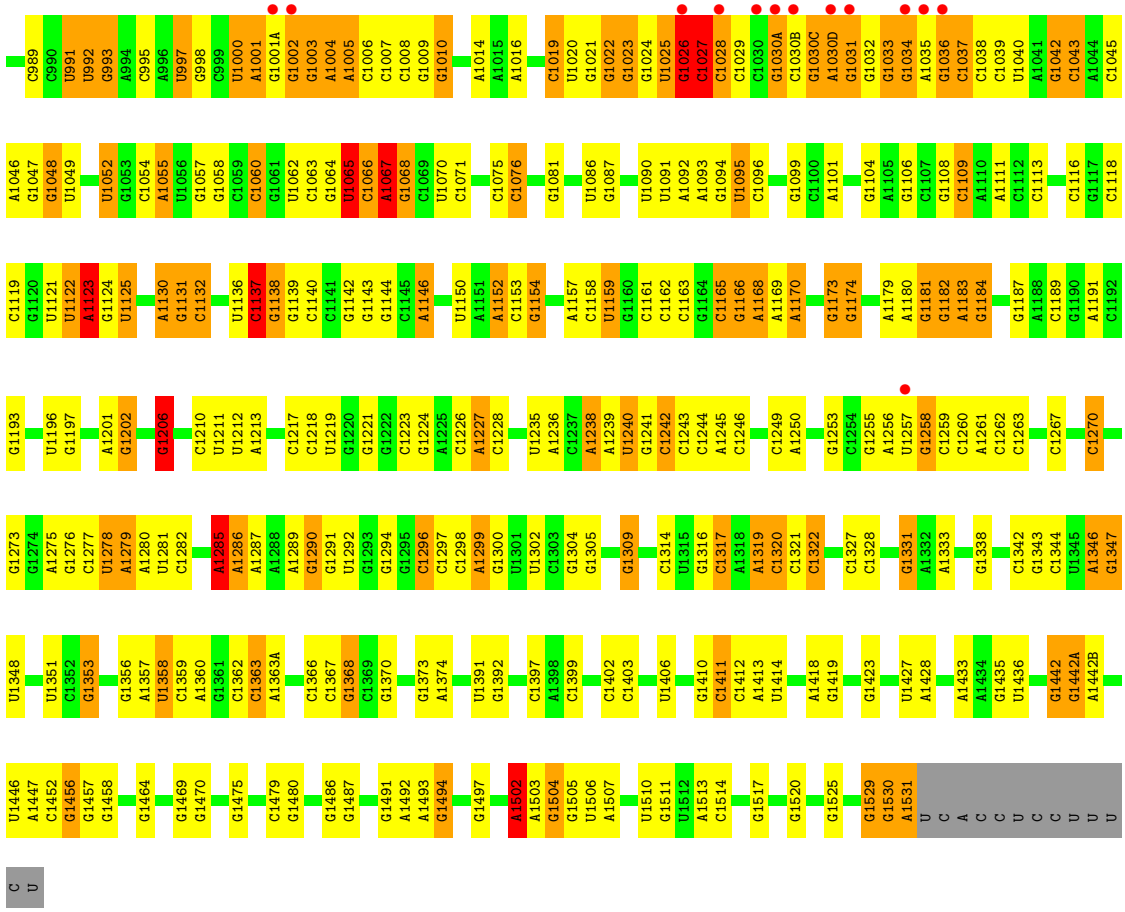
3 Residue-property plots (i)

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

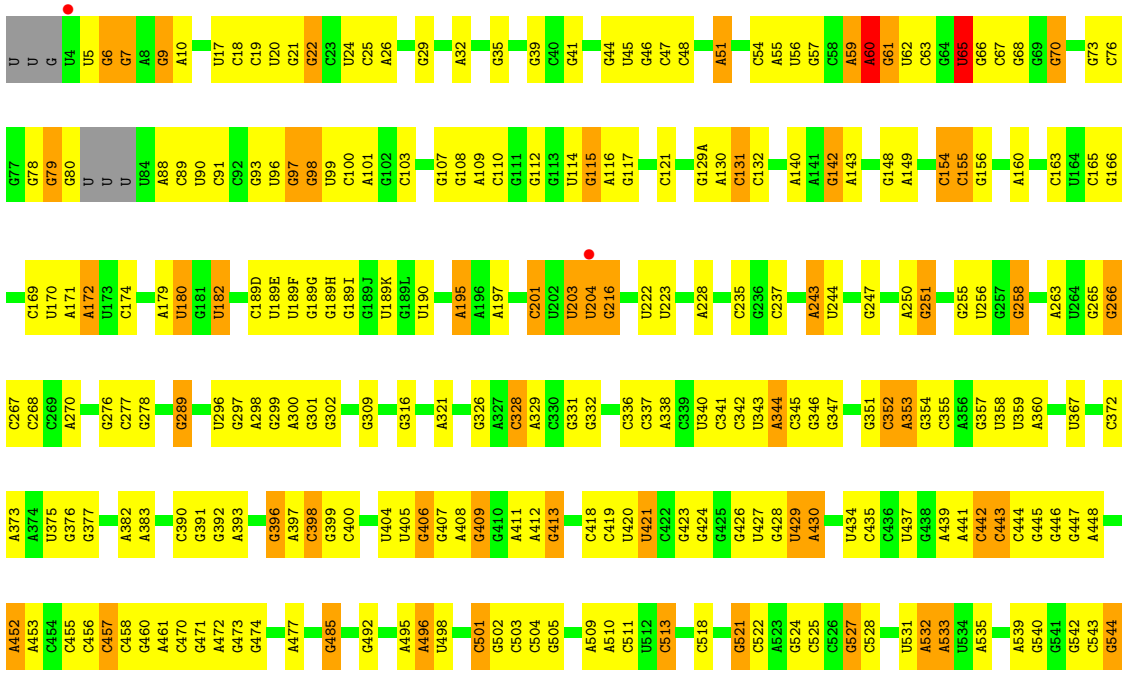
Chain AA:

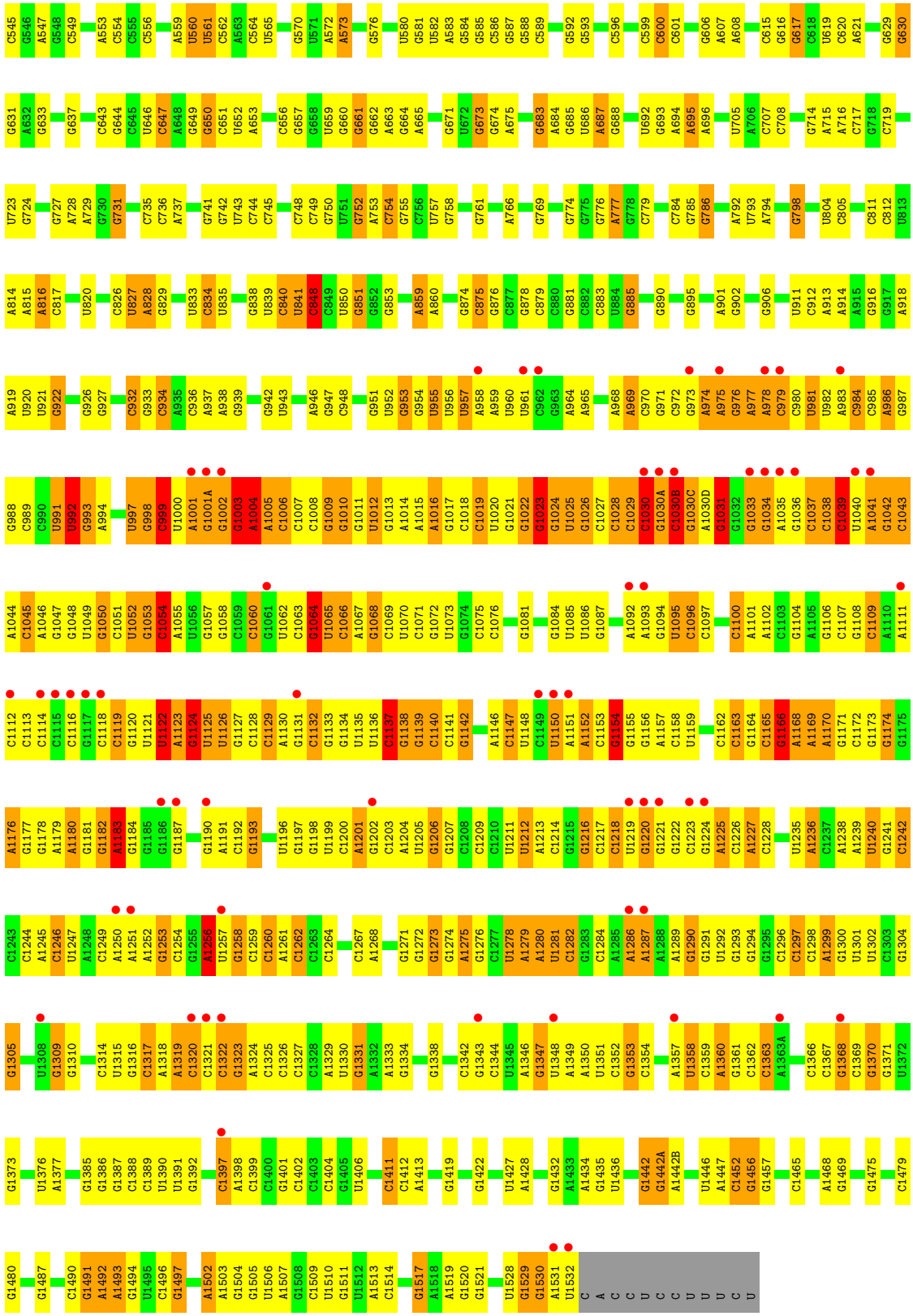




- Molecule 1: 16S Ribosomal RNA

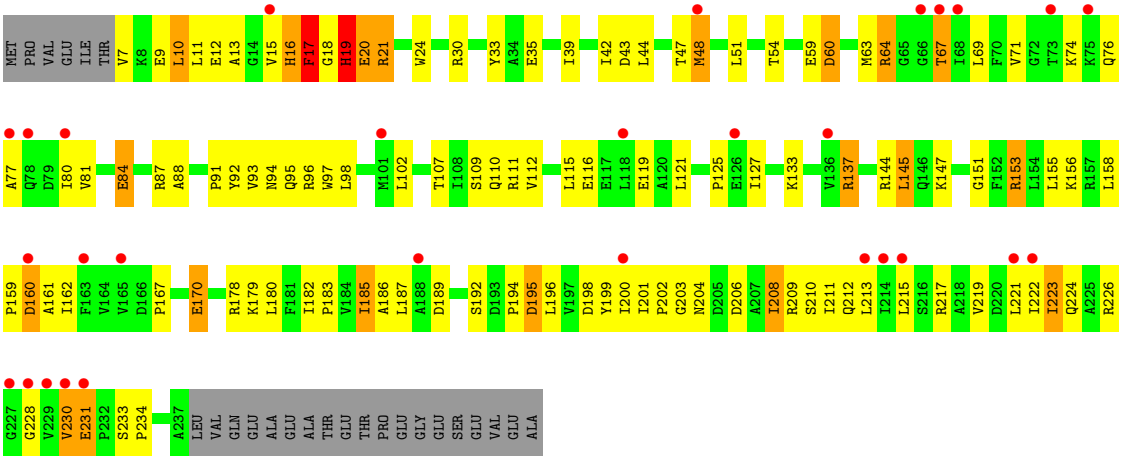
Chain CA:





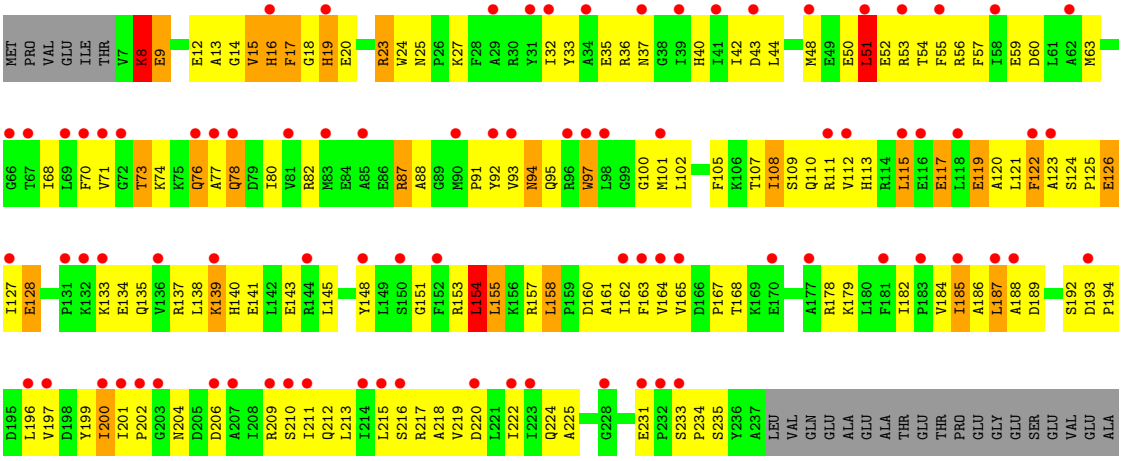
- Molecule 2: 30S ribosomal protein S2

Chain AB:



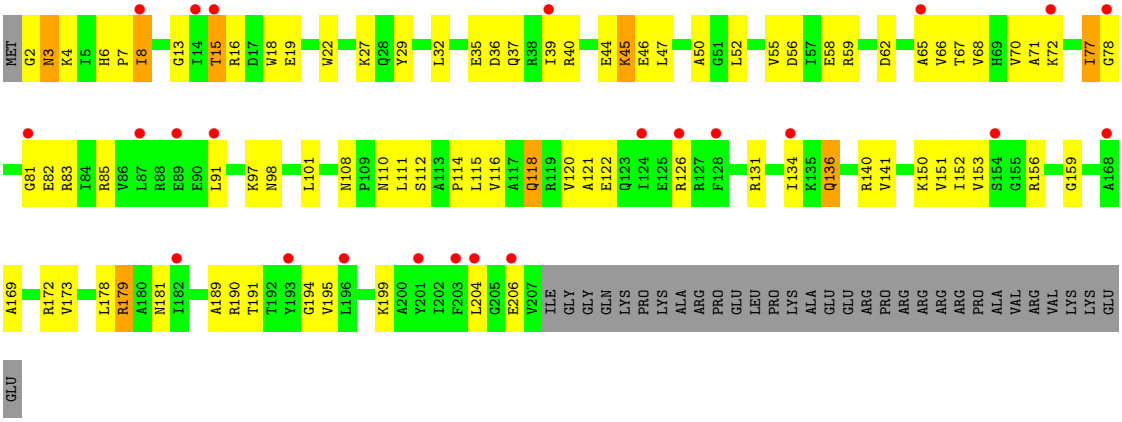
- Molecule 2: 30S ribosomal protein S2

Chain CB:



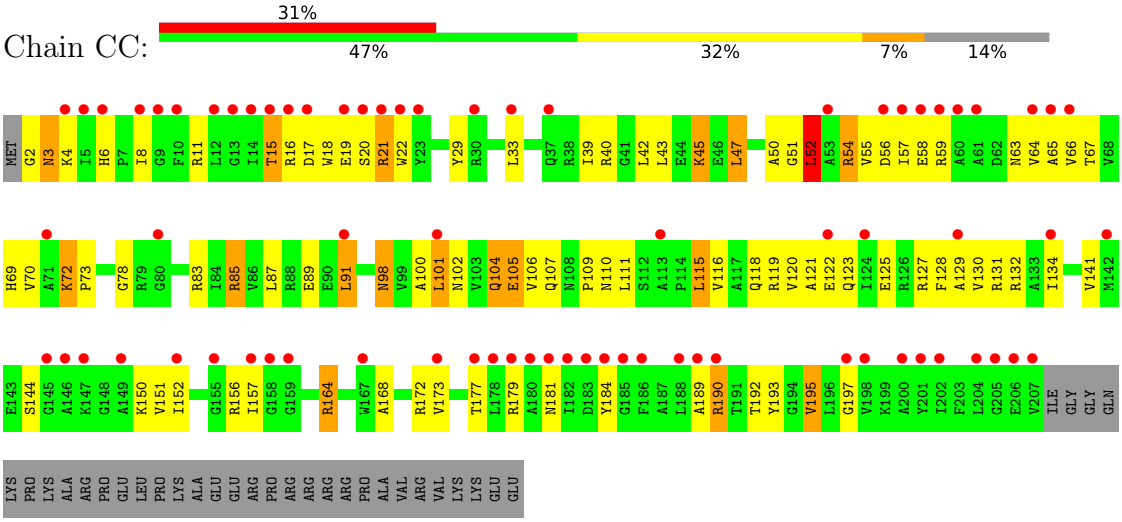
- Molecule 3: 30S ribosomal protein S3

Chain AC:



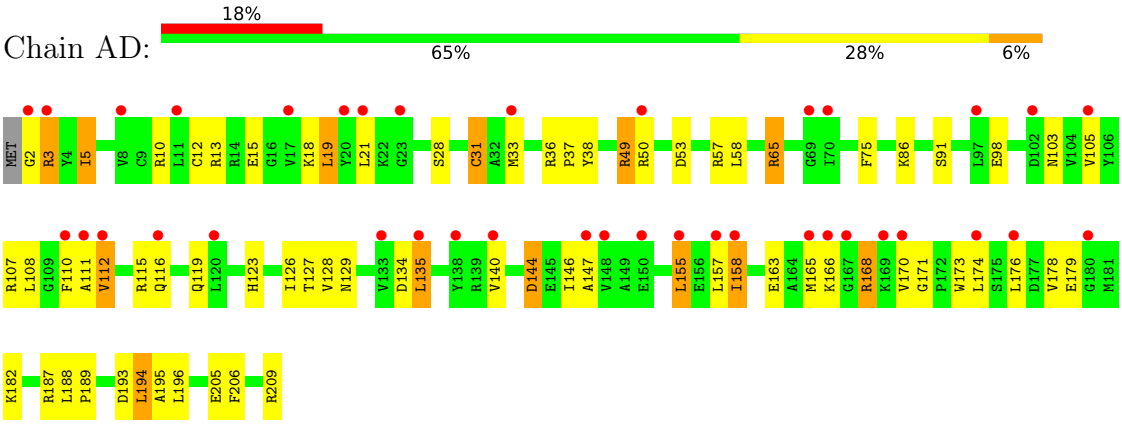
- Molecule 3: 30S ribosomal protein S3

Chain CC:



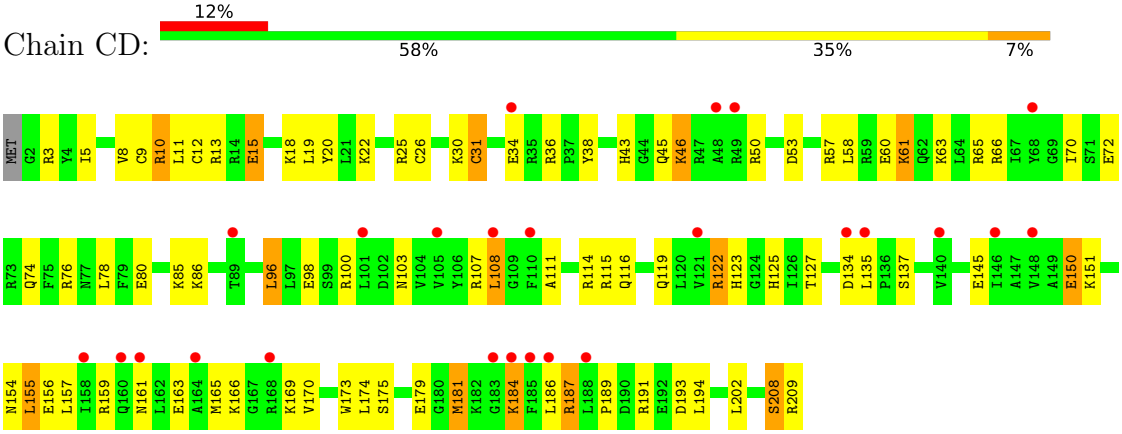
- Molecule 4: 30S ribosomal protein S4

Chain AD:



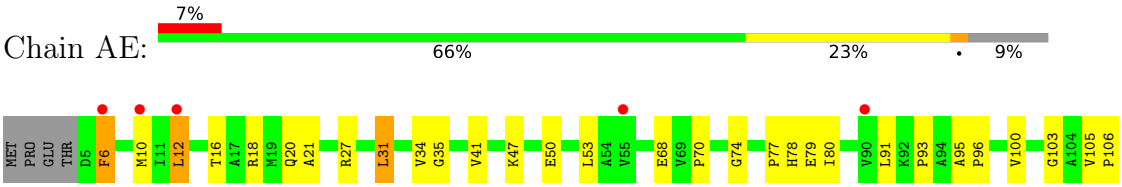
- Molecule 4: 30S ribosomal protein S4

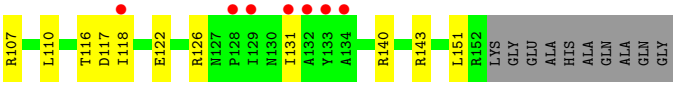
Chain CD:



- Molecule 5: 30S ribosomal protein S5

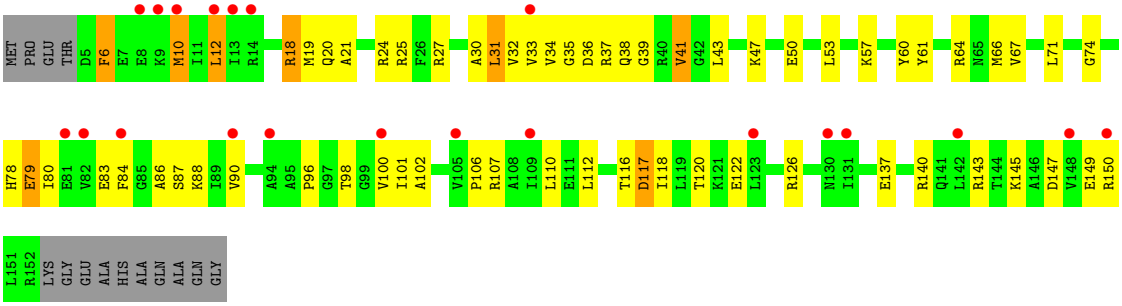
Chain AE:





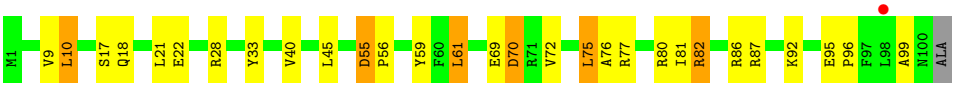
• Molecule 5: 30S ribosomal protein S5

Chain CE:



• Molecule 6: 30S ribosomal protein S6

Chain AF:

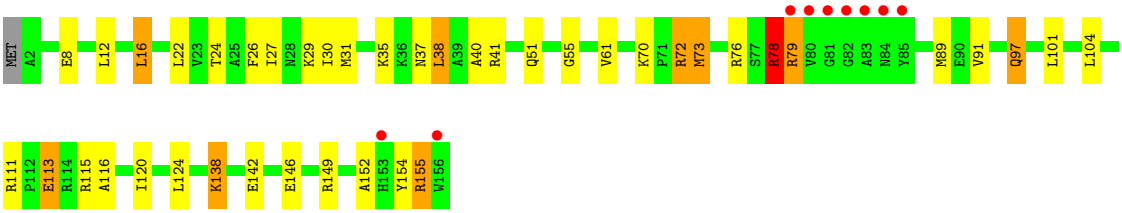


• Molecule 6: 30S ribosomal protein S6

Chain CF:

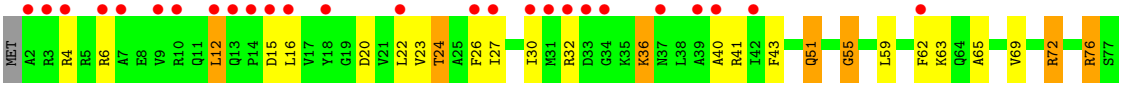
• Molecule 7: 30S ribosomal protein S7

Chain AG:



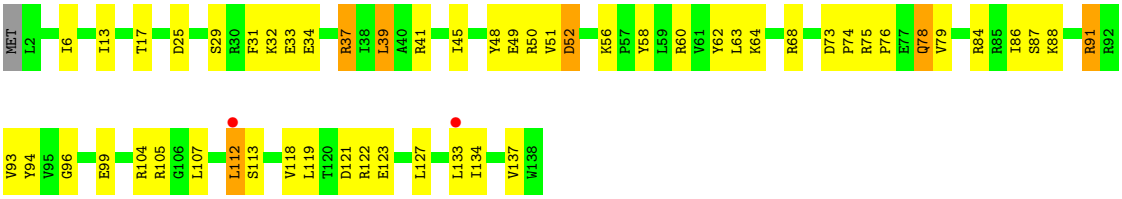
• Molecule 7: 30S ribosomal protein S7

Chain CG:



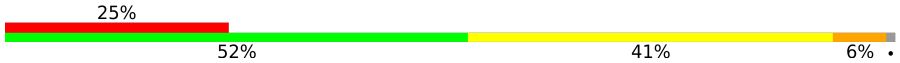
• Molecule 8: 30S ribosomal protein S8

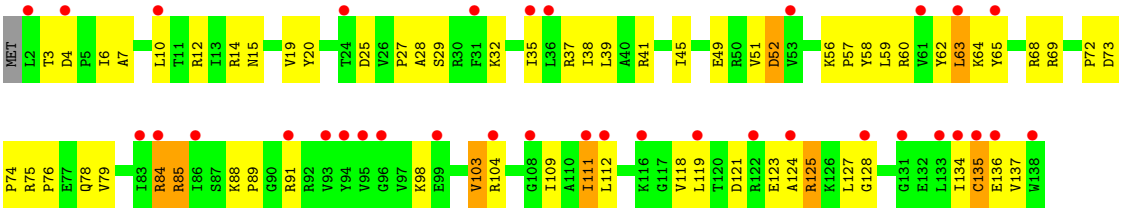
Chain AH:



• Molecule 8: 30S ribosomal protein S8

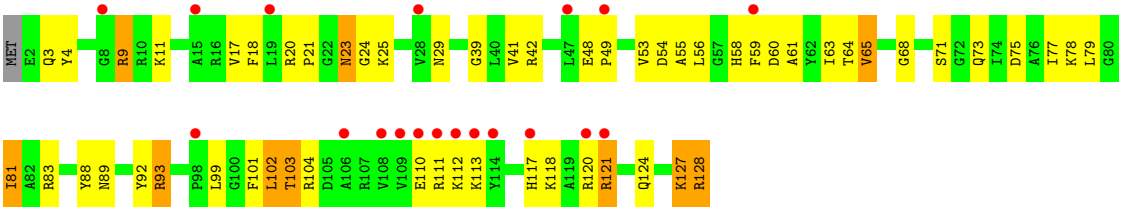
Chain CH:





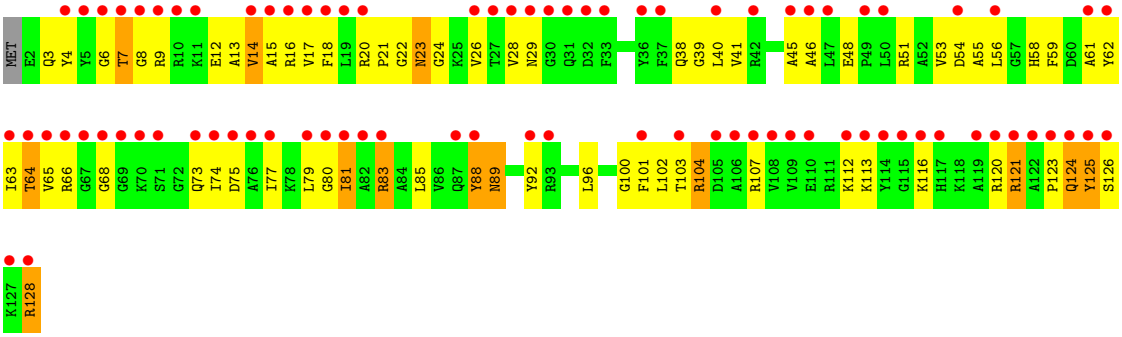
• Molecule 9: 30S ribosomal protein S9

Chain AI:



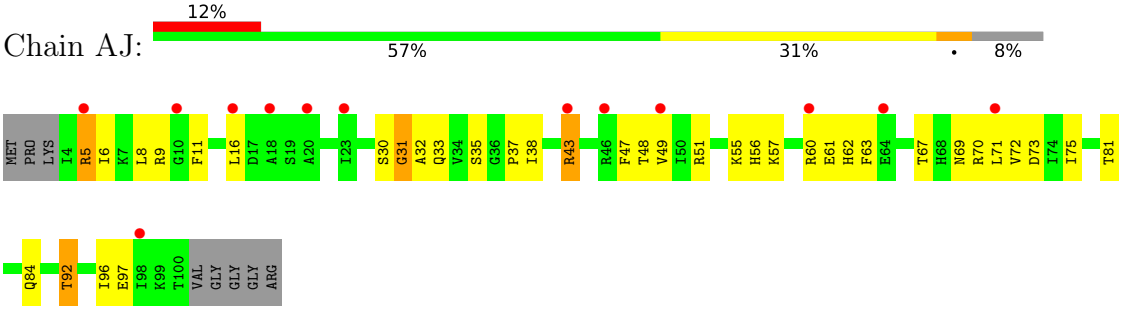
• Molecule 9: 30S ribosomal protein S9

Chain CI:



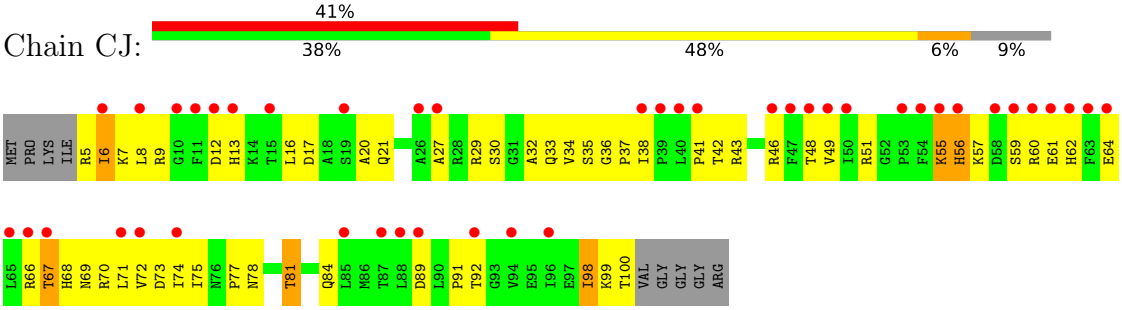
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



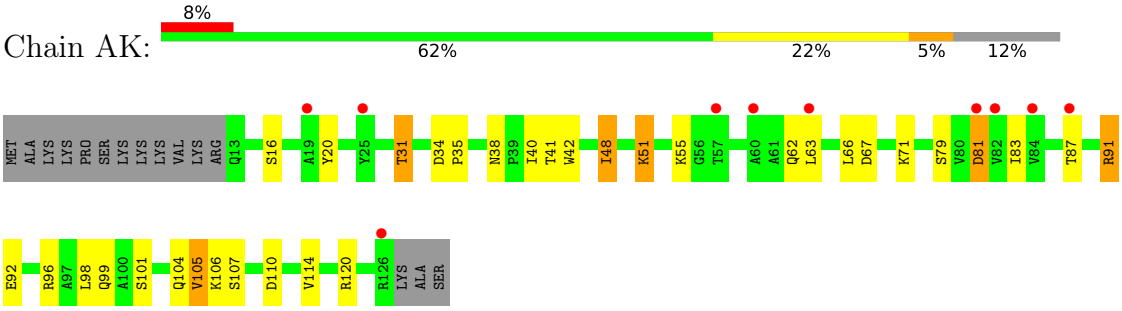
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



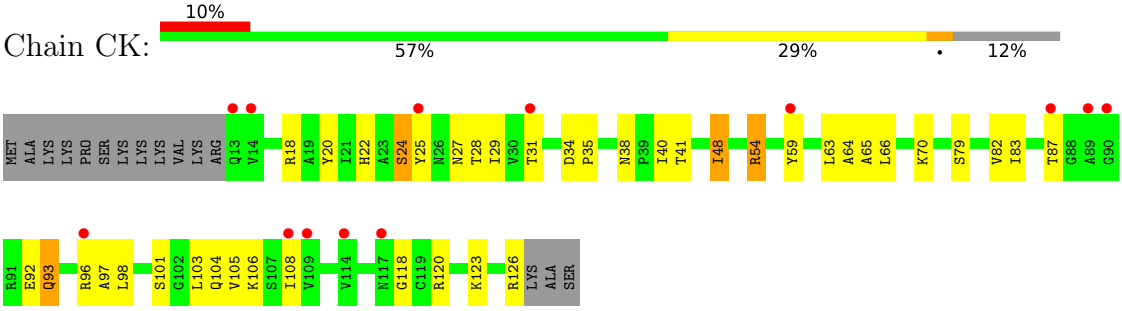
• Molecule 11: 30S ribosomal protein S11

Chain AK:



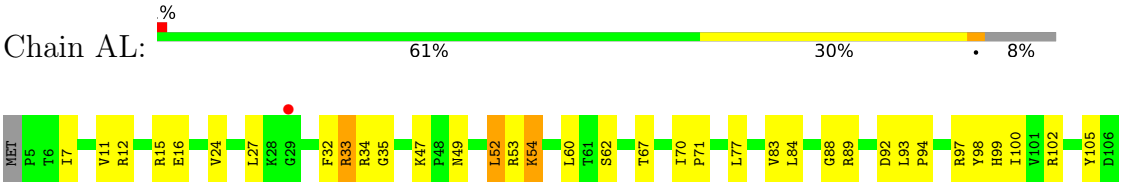
• Molecule 11: 30S ribosomal protein S11

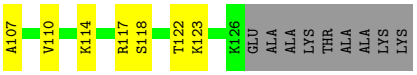
Chain CK:



• Molecule 12: 30S ribosomal protein S12

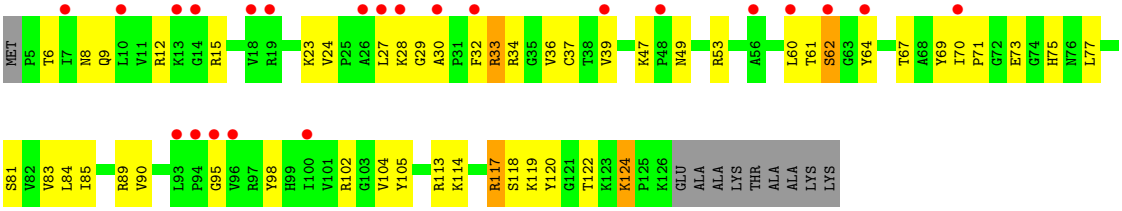
Chain AL:





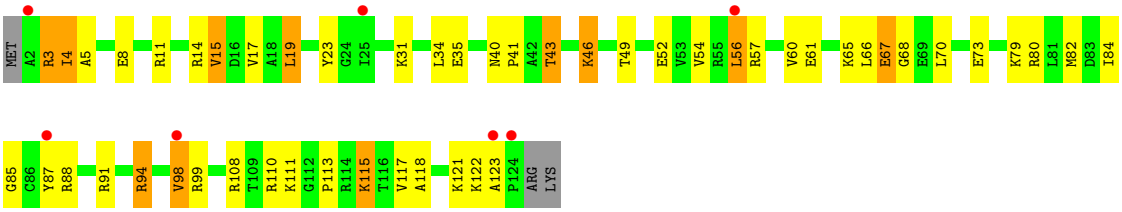
• Molecule 12: 30S ribosomal protein S12

Chain CL:



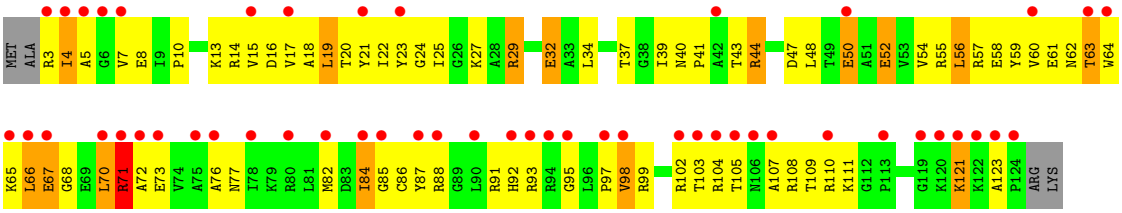
• Molecule 13: 30S ribosomal protein S13

Chain AM:



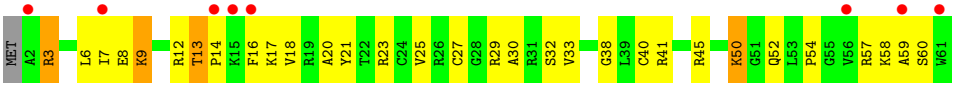
• Molecule 13: 30S ribosomal protein S13

Chain CM:



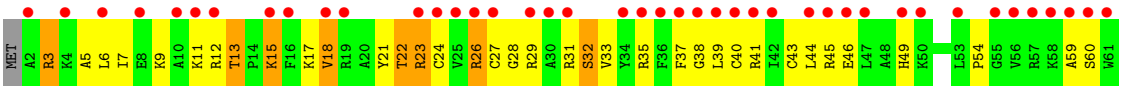
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



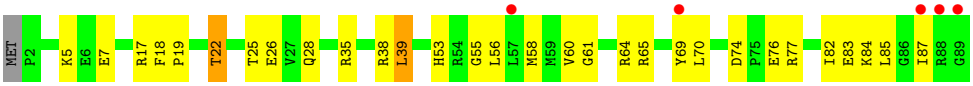
• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



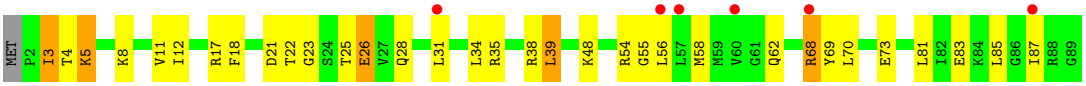
• Molecule 15: 30S ribosomal protein S15

Chain AO:



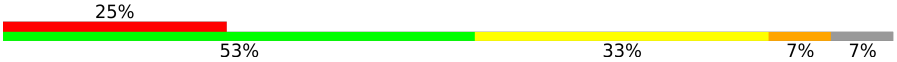
• Molecule 15: 30S ribosomal protein S15

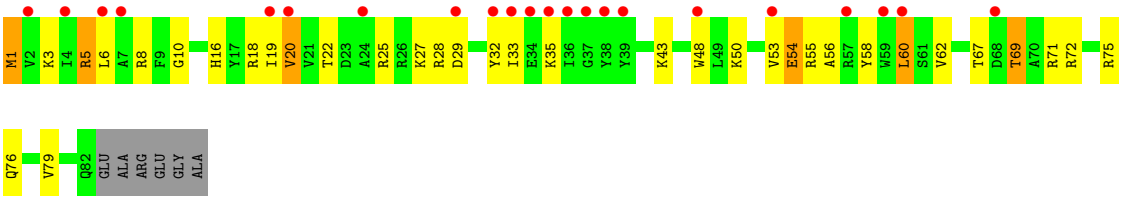
Chain CO:



• Molecule 16: 30S ribosomal protein S16

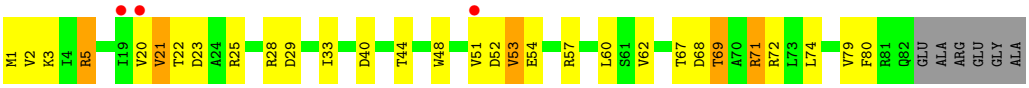
Chain AP:





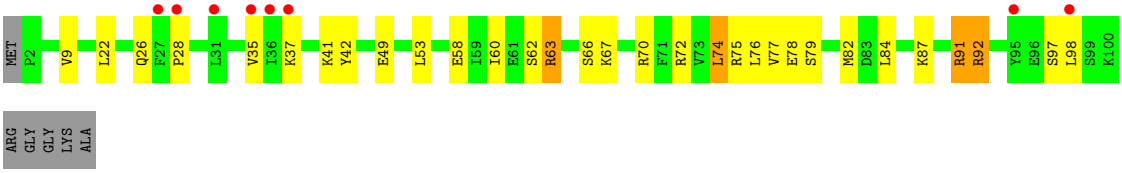
• Molecule 16: 30S ribosomal protein S16

Chain CP:



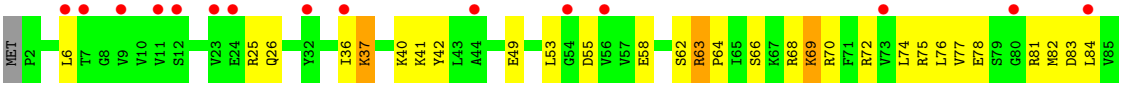
• Molecule 17: 30S ribosomal protein S17

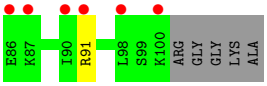
Chain AQ:



• Molecule 17: 30S ribosomal protein S17

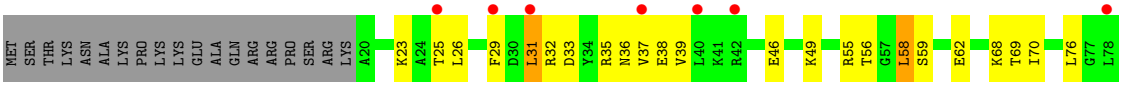
Chain CQ:

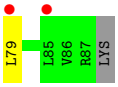




• Molecule 18: 30S ribosomal protein S18

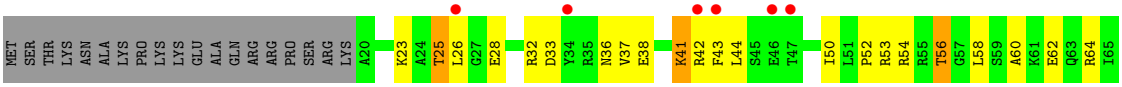
Chain AR:

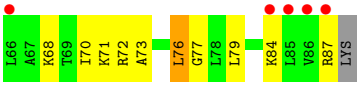




• Molecule 18: 30S ribosomal protein S18

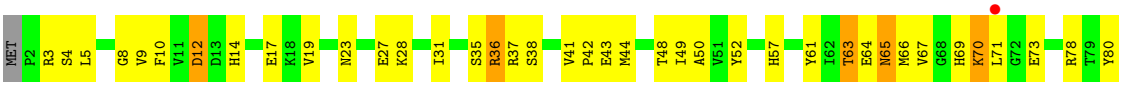
Chain CR:





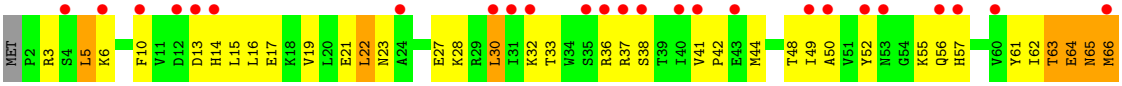
• Molecule 19: 30S ribosomal protein S19

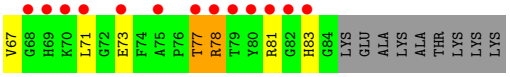
Chain AS:



• Molecule 19: 30S ribosomal protein S19

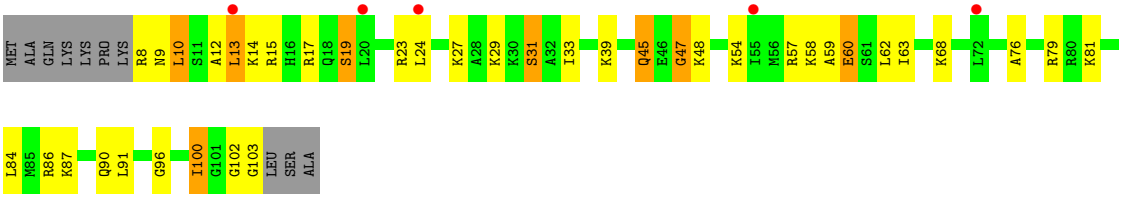
Chain CS:





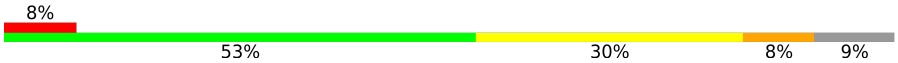
• Molecule 20: 30S ribosomal protein S20

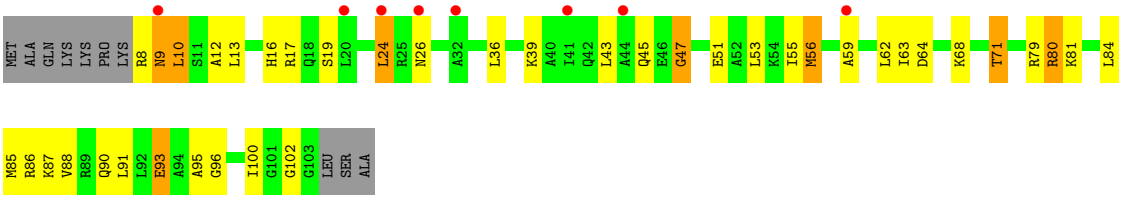
Chain AT:



• Molecule 20: 30S ribosomal protein S20

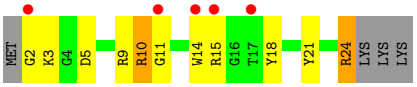
Chain CT:





• Molecule 21: 30S ribosomal protein Thx

Chain AU:

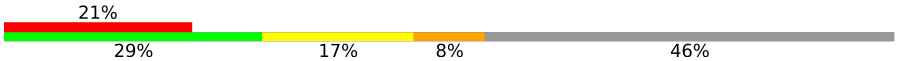


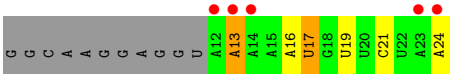
• Molecule 21: 30S ribosomal protein Thx

Chain CU:

• Molecule 22: mRNA

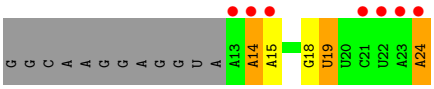
Chain AV:





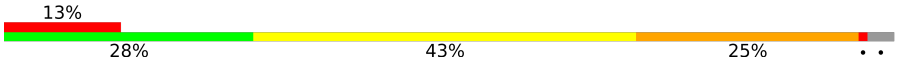
• Molecule 22: mRNA

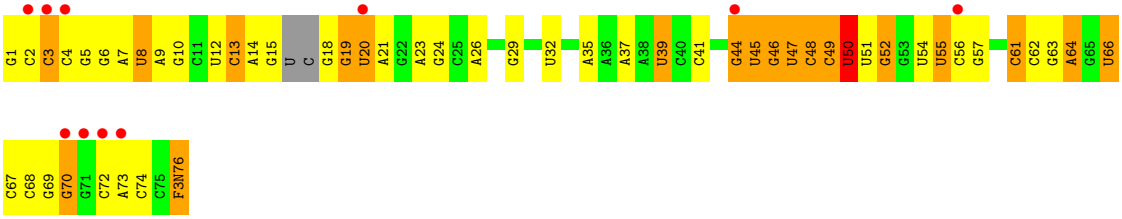
Chain CV:



• Molecule 23: A-site tRNA

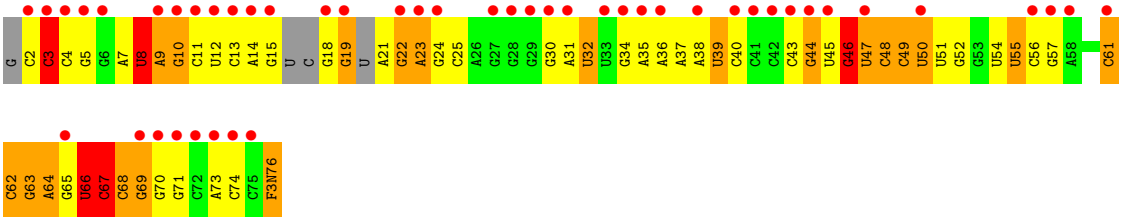
Chain AW:





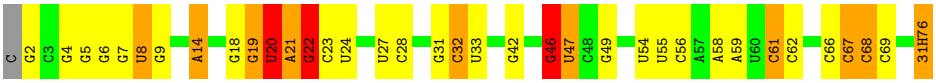
• Molecule 23: A-site tRNA

Chain CW:



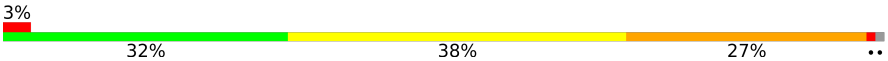
• Molecule 24: P-site tRNA

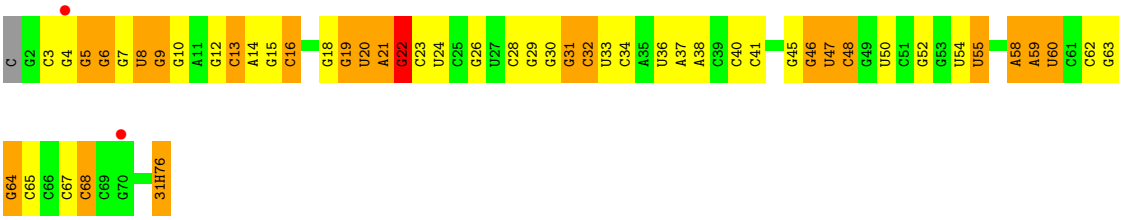
Chain AX:



• Molecule 24: P-site tRNA

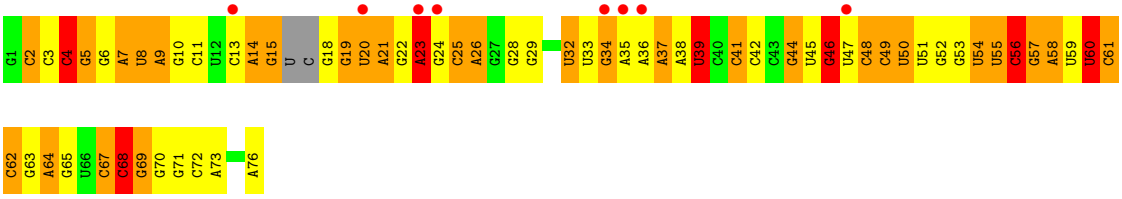
Chain CX:





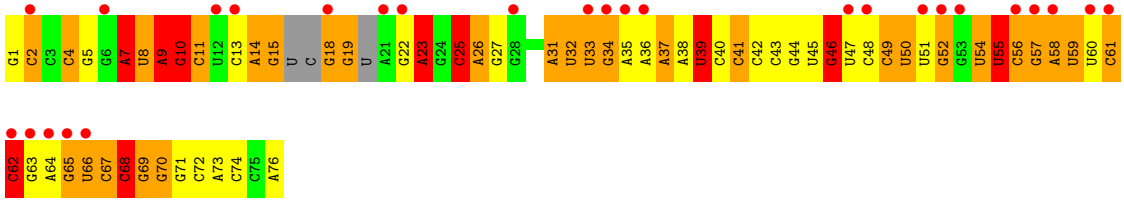
• Molecule 25: E-site tRNA

Chain AY:



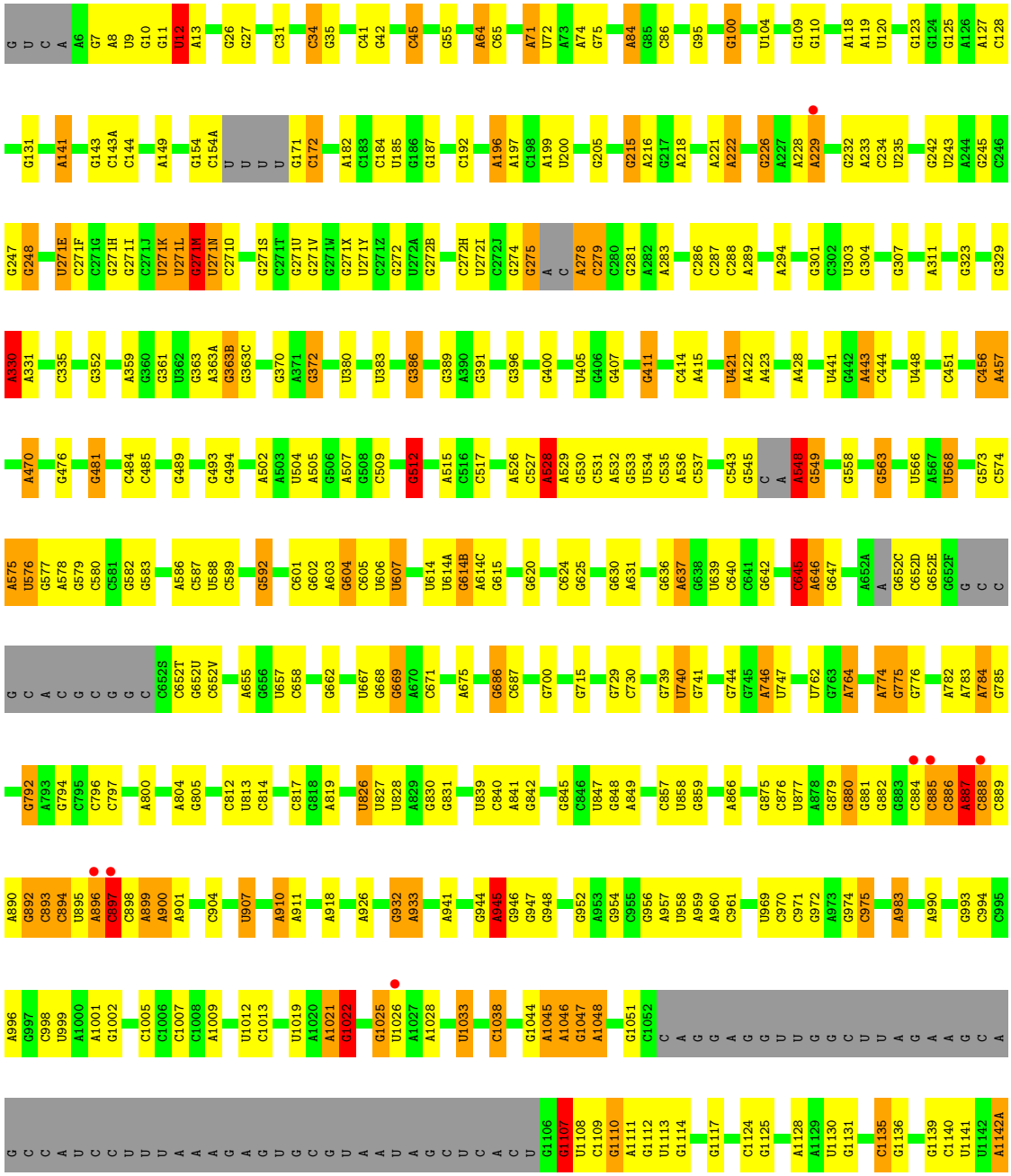
• Molecule 25: E-site tRNA

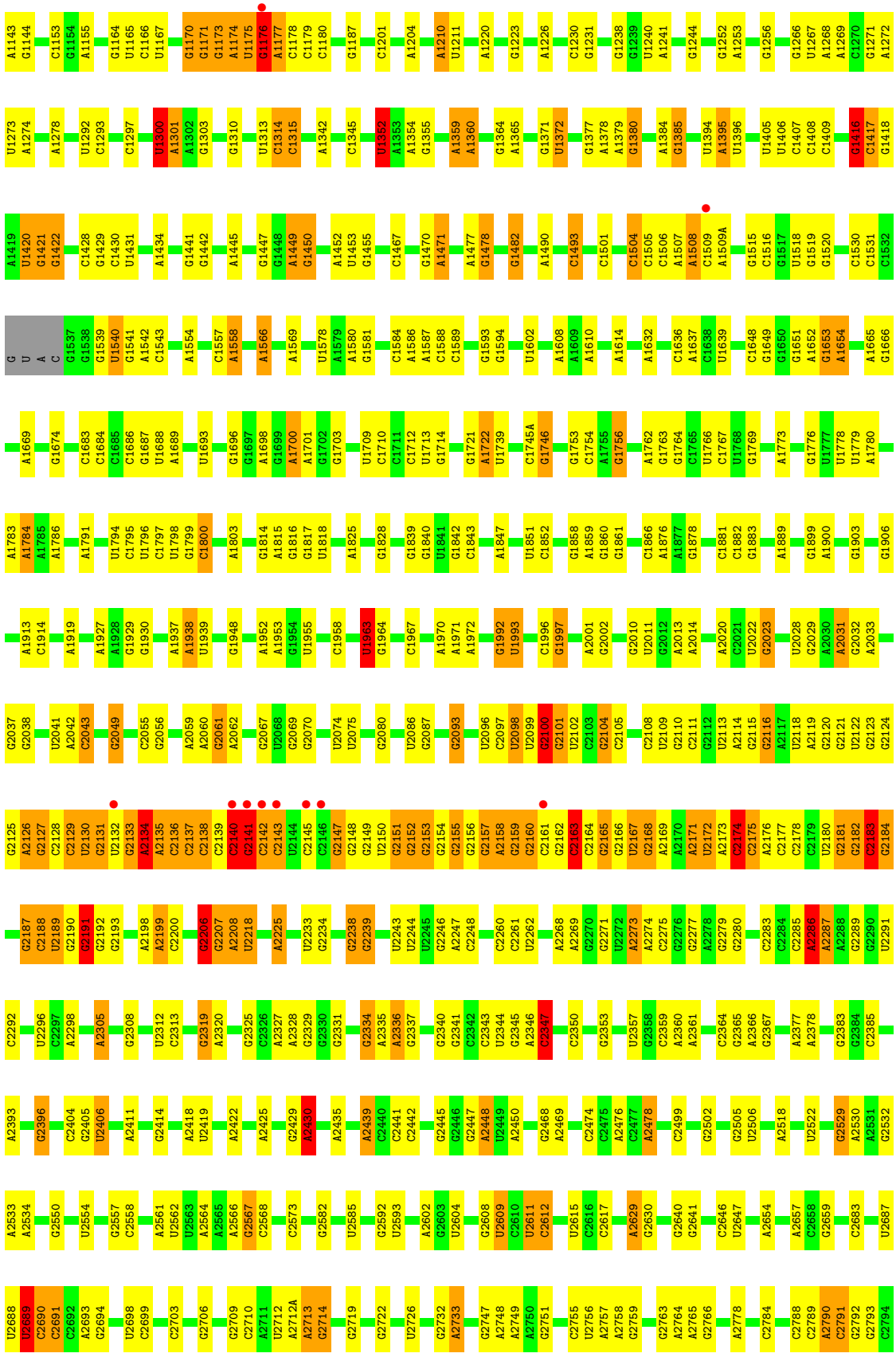
Chain CY:



- Molecule 26: 23S Ribosomal RNA

Chain BA:

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U1273 A1274 A1278 U1292 C1293 C1297 U1300 A1301 A1302 G1303 G1310 U1313 C1314 C1315 A1342 C1345 U1352 A1353 A1354 G1355 A1359 A1360 G1364 A1365 G1371 U1372 G1377 A1378 A1379 G1380 A1384 G1385 U1394 A1395 U1396 U1405 U1406 C1407 C1408 C1409 G1416 C1417 G1418
A1419 U1420 G1421 G1422 C1428 G1429 C1430 U1431 A1434 G1441 G1442 A1445 G1447 G1448 A1449 G1450 A1452 U1453 G1455 C1467 G1470 A1471 A1477 G1478 G1482 A1490 C1493 C1501 C1504 C1505 C1506 A1507 A1508 C1509 A1509A G1515 C1516 G1517 U1518 G1519 G1520 C1530 C1531 C1532
G U A C G1537 G1538 G1539 U1540 G1541 A1542 C1543 A1554 C1557 A1558 A1566 A1569 U1578 A1579 A1580 G1581 C1584 A1586 A1587 C1588 C1589 G1593 G1594 U1602 A1608 A1609 A1610 A1614 A1632 C1636 A1637 C1638 U1639 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1665 G1666
A1669 G1674 C1683 C1684 C1685 C1686 G1687 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 U1709 C1710 C1711 C1712 U1713 G1714 G1721 A1722 U1739 C1745A G1746 G1753 C1754 A1755 G1756 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 A1773 G1776 U1777 U1778 U1779 A1780
A1783 A1784 A1785 A1786 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 A1803 G1814 A1815 G1816 G1817 U1818 A1825 G1828 G1839 G1840 U1841 G1842 C1843 A1847 U1851 C1852 G1858 A1859 G1860 G1861 C1866 A1876 A1877 G1878 C1881 C1882 G1883 A1889 G1899 A1900 G1903 G1906
A1913 C1914 A1919 A1927 A1928 G1929 G1930 A1937 A1938 U1939 G1948 A1952 A1953 G1954 U1955 C1958 U1963 G1964 C1967 A1970 A1971 A1972 G1992 U1993 C1996 G1997 A2001 G2002 G2010 U2011 G2012 A2013 A2014 A2020 C2021 U2022 G2023 U2028 G2029 A2030 A2031 G2032 A2033
G2037 G2038 U2041 A2042 C2043 G2049 C2055 G2056 A2059 A2060 G2061 A2062 C2067 U2068 G2069 G2070 U2074 U2075 G2080 U2086 G2087 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124
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G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 A2199 C2200 G2206 G2207 A2208 U2218 A2225 U2233 G2234 G2238 G2239 U2243 U2244 U2245 G2246 A2247 C2248 C2260 C2261 U2262 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291
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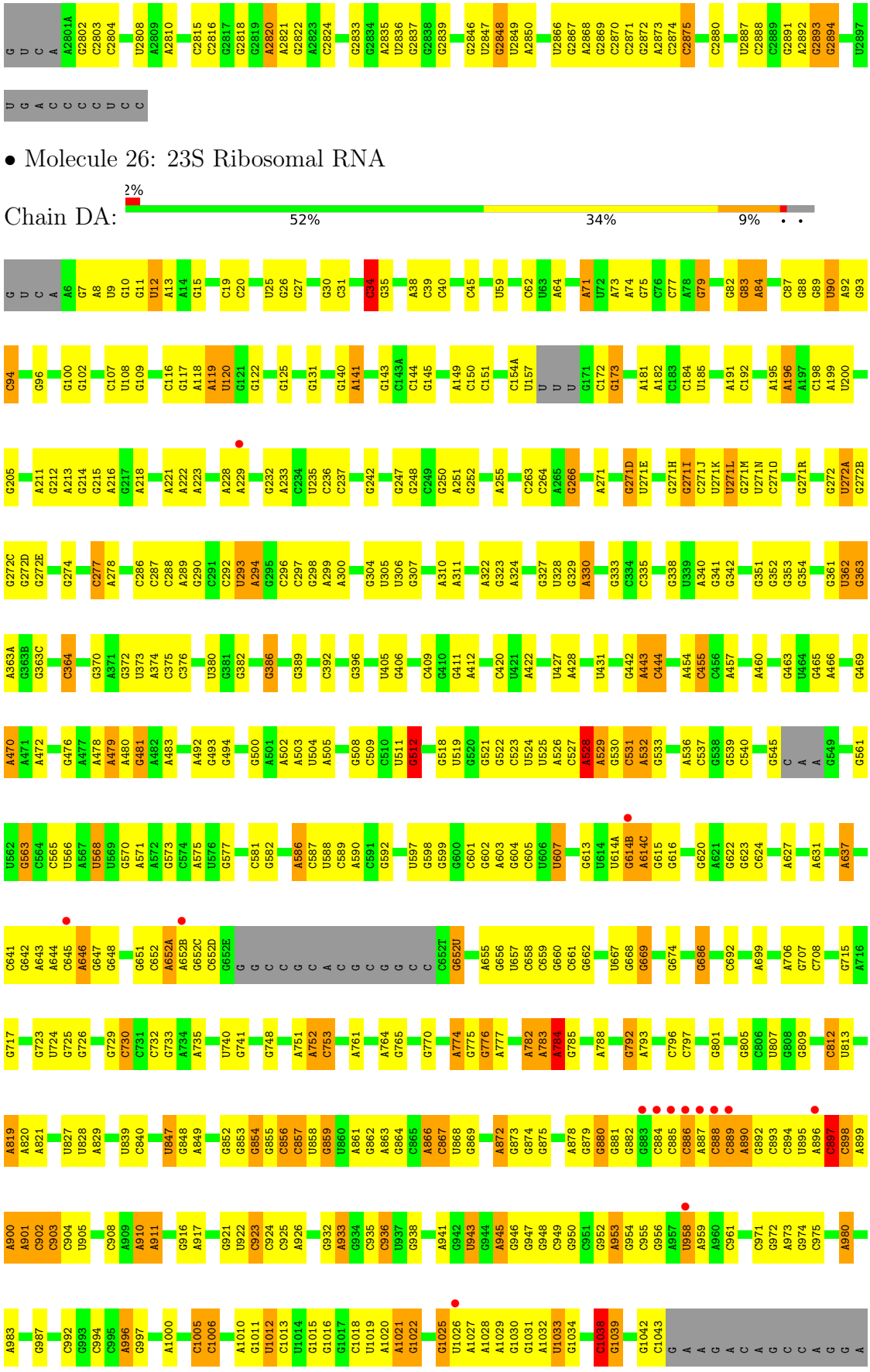
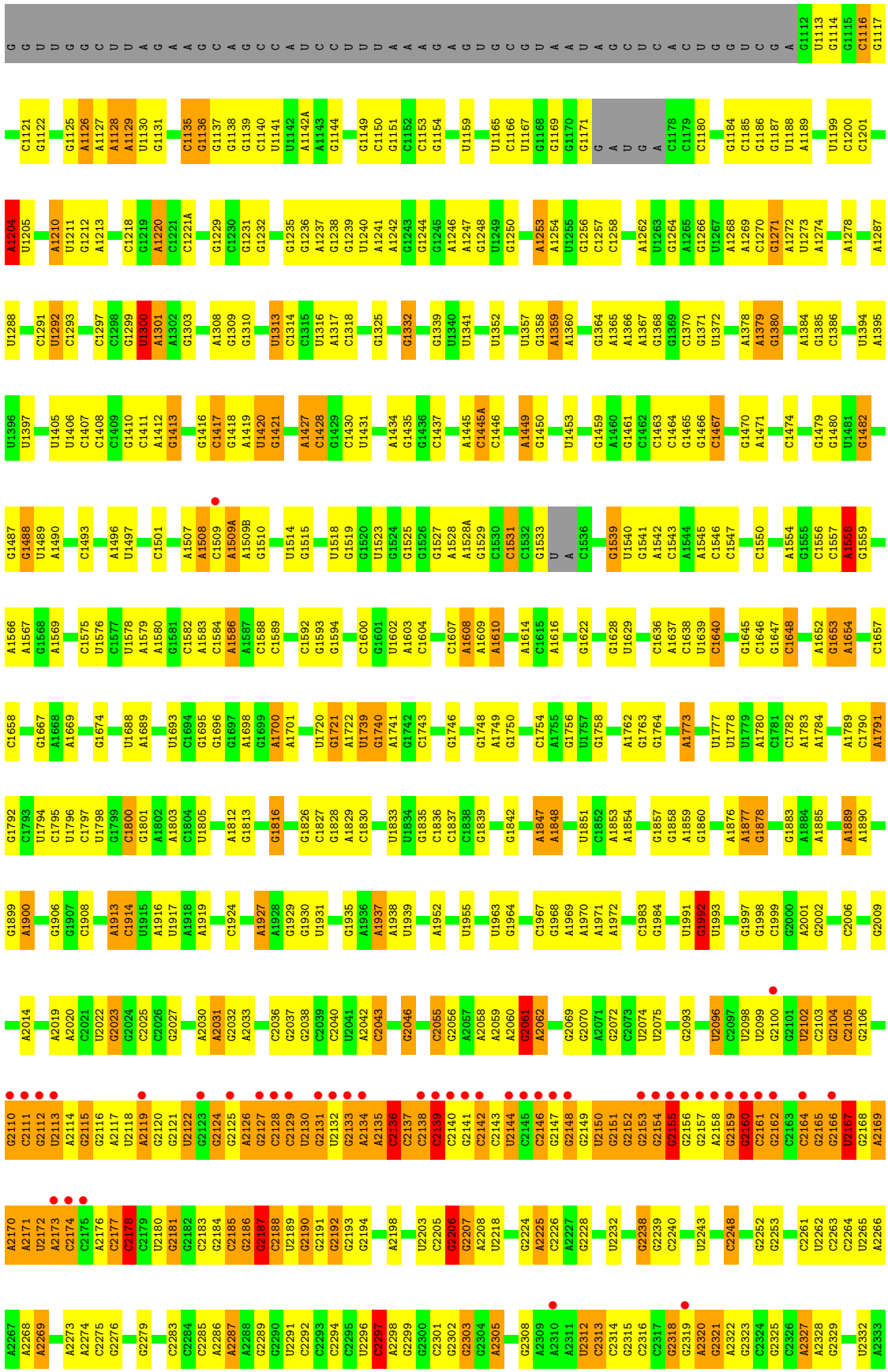
U2688 U2689 C2690 C2691 C2692 A2693 G2694 U2698 C2699 C2703 G2706 G2709 C2710 A2711 U2712 A2712A A2713 G2714 G2719 G2722 U2726 G2732 A2733 G2747 A2748 A2749 A2750 G2751 C2755 U2756 A2757 A2758 G2759 G2763 A2764 A2765 G2766 A2778 C2784 C2788 C2789 A2790 C2791 G2792 G2793 C2794



• Molecule 26: 23S Ribosomal RNA

Chain DA: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A1204 U1205 A1210 U1211 G1212 A1213 C1218 G1219 A1220 C1221 C1221A G1229 C1230 G1231 G1232 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 G1248 U1249 G1250 A1253 A1254 U1255 G1256 C1257 C1258 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1278 A1287
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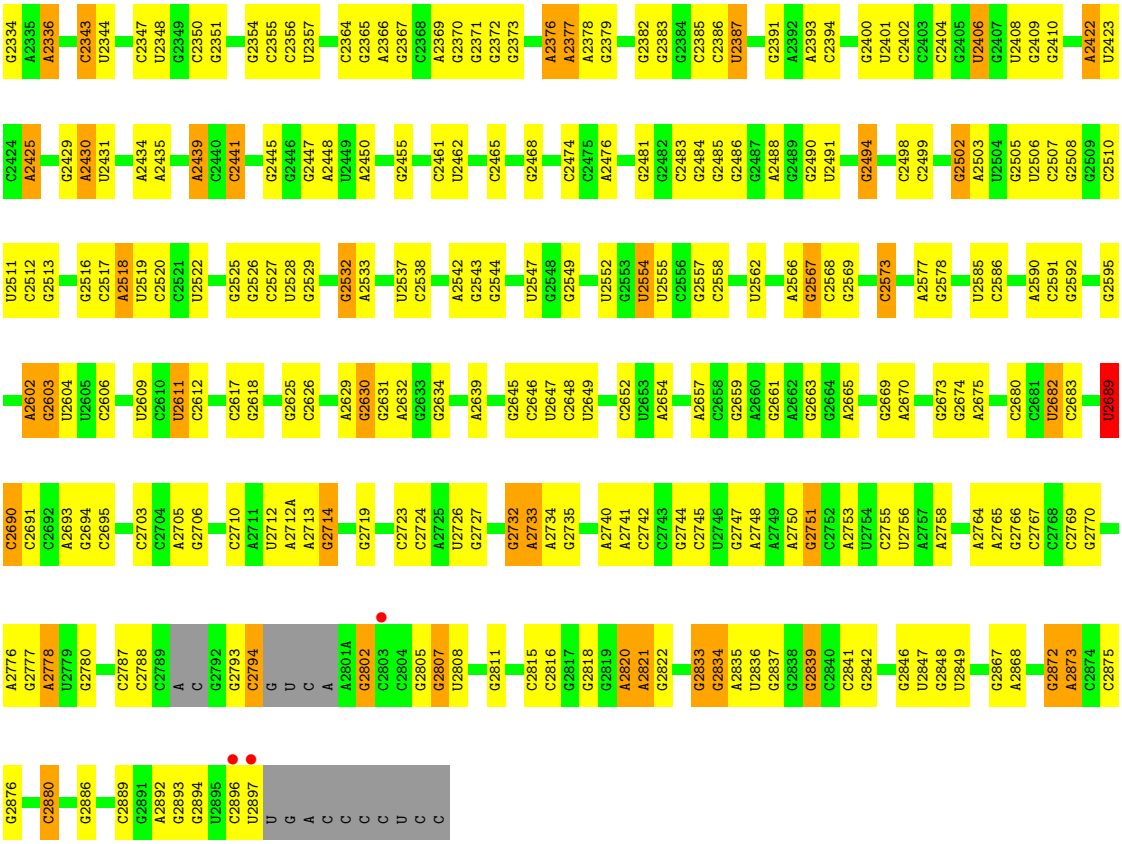
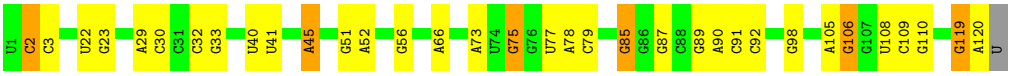


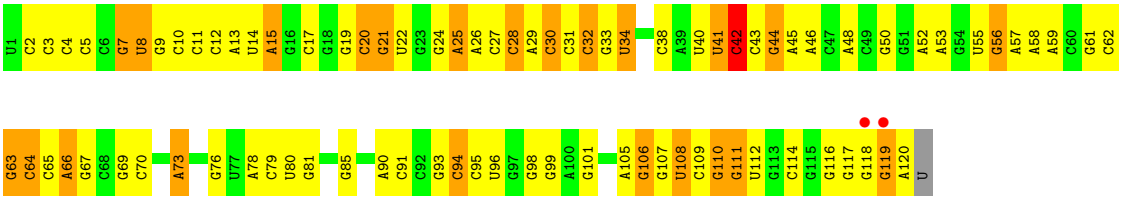
- Molecule 27: 5S Ribosomal RNA

Chain BB:



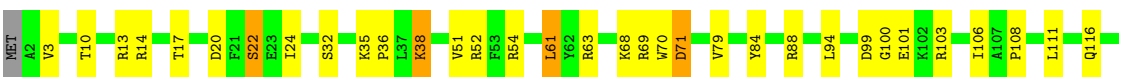
- Molecule 27: 5S Ribosomal RNA

Chain DB:



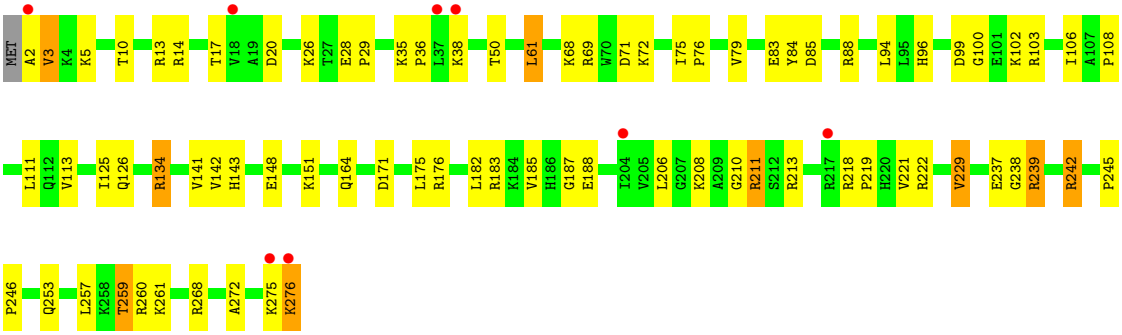
- Molecule 28: 50S ribosomal protein L2

Chain BD:



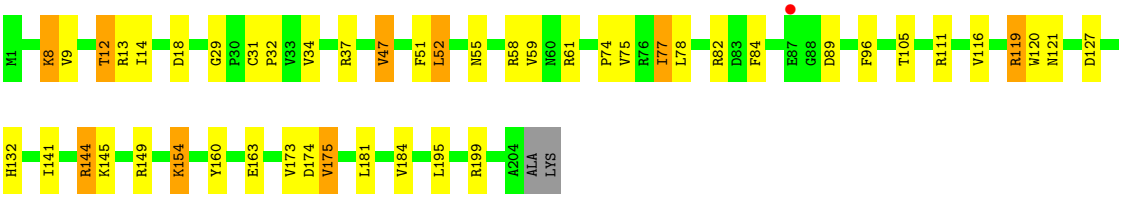
• Molecule 28: 50S ribosomal protein L2

Chain DD:



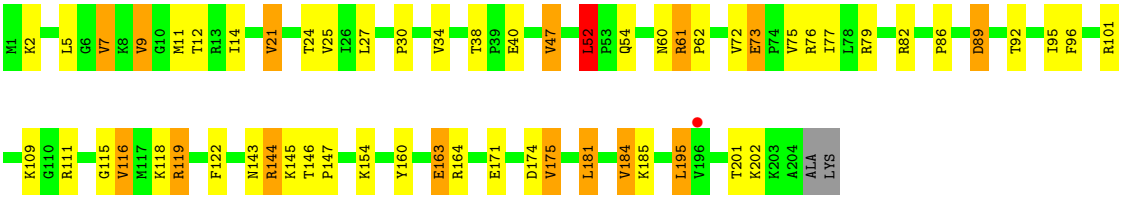
• Molecule 29: 50S ribosomal protein L3

Chain BE:



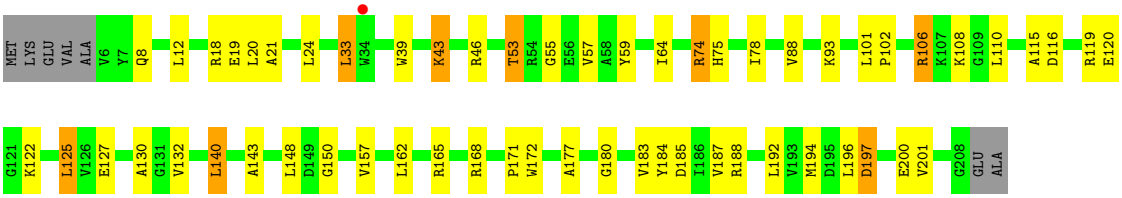
• Molecule 29: 50S ribosomal protein L3

Chain DE:



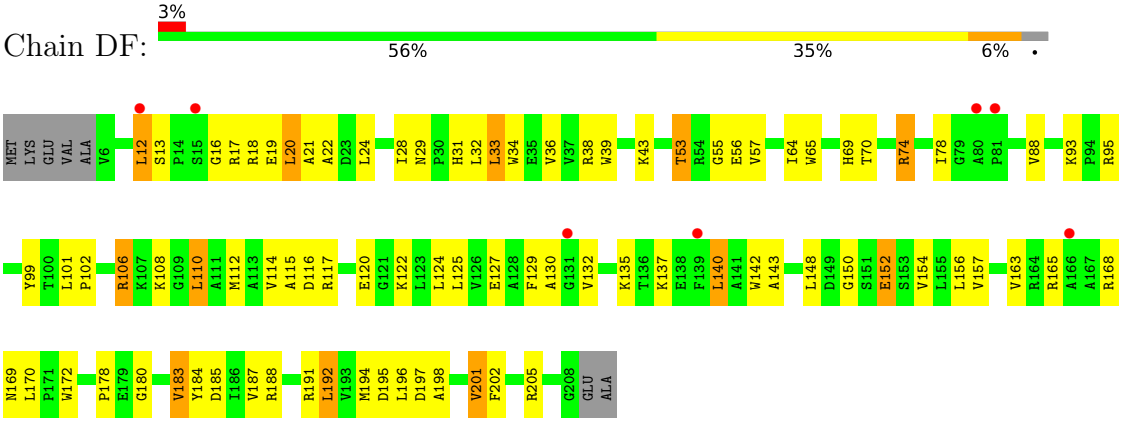
• Molecule 30: 50S ribosomal protein L4

Chain BF:



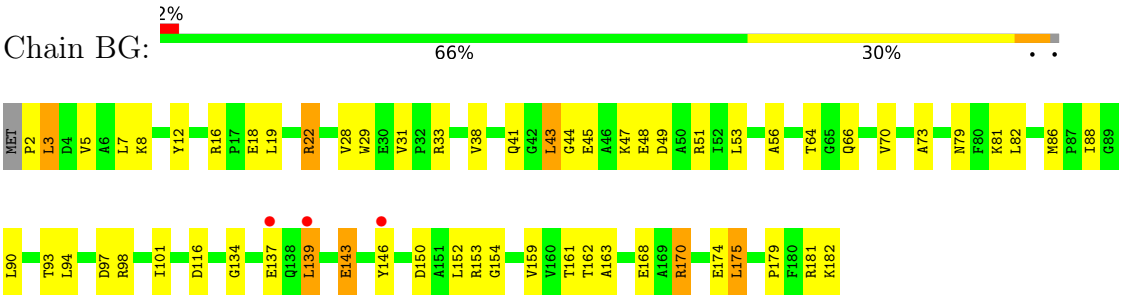
• Molecule 30: 50S ribosomal protein L4

Chain DF:



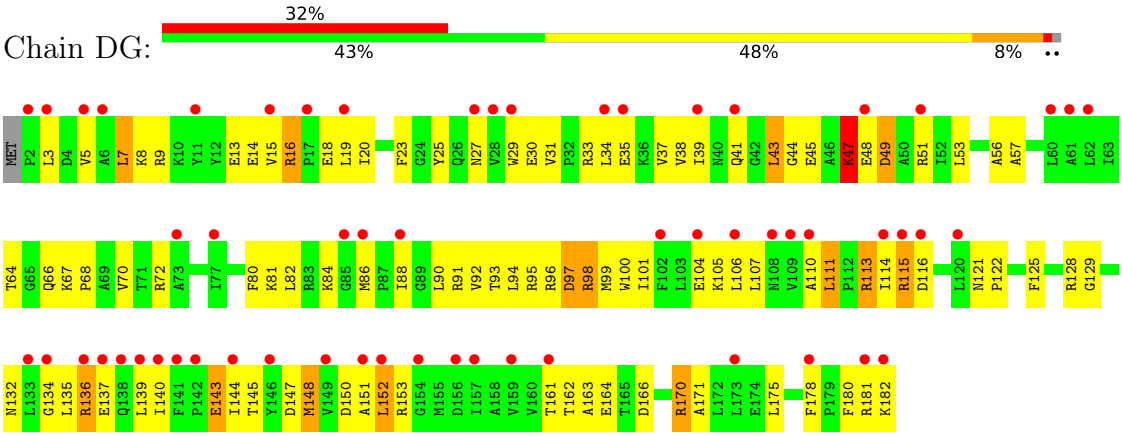
• Molecule 31: 50S ribosomal protein L5

Chain BG:



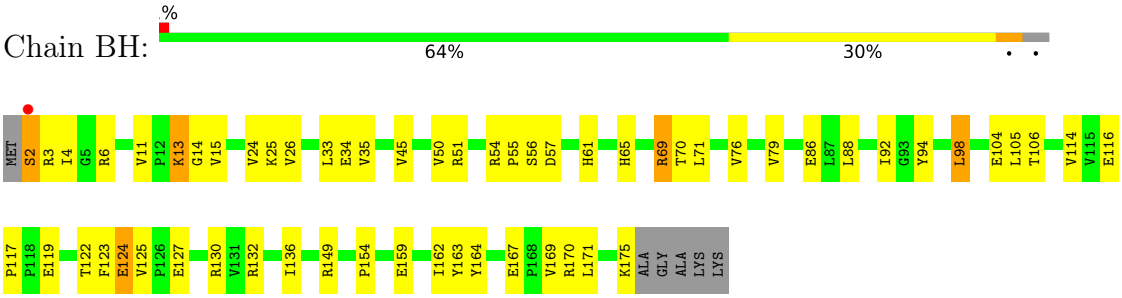
• Molecule 31: 50S ribosomal protein L5

Chain DG:



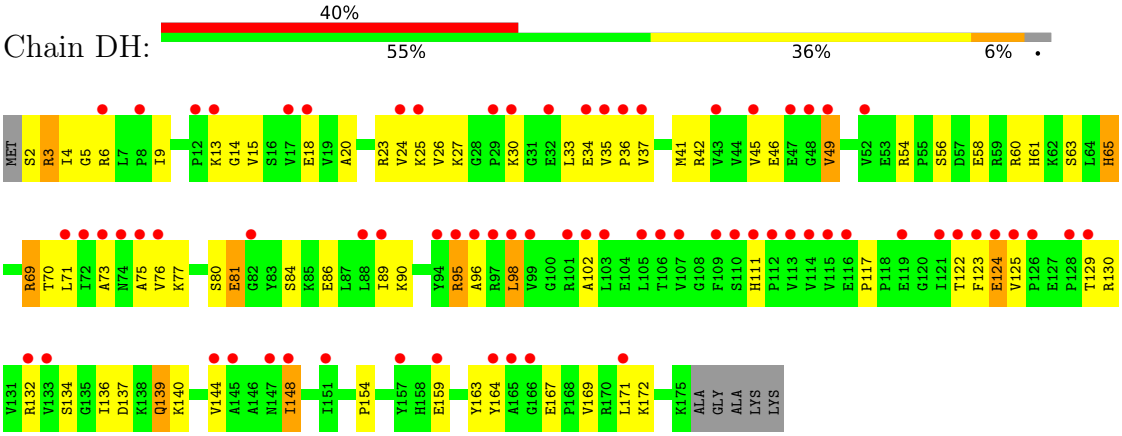
• Molecule 32: 50S ribosomal protein L6

Chain BH:



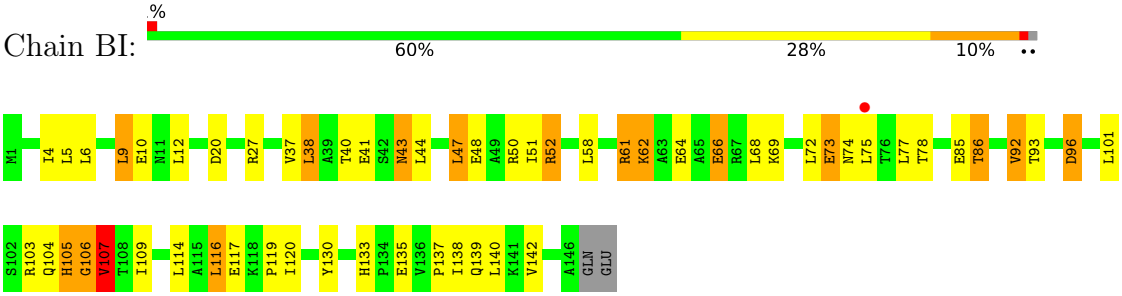
• Molecule 32: 50S ribosomal protein L6

Chain DH:



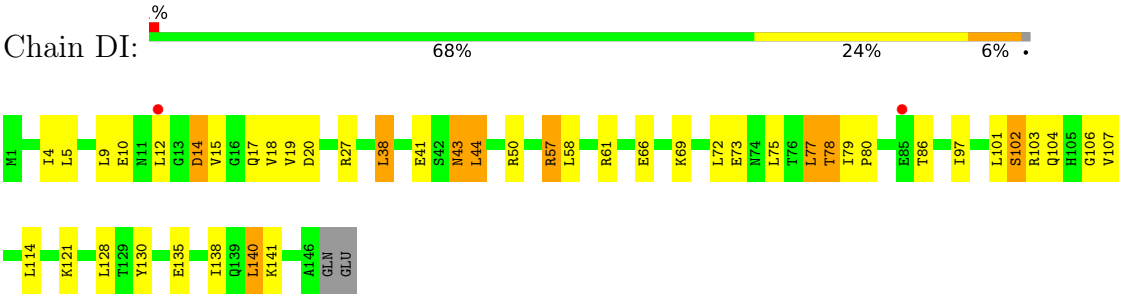
- Molecule 33: 50S ribosomal protein L9

Chain BI:



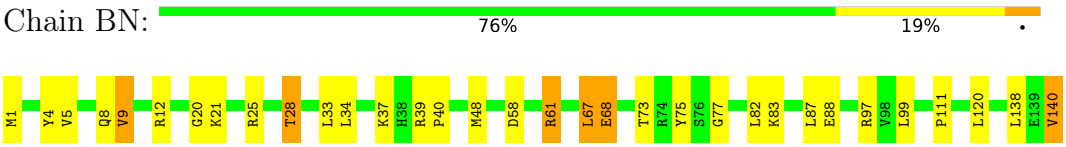
- Molecule 33: 50S ribosomal protein L9

Chain DI:



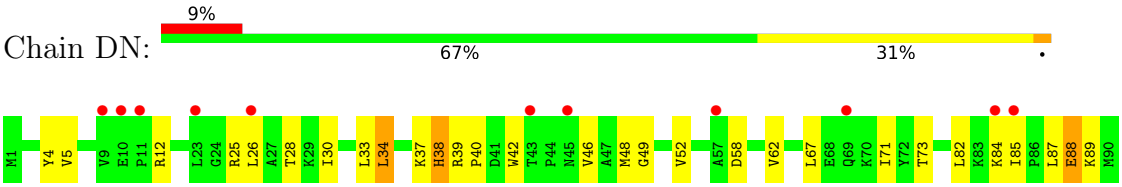
- Molecule 34: 50S ribosomal protein L13

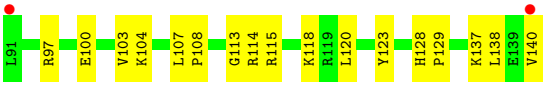
Chain BN:



- Molecule 34: 50S ribosomal protein L13

Chain DN:



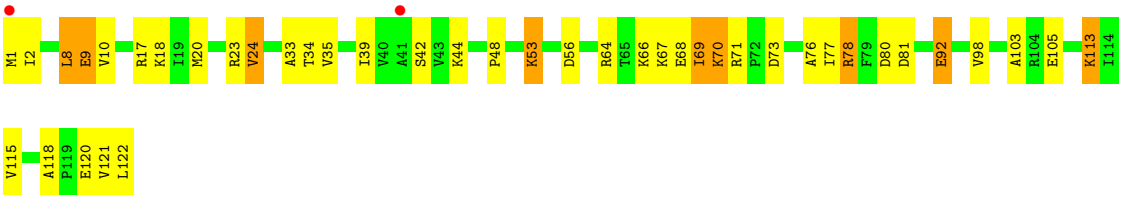


• Molecule 35: 50S ribosomal protein L14

Chain BO:

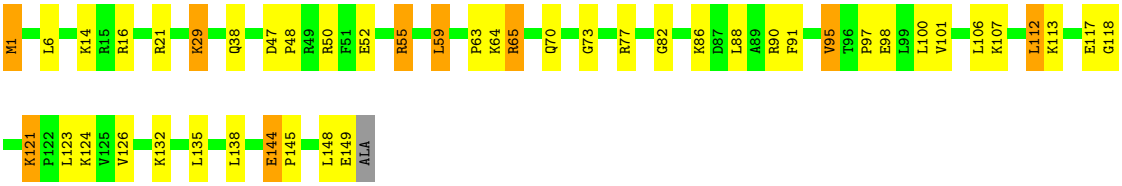
• Molecule 35: 50S ribosomal protein L14

Chain DO:



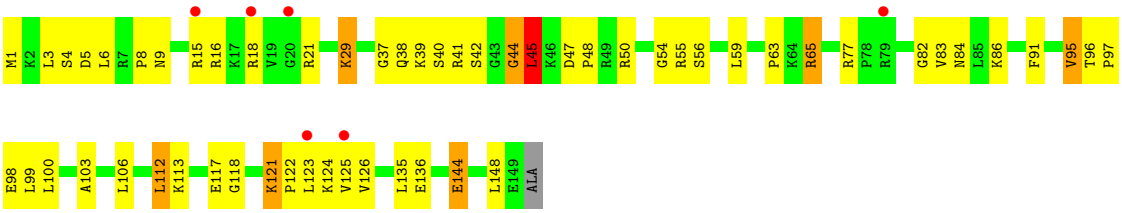
• Molecule 36: 50S ribosomal protein L15

Chain BP:



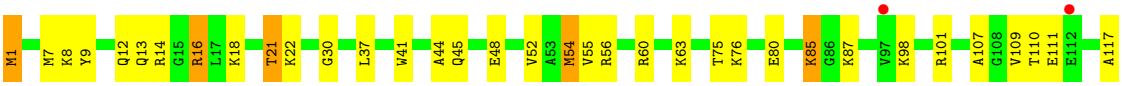
• Molecule 36: 50S ribosomal protein L15

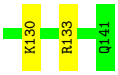
Chain DP:



• Molecule 37: 50S ribosomal protein L16

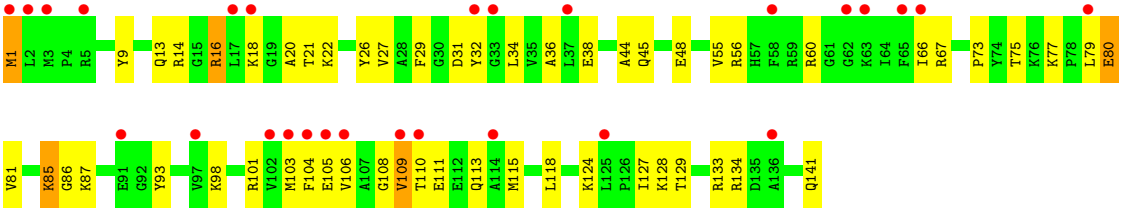
Chain BQ:





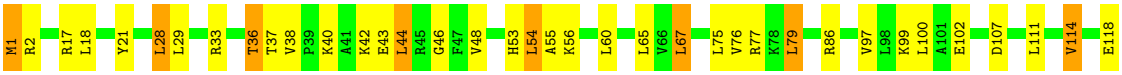
• Molecule 37: 50S ribosomal protein L16

Chain DQ:



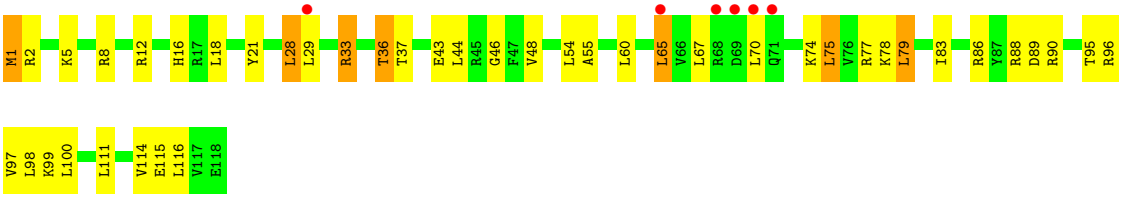
• Molecule 38: 50S ribosomal protein L17

Chain BR:



• Molecule 38: 50S ribosomal protein L17

Chain DR:

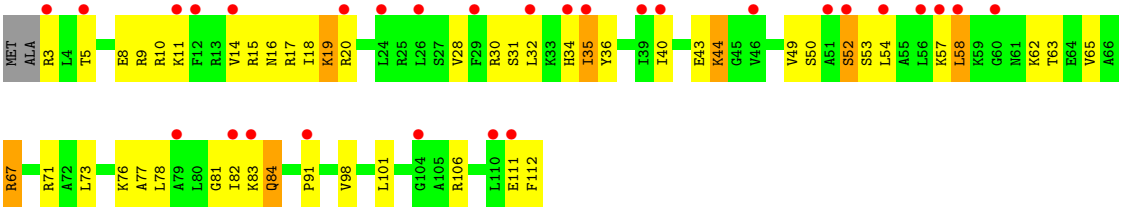


• Molecule 39: 50S ribosomal protein L18

Chain BS:

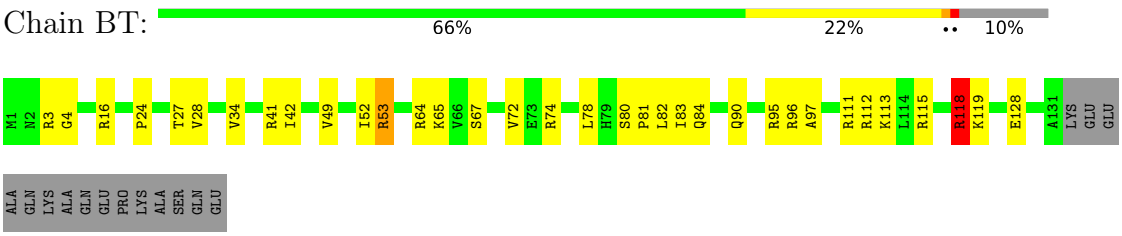
• Molecule 39: 50S ribosomal protein L18

Chain DS:



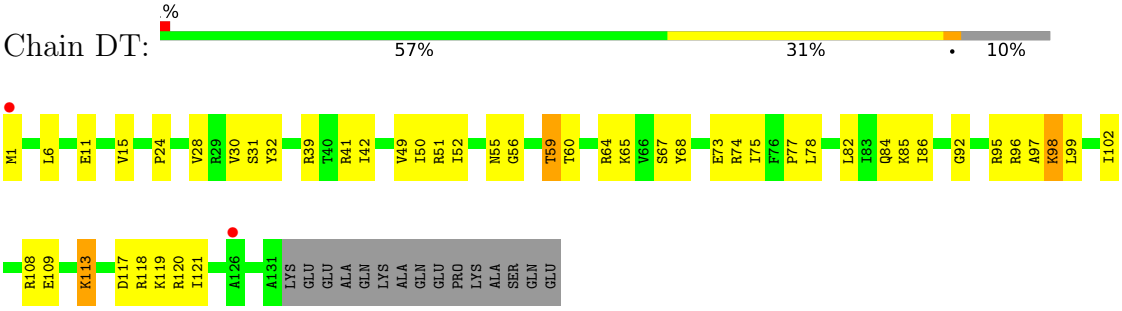
• Molecule 40: 50S ribosomal protein L19

Chain BT:



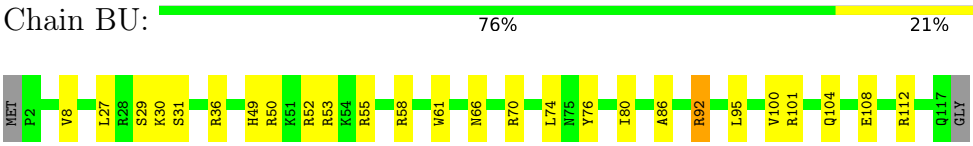
• Molecule 40: 50S ribosomal protein L19

Chain DT:



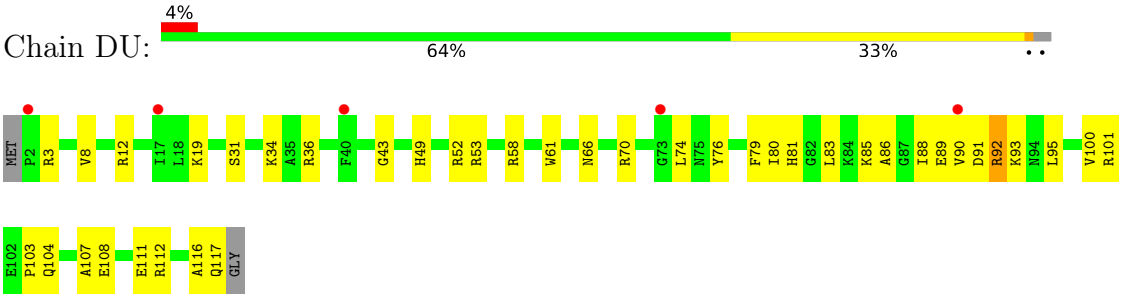
• Molecule 41: 50S ribosomal protein L20

Chain BU:



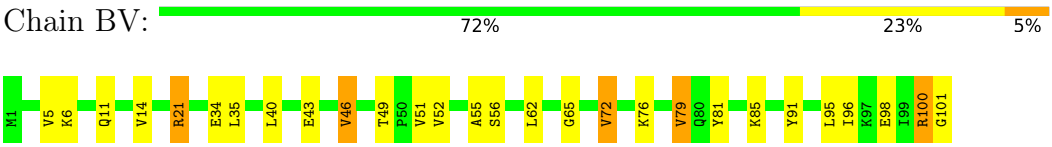
• Molecule 41: 50S ribosomal protein L20

Chain DU:



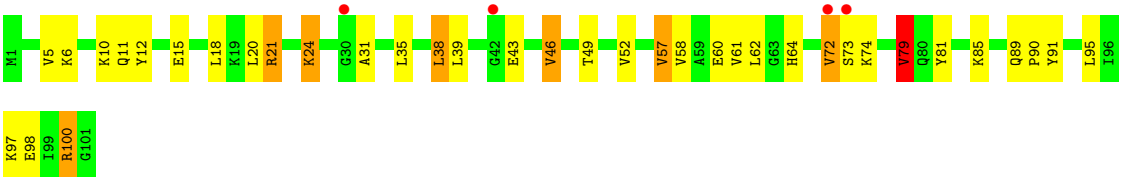
• Molecule 42: 50S ribosomal protein L21

Chain BV:



• Molecule 42: 50S ribosomal protein L21

Chain DV:

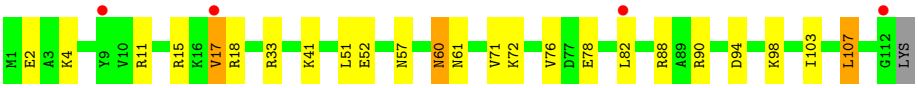


• Molecule 43: 50S ribosomal protein L22

Chain BW:

• Molecule 43: 50S ribosomal protein L22

Chain DW:

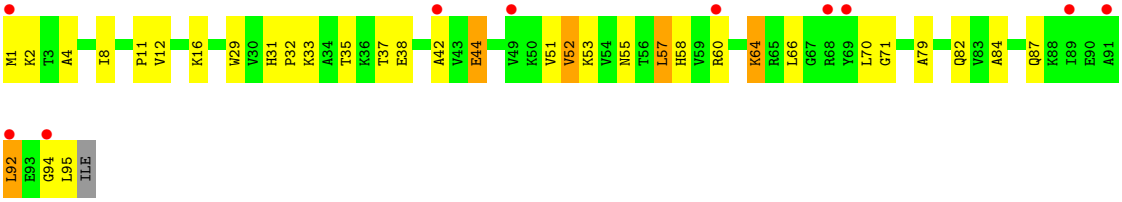


• Molecule 44: 50S ribosomal protein L23

Chain BX:

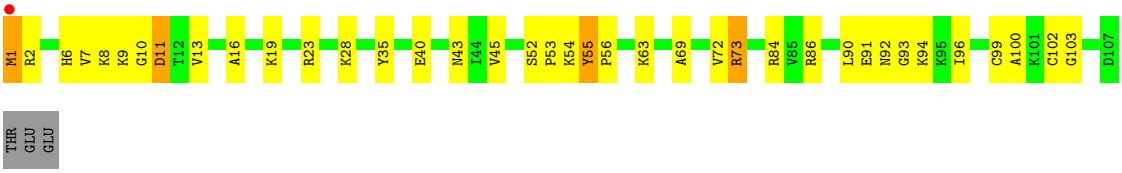
• Molecule 44: 50S ribosomal protein L23

Chain DX:



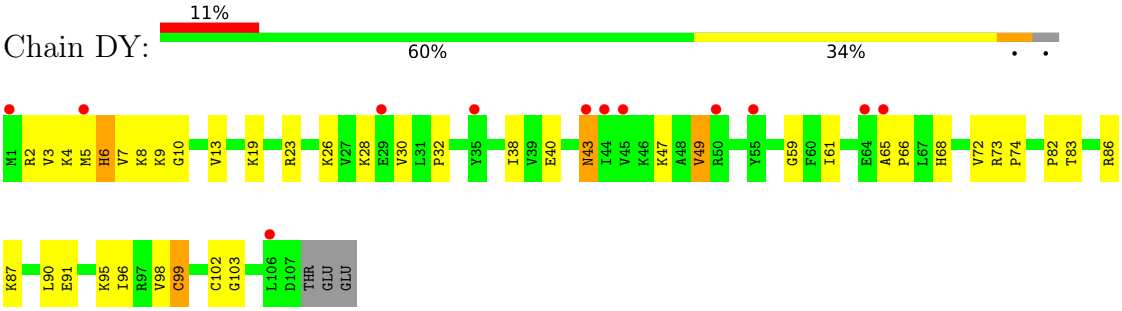
• Molecule 45: 50S ribosomal protein L24

Chain BY:



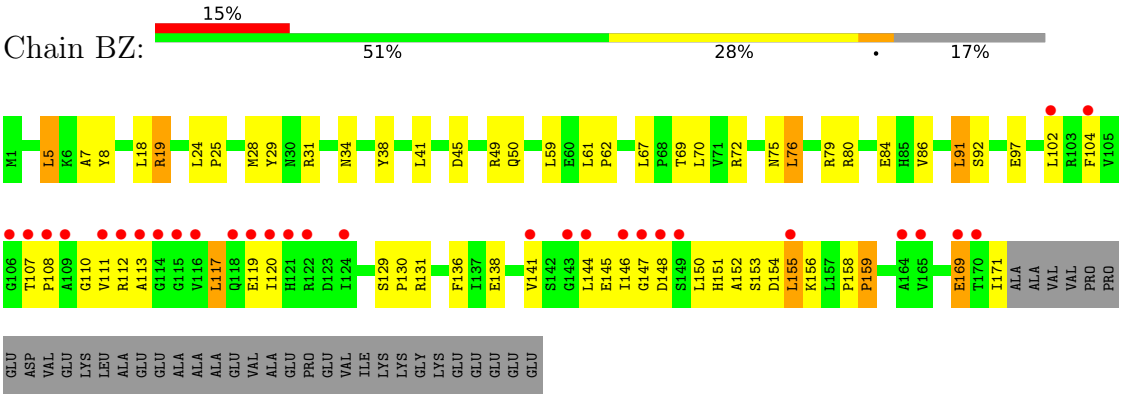
• Molecule 45: 50S ribosomal protein L24

Chain DY:



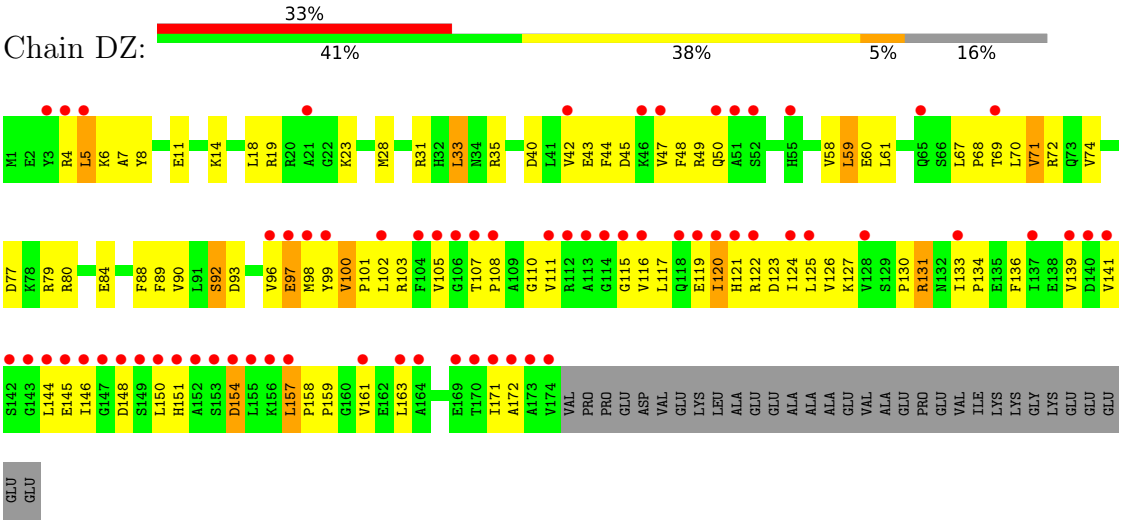
- Molecule 46: 50S ribosomal protein L25

Chain BZ:



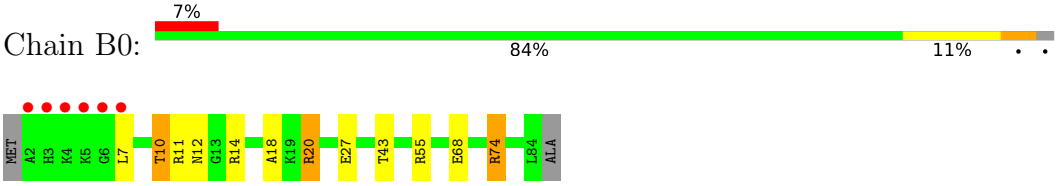
- Molecule 46: 50S ribosomal protein L25

Chain DZ:



- Molecule 47: 50S ribosomal protein L27

Chain B0:



- Molecule 47: 50S ribosomal protein L27

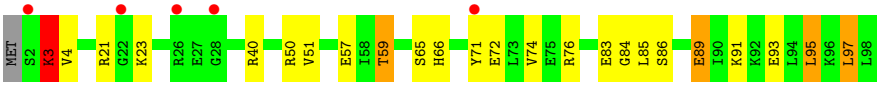
Chain D0:

• Molecule 48: 50S ribosomal protein L28

Chain B1:

• Molecule 48: 50S ribosomal protein L28

Chain D1:

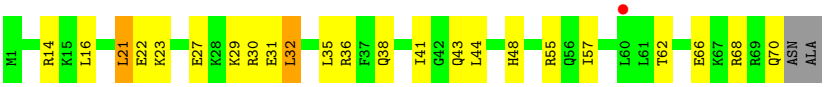


• Molecule 49: 50S ribosomal protein L29

Chain B2:

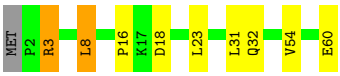
• Molecule 49: 50S ribosomal protein L29

Chain D2:



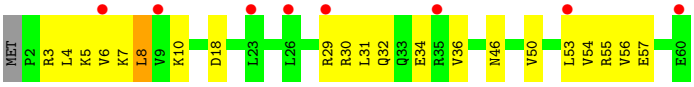
• Molecule 50: 50S ribosomal protein L30

Chain B3:



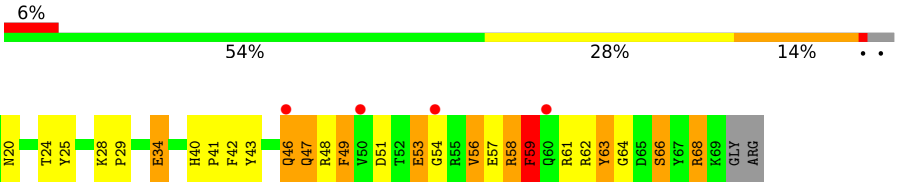
• Molecule 50: 50S ribosomal protein L30

Chain D3:



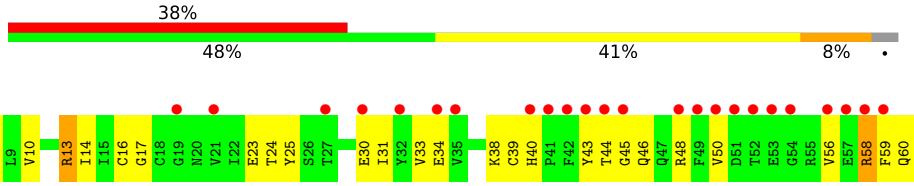
• Molecule 51: 50S ribosomal protein L31

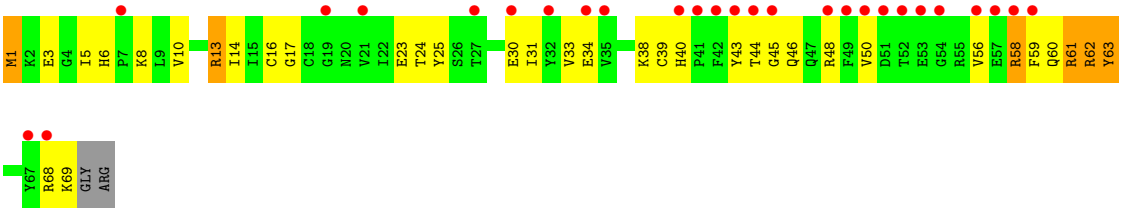
Chain B4:



• Molecule 51: 50S ribosomal protein L31

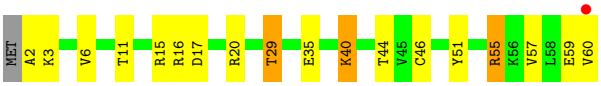
Chain D4:





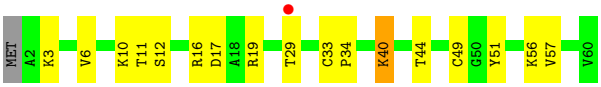
• Molecule 52: 50S ribosomal protein L32

Chain B5:



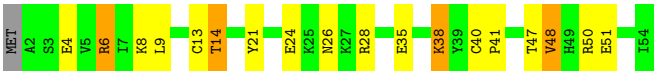
• Molecule 52: 50S ribosomal protein L32

Chain D5:



• Molecule 53: 50S ribosomal protein L33

Chain B6:

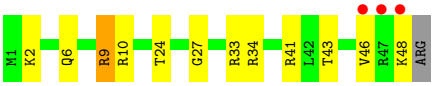


• Molecule 53: 50S ribosomal protein L33

Chain D6:

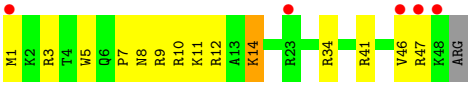
• Molecule 54: 50S ribosomal protein L34

Chain B7:



• Molecule 54: 50S ribosomal protein L34

Chain D7:



• Molecule 55: 50S ribosomal protein L35

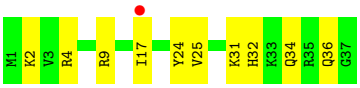
Chain B8:

• Molecule 55: 50S ribosomal protein L35

Chain D8:

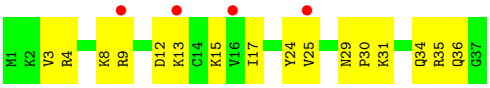
• Molecule 56: 50S ribosomal protein L36

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	209.45Å 448.85Å 619.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.90 – 2.60 224.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (151.90-2.60) 99.9 (224.43-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.223 , 0.264 0.224 , 0.265	Depositor DCC
R_{free} test set	88430 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	297127	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: MIA, F3N, 5MC, 7MG, MG, SF4, K, 31H, ZN, 5MU, PSU, 4SU

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	0.38	0/36027	0.91	43/56227 (0.1%)
1	CA	0.41	8/36170 (0.0%)	1.01	101/56452 (0.2%)
2	AB	0.30	0/1881	0.62	0/2542
2	CB	0.33	0/1860	0.67	2/2518 (0.1%)
3	AC	0.27	0/1576	0.52	0/2130
3	CC	0.31	0/1568	0.61	1/2122 (0.0%)
4	AD	0.29	0/1689	0.55	0/2267
4	CD	0.30	0/1708	0.55	0/2289
5	AE	0.30	0/1145	0.54	0/1543
5	CE	0.33	0/1149	0.61	0/1548
6	AF	0.30	0/825	0.52	0/1118
6	CF	0.32	0/833	0.55	0/1128
7	AG	0.28	0/1250	0.50	0/1679
7	CG	0.27	0/1254	0.53	0/1683
8	AH	0.28	0/1108	0.52	0/1494
8	CH	0.29	0/1108	0.54	0/1494
9	AI	0.29	0/1005	0.57	0/1350
9	CI	0.31	0/997	0.64	0/1343
10	AJ	0.27	0/722	0.54	0/982
10	CJ	0.33	0/727	0.62	0/988
11	AK	0.28	0/848	0.51	0/1149
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.33	0/946	0.52	0/1274
12	CL	0.30	0/946	0.58	0/1274
13	AM	0.31	0/977	0.60	0/1310
13	CM	0.31	0/961	0.62	1/1291 (0.1%)
14	AN	0.32	0/501	0.53	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.52	0/985
15	CO	0.29	0/739	0.54	0/985
16	AP	0.31	0/697	0.54	0/939
16	CP	0.29	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.29	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.54	0/746
18	CR	0.29	0/560	0.56	0/746
19	AS	0.30	0/676	0.58	0/911
19	CS	0.33	0/661	0.71	0/893
20	AT	0.29	0/730	0.57	0/965
20	CT	0.28	0/733	0.55	0/969
21	AU	0.27	0/203	0.50	0/266
21	CU	0.33	0/203	0.53	0/266
22	AV	0.39	0/310	0.96	1/480 (0.2%)
22	CV	0.42	0/282	0.99	2/437 (0.5%)
23	AW	0.47	0/1577	1.20	7/2454 (0.3%)
23	CW	0.53	0/1531	1.28	9/2379 (0.4%)
24	AX	0.53	2/1700 (0.1%)	1.20	22/2650 (0.8%)
24	CX	0.46	0/1700	1.15	6/2650 (0.2%)
25	AY	0.58	0/1602	1.35	20/2493 (0.8%)
25	CY	0.59	0/1579	1.40	25/2455 (1.0%)
26	BA	0.50	1/68013 (0.0%)	0.93	91/106165 (0.1%)
26	DA	0.41	1/67542 (0.0%)	0.92	74/105428 (0.1%)
27	BB	0.41	0/2878	0.86	1/4490 (0.0%)
27	DB	0.44	0/2878	0.92	2/4490 (0.0%)
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2192	0.57	0/2951
29	BE	0.37	0/1592	0.57	0/2149
29	DE	0.33	0/1592	0.55	0/2149
30	BF	0.34	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.55	0/2188
31	BG	0.31	0/1450	0.54	1/1959 (0.1%)
31	DG	0.33	0/1449	0.60	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.29	0/1356	0.54	0/1834
33	BI	0.28	0/1100	0.56	0/1501
33	DI	0.29	0/1088	0.55	0/1484
34	BN	0.34	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.52	0/1543
35	BO	0.37	0/943	0.57	0/1269
35	DO	0.31	0/943	0.55	1/1269 (0.1%)
36	BP	0.35	0/1156	0.57	0/1537
36	DP	0.32	0/1152	0.61	1/1533 (0.1%)
37	BQ	0.35	0/1143	0.53	0/1527
37	DQ	0.32	0/1143	0.53	0/1527
38	BR	0.36	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DR	0.30	0/982	0.53	0/1312
39	BS	0.31	0/887	0.56	0/1180
39	DS	0.28	0/880	0.56	0/1172
40	BT	0.34	0/1105	0.56	1/1477 (0.1%)
40	DT	0.31	0/1097	0.53	0/1468
41	BU	0.39	0/977	0.56	0/1301
41	DU	0.30	0/977	0.54	0/1301
42	BV	0.36	0/782	0.58	0/1049
42	DV	0.32	0/782	0.57	1/1049 (0.1%)
43	BW	0.39	0/897	0.56	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.38	0/764	0.57	1/1025 (0.1%)
44	DX	0.33	0/764	0.58	1/1025 (0.1%)
45	BY	0.35	0/819	0.57	0/1095
45	DY	0.32	0/819	0.55	0/1095
46	BZ	0.32	0/1379	0.58	0/1873
46	DZ	0.30	0/1390	0.56	0/1890
47	B0	0.35	0/662	0.55	0/881
47	D0	0.32	0/662	0.53	0/881
48	B1	0.35	0/762	0.54	0/1014
48	D1	0.31	0/762	0.53	0/1014
49	B2	0.31	0/590	0.53	0/781
49	D2	0.28	0/590	0.46	0/781
50	B3	0.34	0/474	0.57	0/635
50	D3	0.27	0/469	0.55	0/630
51	B4	0.31	0/571	0.70	0/768
51	D4	0.32	0/545	0.67	0/737
52	B5	0.35	0/469	0.65	0/635
52	D5	0.31	0/469	0.50	0/635
53	B6	0.37	0/460	0.52	0/613
53	D6	0.29	0/456	0.49	0/608
54	B7	0.40	0/426	0.57	0/561
54	D7	0.33	0/426	0.54	0/561
55	B8	0.37	0/525	0.59	0/691
55	D8	0.32	0/525	0.51	0/691
56	B9	0.37	0/310	0.50	0/407
56	D9	0.33	0/310	0.52	0/407
All	All	0.41	12/316594 (0.0%)	0.87	415/473940 (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	2
2	CB	0	1
7	AG	0	2
20	CT	0	1
33	BI	0	1
35	BO	0	1
39	BS	0	1
51	B4	0	1
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-10.90	1.29	1.37
1	CA	1119	C	N3-C4	-10.71	1.26	1.33
1	CA	1154	G	C6-N1	-10.47	1.32	1.39
26	DA	528	A	N9-C4	-6.80	1.33	1.37
1	CA	1154	G	N7-C5	-6.78	1.35	1.39

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1119	C	N1-C2-O2	35.97	140.48	118.90
1	CA	1154	G	C5-C6-O6	25.44	143.86	128.60
1	CA	1154	G	N3-C2-N2	24.34	136.94	119.90
1	CA	1154	G	N1-C2-N2	-21.83	96.56	116.20
1	CA	1119	C	N3-C2-O2	-21.82	106.63	121.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide
7	AG	79	ARG	Peptide
33	BI	9	LEU	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	32185	0	16245	536	0
1	CA	32312	0	16307	762	0
2	AB	1846	0	1867	81	0
2	CB	1825	0	1828	119	0
3	AC	1552	0	1546	60	0
3	CC	1544	0	1524	70	0
4	AD	1659	0	1676	56	0
4	CD	1678	0	1718	67	0
5	AE	1129	0	1185	27	0
5	CE	1133	0	1191	46	0
6	AF	812	0	804	18	0
6	CF	820	0	814	19	0
7	AG	1231	0	1238	21	0
7	CG	1235	0	1249	39	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	986	0	995	43	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	44	0
11	AK	833	0	836	19	0
11	CK	833	0	836	22	0
12	AL	930	0	980	27	0
12	CL	930	0	980	33	0
13	AM	966	0	1024	40	0
13	CM	950	0	988	74	0
14	AN	492	0	529	26	0
14	CN	492	0	529	34	0
15	AO	728	0	760	20	0
15	CO	728	0	760	22	0
16	AP	681	0	697	27	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	26	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	12	0
18	CR	555	0	618	24	0
19	AS	661	0	675	31	0
19	CS	646	0	644	40	0
20	AT	728	0	798	26	0
20	CT	731	0	807	26	0
21	AU	199	0	208	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	9	0
22	AV	277	0	140	3	0
22	CV	252	0	130	6	0
23	AW	1599	0	830	42	0
23	CW	1552	0	794	51	0
24	AX	1635	0	839	23	0
24	CX	1635	0	839	36	0
25	AY	1581	0	805	82	0
25	CY	1561	0	796	94	0
26	BA	60729	0	30622	666	0
26	DA	60311	0	30412	876	0
27	BB	2573	0	1306	20	0
27	DB	2573	0	1306	76	0
28	BD	2136	0	2218	42	0
28	DD	2142	0	2229	58	0
29	BE	1559	0	1618	25	0
29	DE	1559	0	1618	39	0
30	BF	1584	0	1625	39	0
30	DF	1580	0	1619	60	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	90	0
32	BH	1330	0	1407	34	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	37	0
33	DI	1073	0	1106	22	0
34	BN	1117	0	1184	23	0
34	DN	1117	0	1184	26	0
35	BO	933	0	996	25	0
35	DO	933	0	996	32	0
36	BP	1139	0	1223	41	0
36	DP	1135	0	1212	52	0
37	BQ	1122	0	1179	28	0
37	DQ	1122	0	1179	40	0
38	BR	968	0	1033	22	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	20	0
39	DS	870	0	923	33	0
40	BT	1091	0	1151	26	0
40	DT	1083	0	1136	37	0
41	BU	959	0	1019	18	0
41	DU	959	0	1018	30	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	24	0
43	BW	886	0	940	17	0
43	DW	886	0	940	13	0
44	BX	750	0	814	15	0
44	DX	750	0	814	27	0
45	BY	806	0	881	27	0
45	DY	806	0	881	30	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	70	0
47	B0	653	0	674	13	0
47	D0	653	0	674	22	0
48	B1	755	0	826	16	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	14	0
50	B3	469	0	518	6	0
50	D3	464	0	514	13	0
51	B4	558	0	544	37	0
51	D4	532	0	503	25	0
52	B5	455	0	465	14	0
52	D5	455	0	465	13	0
53	B6	453	0	473	13	0
53	D6	449	0	469	12	0
54	B7	418	0	467	10	0
54	D7	418	0	467	13	0
55	B8	517	0	582	17	0
55	D8	517	0	582	15	0
56	B9	307	0	335	7	0
56	D9	307	0	335	11	0
57	AA	216	0	0	0	0
57	AB	1	0	0	0	0
57	AE	1	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	2	0	0	0	0
57	AN	2	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0
57	AW	2	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B0	2	0	0	0	0
57	B2	1	0	0	0	0
57	B4	1	0	0	0	0
57	B5	3	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	2	0	0	0	0
57	B9	1	0	0	0	0
57	BA	814	0	0	0	0
57	BB	23	0	0	0	0
57	BD	10	0	0	0	0
57	BE	6	0	0	0	0
57	BF	11	0	0	0	0
57	BG	2	0	0	0	0
57	BH	1	0	0	0	0
57	BN	3	0	0	0	0
57	BO	1	0	0	0	0
57	BP	2	0	0	0	0
57	BQ	2	0	0	0	0
57	BR	2	0	0	0	0
57	BU	4	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	2	0	0	0	0
57	CA	169	0	0	0	0
57	CD	1	0	0	0	0
57	CE	2	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	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	664	0	0	0	0
57	DB	13	0	0	0	0
57	DD	4	0	0	0	0
57	DE	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	2	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
57	DW	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	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
61	AA	210	0	0	13	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	1	0
61	AM	2	0	0	0	0
61	AV	2	0	0	0	0
61	AW	4	0	0	0	0
61	AX	4	0	0	0	0
61	AY	1	0	0	0	0
61	B0	6	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	4	0	0	0	0
61	B6	2	0	0	0	0
61	B7	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	13	0	0	0	0
61	B9	1	0	0	0	0
61	BA	1406	0	0	56	0
61	BB	37	0	0	1	0
61	BD	15	0	0	2	0
61	BE	17	0	0	4	0
61	BF	11	0	0	0	0
61	BG	3	0	0	0	0
61	BH	1	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	13	0	0	0	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BS	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	3	0	0	1	0
61	BX	3	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	156	0	0	11	0
61	CE	2	0	0	0	0
61	CH	1	0	0	0	0
61	CJ	1	0	0	0	0
61	CK	1	0	0	0	0
61	CL	1	0	0	1	0
61	CT	1	0	0	0	0
61	CW	2	0	0	2	0
61	CX	2	0	0	0	0
61	CY	1	0	0	0	0
61	D0	4	0	0	0	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D5	1	0	0	0	0
61	D6	1	0	0	0	0
61	D8	3	0	0	0	0
61	DA	989	0	0	44	0
61	DB	9	0	0	0	0
61	DD	18	0	0	3	0
61	DE	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DF	4	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	4	0
61	DQ	1	0	0	0	0
61	DT	4	0	0	0	0
61	DU	1	0	0	0	0
61	DV	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	1	0	0	0	0
All	All	297127	0	196404	5502	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 12.

The worst 5 of 5502 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)
26:DA:2139:C:N4	26:DA:2152:G:H1	1.46	1.14
1:CA:999:C:N4	1:CA:1042:G:H1	1.48	1.12
25:AY:49:C:N4	25:AY:65:G:H1	1.51	1.09
1:CA:985:C:N4	1:CA:1220:G:H1	1.50	1.09
1:CA:998:G:H1	1:CA:1043:C:N4	1.51	1.09

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%)	13 (6%)	8 (4%)	3 5
2	CB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	29	52
3	CC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
4	CD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	52
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	142 (97%)	3 (2%)	1 (1%)	22	43
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	AG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	22	43
7	CG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	22	43
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
9	AI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	19	39
9	CI	125/128 (98%)	120 (96%)	4 (3%)	1 (1%)	19	39
10	AJ	95/105 (90%)	85 (90%)	8 (8%)	2 (2%)	7	13
10	CJ	94/105 (90%)	84 (89%)	6 (6%)	4 (4%)	2	3
11	AK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	17	35
11	CK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	17	35
12	AL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
12	CL	120/132 (91%)	117 (98%)	2 (2%)	1 (1%)	19	39
13	AM	121/126 (96%)	116 (96%)	4 (3%)	1 (1%)	19	39
13	CM	120/126 (95%)	113 (94%)	4 (3%)	3 (2%)	5	9
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	12	24
17	AQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	82/93 (88%)	76 (93%)	5 (6%)	1 (1%)	13	27
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	2	2
20	CT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	2	2
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34	57
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	22	43
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	52
29	DE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	52
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	52
30	DF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	52
31	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	25	47
31	DG	179/182 (98%)	168 (94%)	8 (4%)	3 (2%)	9	18
32	BH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
32	DH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
33	BI	144/148 (97%)	132 (92%)	7 (5%)	5 (4%)	3	5
33	DI	144/148 (97%)	135 (94%)	8 (6%)	1 (1%)	22	43
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
36	BP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	22	43
36	DP	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11	22
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	43
38	BR	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
38	DR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
39	BS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
39	DS	108/112 (96%)	107 (99%)	0	1 (1%)	17	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
40	DT	129/146 (88%)	126 (98%)	3 (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%)	5 (5%)	1 (1%)	15	32
42	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	32
43	BW	110/113 (97%)	110 (100%)	0	0	100	100
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	30
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	47
46	DZ	172/206 (84%)	159 (92%)	13 (8%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	13	27
48	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
48	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
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%)	54 (81%)	9 (13%)	4 (6%)	1	1
51	D4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	3
52	B5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	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%)	45 (98%)	1 (2%)	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	12
55	B8	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	11410/12128 (94%)	10945 (96%)	381 (3%)	84 (1%)	22	43

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	19	HIS
2	AB	231	GLU
9	AI	54	ASP
10	AJ	56	HIS

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%)	155 (81%)	37 (19%)	1	2
2	CB	187/220 (85%)	151 (81%)	36 (19%)	1	2
3	AC	143/188 (76%)	127 (89%)	16 (11%)	6	10
3	CC	141/188 (75%)	116 (82%)	25 (18%)	2	3
4	AD	170/181 (94%)	147 (86%)	23 (14%)	4	6
4	CD	174/181 (96%)	147 (84%)	27 (16%)	2	4
5	AE	113/123 (92%)	106 (94%)	7 (6%)	18	37
5	CE	114/123 (93%)	99 (87%)	15 (13%)	4	7
6	AF	84/90 (93%)	74 (88%)	10 (12%)	5	9
6	CF	86/90 (96%)	79 (92%)	7 (8%)	11	23
7	AG	119/127 (94%)	99 (83%)	20 (17%)	2	3
7	CG	120/127 (94%)	106 (88%)	14 (12%)	5	10
8	AH	114/119 (96%)	101 (89%)	13 (11%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	114/119 (96%)	97 (85%)	17 (15%)	3	5
9	AI	91/99 (92%)	73 (80%)	18 (20%)	1	2
9	CI	89/99 (90%)	69 (78%)	20 (22%)	1	1
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	9	18
10	CJ	69/92 (75%)	61 (88%)	8 (12%)	5	10
11	AK	83/99 (84%)	74 (89%)	9 (11%)	6	12
11	CK	83/99 (84%)	72 (87%)	11 (13%)	4	7
12	AL	97/109 (89%)	88 (91%)	9 (9%)	9	17
12	CL	97/109 (89%)	85 (88%)	12 (12%)	4	8
13	AM	95/101 (94%)	81 (85%)	14 (15%)	3	5
13	CM	92/101 (91%)	74 (80%)	18 (20%)	1	2
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	2
14	CN	49/50 (98%)	37 (76%)	12 (24%)	0	1
15	AO	78/80 (98%)	70 (90%)	8 (10%)	7	13
15	CO	78/80 (98%)	67 (86%)	11 (14%)	3	6
16	AP	69/74 (93%)	58 (84%)	11 (16%)	2	4
16	CP	68/74 (92%)	59 (87%)	9 (13%)	4	7
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	28
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	6	12
18	AR	59/77 (77%)	50 (85%)	9 (15%)	2	4
18	CR	59/77 (77%)	46 (78%)	13 (22%)	1	1
19	AS	70/80 (88%)	59 (84%)	11 (16%)	2	4
19	CS	67/80 (84%)	54 (81%)	13 (19%)	1	2
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3	5
20	CT	71/82 (87%)	62 (87%)	9 (13%)	4	8
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	3
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	3
28	BD	215/218 (99%)	196 (91%)	19 (9%)	10	19
28	DD	216/218 (99%)	200 (93%)	16 (7%)	13	28
29	BE	164/166 (99%)	145 (88%)	19 (12%)	5	10
29	DE	164/166 (99%)	141 (86%)	23 (14%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BF	160/166 (96%)	142 (89%)	18 (11%)	6	10
30	DF	159/166 (96%)	138 (87%)	21 (13%)	4	7
31	BG	143/156 (92%)	127 (89%)	16 (11%)	6	10
31	DG	142/156 (91%)	119 (84%)	23 (16%)	2	4
32	BH	144/148 (97%)	129 (90%)	15 (10%)	7	13
32	DH	144/148 (97%)	124 (86%)	20 (14%)	3	6
33	BI	110/124 (89%)	88 (80%)	22 (20%)	1	2
33	DI	107/124 (86%)	87 (81%)	20 (19%)	1	2
34	BN	118/119 (99%)	101 (86%)	17 (14%)	3	5
34	DN	118/119 (99%)	101 (86%)	17 (14%)	3	5
35	BO	100/100 (100%)	92 (92%)	8 (8%)	12	24
35	DO	100/100 (100%)	89 (89%)	11 (11%)	6	11
36	BP	116/116 (100%)	104 (90%)	12 (10%)	7	13
36	DP	115/116 (99%)	103 (90%)	12 (10%)	7	13
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	5
37	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	8
38	BR	101/101 (100%)	83 (82%)	18 (18%)	2	3
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	5
39	BS	87/88 (99%)	79 (91%)	8 (9%)	9	17
39	DS	85/88 (97%)	74 (87%)	11 (13%)	4	7
40	BT	115/127 (91%)	107 (93%)	8 (7%)	15	30
40	DT	113/127 (89%)	105 (93%)	8 (7%)	14	29
41	BU	93/94 (99%)	86 (92%)	7 (8%)	13	27
41	DU	93/94 (99%)	87 (94%)	6 (6%)	17	34
42	BV	80/82 (98%)	70 (88%)	10 (12%)	4	8
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	3
43	BW	90/92 (98%)	83 (92%)	7 (8%)	12	25
43	DW	90/92 (98%)	84 (93%)	6 (7%)	16	33
44	BX	77/78 (99%)	72 (94%)	5 (6%)	17	34
44	DX	77/78 (99%)	70 (91%)	7 (9%)	9	18
45	BY	85/91 (93%)	77 (91%)	8 (9%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DY	85/91 (93%)	78 (92%)	7 (8%)	11	22
46	BZ	145/179 (81%)	128 (88%)	17 (12%)	5	10
46	DZ	145/179 (81%)	127 (88%)	18 (12%)	4	8
47	B0	65/67 (97%)	61 (94%)	4 (6%)	18	37
47	D0	65/67 (97%)	59 (91%)	6 (9%)	9	17
48	B1	80/83 (96%)	72 (90%)	8 (10%)	7	14
48	D1	80/83 (96%)	71 (89%)	9 (11%)	6	10
49	B2	65/67 (97%)	59 (91%)	6 (9%)	9	17
49	D2	65/67 (97%)	60 (92%)	5 (8%)	13	25
50	B3	51/52 (98%)	47 (92%)	4 (8%)	12	25
50	D3	50/52 (96%)	47 (94%)	3 (6%)	19	39
51	B4	60/63 (95%)	51 (85%)	9 (15%)	3	5
51	D4	53/63 (84%)	38 (72%)	15 (28%)	0	1
52	B5	50/52 (96%)	46 (92%)	4 (8%)	12	24
52	D5	50/52 (96%)	48 (96%)	2 (4%)	31	57
53	B6	51/52 (98%)	45 (88%)	6 (12%)	5	9
53	D6	50/52 (96%)	47 (94%)	3 (6%)	19	39
54	B7	41/42 (98%)	39 (95%)	2 (5%)	25	48
54	D7	41/42 (98%)	39 (95%)	2 (5%)	25	48
55	B8	54/55 (98%)	50 (93%)	4 (7%)	13	28
55	D8	54/55 (98%)	50 (93%)	4 (7%)	13	28
56	B9	34/34 (100%)	33 (97%)	1 (3%)	42	68
56	D9	34/34 (100%)	33 (97%)	1 (3%)	42	68
All	All	9336/10066 (93%)	8180 (88%)	1156 (12%)	4	8

5 of 1156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	DH	42	ARG
53	D6	6	ARG
33	DI	77	LEU
32	DH	41	MET
39	DS	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
51	B4	46	GLN
33	DI	43	ASN
4	CD	77	ASN
31	DG	108	ASN
43	DW	60	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	361 (24%)	19 (1%)
1	CA	1501/1521 (98%)	370 (24%)	25 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	3 (27%)	0
23	AW	70/76 (92%)	27 (38%)	2 (2%)
23	CW	67/76 (88%)	26 (38%)	3 (4%)
24	AX	74/77 (96%)	16 (21%)	0
24	CX	74/77 (96%)	23 (31%)	0
25	AY	71/76 (93%)	37 (52%)	3 (4%)
25	CY	69/76 (90%)	36 (52%)	1 (1%)
26	BA	2812/2915 (96%)	444 (15%)	36 (1%)
26	DA	2791/2915 (95%)	563 (20%)	24 (0%)
27	BB	119/121 (98%)	13 (10%)	0
27	DB	119/121 (98%)	38 (31%)	0
All	All	9284/9620 (96%)	1960 (21%)	113 (1%)

5 of 1960 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2689	U
26	DA	2422	A
1	CA	991	U

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Mol	Chain	Res	Type
26	DA	2318	G
26	DA	1300	U

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

40 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	$\#\|Z\| > 2$
25	PSU	AY	55	25	18,21,22	1.29	2 (11%)	22,30,33	1.95	3 (13%)
23	5MU	CW	54	23	19,22,23	1.41	5 (26%)	28,32,35	1.80	6 (21%)
23	4SU	CW	8	23	18,21,22	1.65	4 (22%)	26,30,33	2.32	5 (19%)
23	PSU	CW	55	23	18,21,22	1.29	2 (11%)	22,30,33	1.95	4 (18%)
24	4SU	CX	8	24	18,21,22	1.90	6 (33%)	26,30,33	1.33	3 (11%)
25	7MG	CY	46	25	22,26,27	1.43	4 (18%)	29,39,42	2.55	9 (31%)
23	7MG	AW	46	23	22,26,27	1.39	4 (18%)	29,39,42	2.41	7 (24%)
25	PSU	CY	39	25	18,21,22	1.53	5 (27%)	22,30,33	2.45	3 (13%)
25	5MU	AY	54	25	19,22,23	1.57	6 (31%)	28,32,35	2.01	6 (21%)
23	PSU	AW	39	23	18,21,22	1.35	2 (11%)	22,30,33	1.80	3 (13%)
25	4SU	AY	8	25	18,21,22	1.66	3 (16%)	26,30,33	2.25	6 (23%)
23	F3N	CW	76	23	30,36,37	1.50	6 (20%)	29,51,54	1.19	1 (3%)
23	MIA	CW	37	23	18,24,32	1.12	2 (11%)	18,35,47	1.23	2 (11%)
25	5MU	CY	54	25	19,22,23	1.35	4 (21%)	28,32,35	2.25	6 (21%)
25	PSU	CY	32	25	18,21,22	1.34	2 (11%)	22,30,33	1.82	4 (18%)
23	5MU	AW	54	23	19,22,23	1.41	4 (21%)	28,32,35	1.87	5 (17%)
23	F3N	AW	76	23	30,36,37	1.49	5 (16%)	29,51,54	1.21	1 (3%)
25	PSU	AY	39	25	18,21,22	1.40	2 (11%)	22,30,33	1.72	3 (13%)
24	5MU	CX	54	24	19,22,23	1.37	4 (21%)	28,32,35	2.14	6 (21%)
24	5MU	AX	54	57,24	19,22,23	1.39	5 (26%)	28,32,35	2.03	6 (21%)
23	4SU	AW	8	23	18,21,22	1.78	4 (22%)	26,30,33	2.00	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	7MG	CW	46	23	22,26,27	1.36	4 (18%)	29,39,42	2.47	8 (27%)
25	4SU	CY	8	25	18,21,22	1.80	4 (22%)	26,30,33	2.39	5 (19%)
25	7MG	AY	46	25	22,26,27	1.26	3 (13%)	29,39,42	2.93	8 (27%)
24	31H	AX	76	57,24	28,34,35	1.20	4 (14%)	23,47,50	1.61	4 (17%)
24	PSU	AX	55	24	18,21,22	1.33	2 (11%)	22,30,33	1.95	4 (18%)
25	MIA	CY	37	25	18,24,32	1.17	2 (11%)	18,35,47	1.27	2 (11%)
23	PSU	CW	32	23	18,21,22	1.30	2 (11%)	22,30,33	1.85	4 (18%)
25	PSU	CY	55	25	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
23	PSU	AW	32	57,23	18,21,22	1.31	2 (11%)	22,30,33	1.88	3 (13%)
24	31H	CX	76	57,24	28,34,35	1.21	3 (10%)	23,47,50	1.51	2 (8%)
23	PSU	AW	55	23	18,21,22	1.40	2 (11%)	22,30,33	1.87	3 (13%)
24	4SU	AX	8	24	18,21,22	2.16	5 (27%)	26,30,33	1.58	4 (15%)
25	PSU	AY	32	25	18,21,22	1.37	2 (11%)	22,30,33	1.78	3 (13%)
23	PSU	CW	39	23	18,21,22	1.37	2 (11%)	22,30,33	1.58	2 (9%)
25	MIA	AY	37	25	18,24,32	1.15	2 (11%)	18,35,47	1.24	2 (11%)
24	5MC	CX	32	24	18,22,23	0.98	2 (11%)	26,32,35	1.22	4 (15%)
24	5MC	AX	32	24	18,22,23	0.97	2 (11%)	26,32,35	1.24	4 (15%)
23	MIA	AW	37	23	24,31,32	2.20	4 (16%)	26,44,47	2.40	9 (34%)
24	PSU	CX	55	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)

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
25	PSU	AY	55	25	-	1/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	2/7/37/38	0/3/3/3
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
25	PSU	CY	39	25	-	2/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	4/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	F3N	CW	76	23	-	5/15/37/38	0/4/4/4
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
25	5MU	CY	54	25	-	2/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	2/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	F3N	AW	76	23	-	0/15/37/38	0/4/4/4
25	PSU	AY	39	25	-	2/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	57,24	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
25	4SU	CY	8	25	-	1/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	4/7/37/38	0/3/3/3
24	31H	AX	76	57,24	-	7/18/40/41	0/3/3/3
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/3/25/34	0/3/3/3
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
25	PSU	CY	55	25	-	2/7/25/26	0/2/2/2
23	PSU	AW	32	57,23	-	0/7/25/26	0/2/2/2
24	31H	CX	76	57,24	-	12/18/40/41	0/3/3/3
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
25	PSU	AY	32	25	-	2/7/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
25	MIA	AY	37	25	-	3/3/25/34	0/3/3/3
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.34	1.53	1.32
23	AW	37	MIA	C2-S10	-6.22	1.70	1.75
24	AX	8	4SU	C4-N3	-5.22	1.32	1.37
23	AW	76	F3N	CB-CG	-4.99	1.39	1.51
25	CY	8	4SU	C4-S4	-4.57	1.59	1.68

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	46	7MG	N9-C4-N3	10.67	141.42	125.47
23	AW	46	7MG	N9-C4-N3	8.36	137.97	125.47
25	CY	46	7MG	N9-C4-N3	8.15	137.66	125.47
25	CY	39	PSU	N1-C2-N3	7.80	123.97	115.13
23	CW	8	4SU	C4-N3-C2	-7.19	120.35	127.34

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
24	AX	76	31H	OCN-CN-N-CA
25	AY	32	PSU	O4'-C4'-C5'-O5'
25	AY	37	MIA	C3'-C4'-C5'-O5'
25	AY	46	7MG	C4'-C5'-O5'-P

There are no ring outliers.

26 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AY	55	PSU	1	0
23	CW	8	4SU	2	0
23	CW	55	PSU	1	0
24	CX	8	4SU	3	0
25	CY	46	7MG	4	0
25	CY	39	PSU	8	0
23	AW	39	PSU	1	0
25	AY	8	4SU	1	0
23	CW	76	F3N	3	0
23	AW	76	F3N	1	0
25	AY	39	PSU	2	0
23	CW	46	7MG	2	0
25	CY	8	4SU	2	0
25	AY	46	7MG	3	0
24	AX	76	31H	1	0
25	CY	37	MIA	3	0
23	CW	32	PSU	1	0
25	CY	55	PSU	2	0
24	CX	76	31H	1	0
23	AW	55	PSU	1	0
24	AX	8	4SU	1	0
23	CW	39	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AY	37	MIA	1	0
24	CX	32	5MC	1	0
24	AX	32	5MC	2	0
24	CX	55	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2063 ligands modelled in this entry, 2061 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	AD	501	4	0,12,12	-	-	-		
58	SF4	CD	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	AD	501	4	-	-	0/6/5/5
58	SF4	CD	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AD	501	SF4	1	0
58	CD	501	SF4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	1497/1521 (98%)	0.04	16 (1%)	80	78	41, 72, 93, 106	0
1	CA	1503/1521 (98%)	0.06	62 (4%)	37	30	43, 75, 94, 106	0
2	AB	231/256 (90%)	0.69	29 (12%)	3	2	68, 82, 89, 95	0
2	CB	231/256 (90%)	1.72	85 (36%)	0	0	68, 83, 90, 96	0
3	AC	206/239 (86%)	0.79	24 (11%)	4	3	69, 79, 87, 94	0
3	CC	206/239 (86%)	1.62	73 (35%)	0	0	70, 82, 90, 94	0
4	AD	208/209 (99%)	1.04	38 (18%)	1	0	57, 72, 81, 87	0
4	CD	208/209 (99%)	0.96	25 (12%)	4	2	60, 72, 81, 89	0
5	AE	148/162 (91%)	0.74	12 (8%)	12	8	58, 71, 81, 85	0
5	CE	148/162 (91%)	1.07	21 (14%)	2	1	60, 74, 83, 86	0
6	AF	100/101 (99%)	0.41	1 (1%)	82	80	52, 67, 75, 85	0
6	CF	100/101 (99%)	0.38	3 (3%)	50	43	57, 71, 81, 85	0
7	AG	155/156 (99%)	0.42	9 (5%)	23	17	66, 76, 85, 96	0
7	CG	155/156 (99%)	1.29	47 (30%)	0	0	68, 77, 86, 97	0
8	AH	137/138 (99%)	0.32	2 (1%)	73	70	62, 72, 79, 83	0
8	CH	137/138 (99%)	1.22	35 (25%)	0	0	64, 74, 80, 85	0
9	AI	127/128 (99%)	0.99	19 (14%)	2	1	62, 80, 87, 89	0
9	CI	127/128 (99%)	2.96	83 (65%)	0	0	69, 82, 89, 91	0
10	AJ	97/105 (92%)	0.82	13 (13%)	3	2	66, 83, 91, 92	0
10	CJ	96/105 (91%)	2.14	43 (44%)	0	0	68, 84, 91, 93	0
11	AK	114/129 (88%)	0.86	10 (8%)	10	7	51, 70, 80, 84	0
11	CK	114/129 (88%)	0.93	13 (11%)	5	3	52, 72, 81, 85	0
12	AL	122/132 (92%)	0.24	1 (0%)	86	84	41, 56, 71, 75	0
12	CL	122/132 (92%)	0.85	23 (18%)	1	0	58, 73, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.46	7 (5%)	23	18	57, 72, 83, 88	0
13	CM	122/126 (96%)	1.98	51 (41%)	0	0	69, 85, 92, 97	0
14	AN	60/61 (98%)	1.05	8 (13%)	3	2	70, 76, 83, 84	0
14	CN	60/61 (98%)	3.05	42 (70%)	0	0	73, 79, 85, 87	0
15	AO	88/89 (98%)	0.53	5 (5%)	23	18	54, 68, 79, 83	0
15	CO	88/89 (98%)	0.55	6 (6%)	17	12	56, 70, 81, 84	0
16	AP	82/88 (93%)	1.40	22 (26%)	0	0	59, 71, 79, 84	0
16	CP	82/88 (93%)	0.65	3 (3%)	41	34	59, 70, 79, 83	0
17	AQ	99/105 (94%)	0.61	8 (8%)	12	8	57, 70, 79, 84	0
17	CQ	99/105 (94%)	1.09	21 (21%)	0	0	60, 71, 79, 84	0
18	AR	68/88 (77%)	0.76	9 (13%)	3	2	59, 69, 81, 84	0
18	CR	68/88 (77%)	0.90	11 (16%)	1	1	58, 70, 81, 85	0
19	AS	84/93 (90%)	0.31	2 (2%)	59	53	70, 81, 87, 92	0
19	CS	83/93 (89%)	2.05	38 (45%)	0	0	74, 83, 90, 94	0
20	AT	96/106 (90%)	0.37	5 (5%)	27	21	59, 71, 80, 83	0
20	CT	96/106 (90%)	0.58	8 (8%)	11	8	59, 71, 80, 83	0
21	AU	23/27 (85%)	1.17	5 (21%)	0	0	70, 75, 78, 82	0
21	CU	23/27 (85%)	2.81	15 (65%)	0	0	71, 78, 81, 82	0
22	AV	13/24 (54%)	1.83	5 (38%)	0	0	58, 77, 95, 100	0
22	CV	12/24 (50%)	2.36	7 (58%)	0	0	64, 81, 93, 95	0
23	AW	66/76 (86%)	1.04	10 (15%)	2	1	66, 95, 102, 105	0
23	CW	64/76 (84%)	3.10	47 (73%)	0	0	70, 96, 101, 106	0
24	AX	71/77 (92%)	-0.01	0	100	100	42, 73, 90, 96	0
24	CX	71/77 (92%)	0.11	2 (2%)	53	46	55, 86, 95, 98	0
25	AY	67/76 (88%)	0.49	8 (11%)	4	3	44, 97, 101, 105	0
25	CY	66/76 (86%)	1.70	27 (40%)	0	0	48, 98, 102, 103	0
26	BA	2819/2915 (96%)	0.52	17 (0%)	89	88	23, 43, 87, 106	0
26	DA	2800/2915 (96%)	-0.10	60 (2%)	63	58	27, 48, 90, 108	0
27	BB	120/121 (99%)	0.49	0	100	100	41, 64, 76, 88	0
27	DB	120/121 (99%)	-0.08	2 (1%)	70	66	48, 70, 80, 91	0
28	BD	275/276 (99%)	0.46	3 (1%)	80	78	24, 41, 58, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DD	275/276 (99%)	0.40	8 (2%) 51 45	28, 44, 61, 79	0
29	BE	204/206 (99%)	0.59	1 (0%) 91 89	23, 46, 65, 83	0
29	DE	204/206 (99%)	0.25	1 (0%) 91 89	26, 50, 67, 84	0
30	BF	203/210 (96%)	0.61	1 (0%) 91 89	25, 51, 76, 86	0
30	DF	203/210 (96%)	0.43	7 (3%) 45 38	28, 56, 78, 88	0
31	BG	181/182 (99%)	0.51	3 (1%) 70 66	55, 72, 83, 93	0
31	DG	181/182 (99%)	1.53	58 (32%) 0 0	64, 76, 85, 93	0
32	BH	174/180 (96%)	0.51	1 (0%) 89 88	50, 66, 75, 82	0
32	DH	174/180 (96%)	1.74	72 (41%) 0 0	56, 71, 79, 83	0
33	BI	146/148 (98%)	0.33	1 (0%) 87 86	49, 74, 83, 87	0
33	DI	146/148 (98%)	0.12	2 (1%) 75 71	50, 74, 83, 87	0
34	BN	140/140 (100%)	0.67	0 100 100	29, 48, 67, 79	0
34	DN	140/140 (100%)	0.80	13 (9%) 8 6	35, 53, 70, 82	0
35	BO	122/122 (100%)	0.28	0 100 100	25, 40, 57, 67	0
35	DO	122/122 (100%)	0.47	2 (1%) 72 68	44, 58, 74, 79	0
36	BP	149/150 (99%)	0.55	0 100 100	25, 55, 75, 80	0
36	DP	149/150 (99%)	0.59	6 (4%) 38 31	28, 58, 78, 83	0
37	BQ	141/141 (100%)	0.76	2 (1%) 75 71	37, 52, 68, 77	0
37	DQ	141/141 (100%)	1.22	27 (19%) 1 0	41, 58, 72, 79	0
38	BR	118/118 (100%)	0.42	0 100 100	22, 34, 50, 59	0
38	DR	118/118 (100%)	0.65	6 (5%) 28 22	38, 53, 64, 75	0
39	BS	110/112 (98%)	0.33	0 100 100	34, 50, 64, 70	0
39	DS	110/112 (98%)	1.42	29 (26%) 0 0	70, 79, 87, 91	0
40	BT	131/146 (89%)	0.38	0 100 100	38, 51, 73, 82	0
40	DT	131/146 (89%)	0.23	2 (1%) 73 70	40, 54, 75, 81	0
41	BU	116/118 (98%)	0.44	0 100 100	17, 30, 50, 63	0
41	DU	116/118 (98%)	0.54	5 (4%) 35 28	40, 59, 79, 85	0
42	BV	101/101 (100%)	0.28	0 100 100	16, 38, 58, 68	0
42	DV	101/101 (100%)	0.33	4 (3%) 38 31	44, 73, 81, 92	0
43	BW	112/113 (99%)	0.38	0 100 100	22, 30, 49, 83	0
43	DW	112/113 (99%)	0.71	4 (3%) 42 35	35, 50, 66, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BX	95/96 (98%)	0.64	0 100 100	31, 46, 67, 83	0
44	DX	95/96 (98%)	0.70	10 (10%) 6 4	36, 50, 68, 83	0
45	BY	107/110 (97%)	0.47	1 (0%) 84 82	42, 58, 73, 84	0
45	DY	107/110 (97%)	0.77	12 (11%) 5 3	47, 61, 75, 84	0
46	BZ	171/206 (83%)	0.95	30 (17%) 1 0	40, 66, 91, 95	0
46	DZ	174/206 (84%)	1.90	67 (38%) 0 0	69, 85, 94, 101	0
47	B0	83/85 (97%)	0.96	6 (7%) 15 11	34, 50, 67, 75	0
47	D0	83/85 (97%)	1.15	10 (12%) 4 2	40, 56, 71, 76	0
48	B1	97/98 (98%)	0.47	2 (2%) 63 58	31, 49, 72, 76	0
48	D1	97/98 (98%)	0.54	5 (5%) 27 21	34, 53, 73, 78	0
49	B2	70/72 (97%)	0.42	0 100 100	33, 49, 64, 82	0
49	D2	70/72 (97%)	0.38	1 (1%) 75 71	58, 69, 78, 82	0
50	B3	59/60 (98%)	0.22	0 100 100	24, 37, 63, 74	0
50	D3	59/60 (98%)	0.92	8 (13%) 3 1	52, 65, 79, 87	0
51	B4	69/71 (97%)	0.46	4 (5%) 23 17	49, 76, 89, 91	0
51	D4	69/71 (97%)	1.72	27 (39%) 0 0	74, 89, 95, 99	0
52	B5	59/60 (98%)	0.42	1 (1%) 70 66	16, 30, 46, 68	0
52	D5	59/60 (98%)	0.30	1 (1%) 70 66	35, 49, 65, 77	0
53	B6	53/54 (98%)	0.31	0 100 100	32, 44, 57, 72	0
53	D6	53/54 (98%)	0.70	3 (5%) 23 18	49, 64, 74, 79	0
54	B7	48/49 (97%)	0.77	3 (6%) 20 15	23, 32, 58, 70	0
54	D7	48/49 (97%)	0.98	5 (10%) 6 4	26, 35, 61, 70	0
55	B8	64/65 (98%)	0.62	0 100 100	34, 42, 50, 65	0
55	D8	64/65 (98%)	0.55	1 (1%) 72 68	37, 46, 54, 65	0
56	B9	37/37 (100%)	0.94	1 (2%) 54 48	36, 51, 65, 73	0
56	D9	37/37 (100%)	0.71	4 (10%) 5 3	43, 55, 68, 76	0
All	All	20895/21748 (96%)	0.54	1598 (7%) 13 10	16, 64, 89, 108	0

The worst 5 of 1598 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CB	165	VAL	12.1
46	DZ	155	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	10.0
46	DZ	107	THR	9.1
46	DZ	171	ILE	8.6

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	0.71	0.25	87,101,108,135	0
23	7MG	CW	46	24/25	0.73	0.33	81,97,101,125	0
25	5MU	CY	54	21/22	0.74	0.49	89,99,105,136	0
25	PSU	CY	55	20/21	0.75	0.41	86,100,107,118	0
23	4SU	CW	8	20/21	0.77	0.29	85,96,117,121	0
25	MIA	CY	37	22/30	0.79	0.30	79,95,102,124	0
25	4SU	CY	8	20/21	0.79	0.16	88,102,112,128	0
24	4SU	CX	8	20/21	0.80	0.13	84,92,105,111	0
23	7MG	AW	46	24/25	0.80	0.21	80,97,112,135	0
25	PSU	CY	39	20/21	0.81	0.27	86,91,104,110	0
25	PSU	AY	55	20/21	0.81	0.20	85,96,106,117	0
25	7MG	AY	46	24/25	0.82	0.18	80,99,107,116	0
25	4SU	AY	8	20/21	0.83	0.13	83,95,104,129	0
25	PSU	AY	32	20/21	0.83	0.26	76,92,107,110	0
25	PSU	CY	32	20/21	0.83	0.26	77,91,109,114	0
23	PSU	AW	55	20/21	0.83	0.27	76,88,103,105	0
23	4SU	AW	8	20/21	0.84	0.17	83,89,107,110	0
23	PSU	CW	55	20/21	0.84	0.34	76,90,103,106	0
25	5MU	AY	54	21/22	0.85	0.20	81,89,99,128	0
23	PSU	AW	32	20/21	0.86	0.26	77,84,98,106	0
25	MIA	AY	37	22/30	0.86	0.22	79,89,101,116	0
23	5MU	CW	54	21/22	0.86	0.23	76,87,97,99	0
25	PSU	AY	39	20/21	0.86	0.25	84,90,102,107	0
23	MIA	CW	37	22/30	0.87	0.30	72,86,92,96	0
23	PSU	CW	32	20/21	0.87	0.48	77,86,95,106	0
23	PSU	CW	39	20/21	0.89	0.43	76,85,92,95	0
24	31H	CX	76	32/33	0.90	0.35	48,68,88,99	0
23	5MU	AW	54	21/22	0.91	0.21	66,80,87,93	0
24	PSU	CX	55	20/21	0.92	0.15	81,87,92,97	0
23	MIA	AW	37	29/30	0.93	0.25	56,65,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	F3N	CW	76	33/34	0.93	0.44	53,69,79,80	0
24	4SU	AX	8	20/21	0.93	0.17	59,69,79,85	0
23	PSU	AW	39	20/21	0.93	0.24	71,82,92,93	0
24	31H	AX	76	32/33	0.94	0.33	31,57,76,77	10
23	F3N	AW	76	33/34	0.94	0.38	44,58,72,77	0
24	5MU	CX	54	21/22	0.94	0.21	71,85,94,104	0
24	PSU	AX	55	20/21	0.94	0.16	52,69,77,77	0
24	5MC	CX	32	21/22	0.95	0.18	63,77,85,87	0
24	5MU	AX	54	21/22	0.96	0.16	46,72,77,86	0
24	5MC	AX	32	21/22	0.97	0.20	50,57,69,76	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	CE	202	1/1	0.26	0.19	95,95,95,95	0
59	ZN	D4	501	1/1	0.33	0.12	162,162,162,162	0
57	MG	AA	1784	1/1	0.34	0.29	72,72,72,72	0
57	MG	DA	3254	1/1	0.43	0.15	68,68,68,68	0
57	MG	BA	3327	1/1	0.47	0.17	39,39,39,39	0
57	MG	CA	3086	1/1	0.48	0.13	93,93,93,93	0
57	MG	BA	3702	1/1	0.49	0.12	39,39,39,39	0
57	MG	DA	3135	1/1	0.49	0.18	63,63,63,63	0
57	MG	AA	1618	1/1	0.55	0.18	68,68,68,68	0
57	MG	DA	3628	1/1	0.57	0.19	77,77,77,77	0
57	MG	BA	3734	1/1	0.57	0.14	65,65,65,65	0
57	MG	CA	3115	1/1	0.58	0.34	82,82,82,82	0
57	MG	DA	3070	1/1	0.59	0.19	65,65,65,65	0
57	MG	DA	3463	1/1	0.60	0.19	44,44,44,44	0
57	MG	DA	3204	1/1	0.60	0.21	68,68,68,68	0
57	MG	DA	3033	1/1	0.60	0.49	68,68,68,68	0
57	MG	BA	3439	1/1	0.61	0.18	36,36,36,36	0
57	MG	DA	3318	1/1	0.62	0.10	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	DA	3057	1/1	0.63	0.20	44,44,44,44	0
57	MG	AX	3007	1/1	0.63	0.30	68,68,68,68	0
57	MG	BA	3154	1/1	0.63	0.21	52,52,52,52	0
57	MG	CA	3003	1/1	0.64	0.16	58,58,58,58	0
57	MG	BA	3693	1/1	0.64	0.16	77,77,77,77	0
57	MG	DA	3516	1/1	0.65	0.21	67,67,67,67	0
57	MG	BA	3272	1/1	0.66	0.26	64,64,64,64	0
57	MG	BA	3710	1/1	0.66	0.79	65,65,65,65	0
57	MG	AA	1743	1/1	0.67	0.17	66,66,66,66	0
57	MG	DA	3116	1/1	0.67	0.16	53,53,53,53	0
57	MG	DA	3487	1/1	0.68	0.12	55,55,55,55	0
57	MG	DA	3099	1/1	0.68	0.18	63,63,63,63	0
57	MG	AA	1713	1/1	0.69	0.11	67,67,67,67	0
57	MG	AA	1679	1/1	0.69	0.19	51,51,51,51	0
57	MG	BA	3569	1/1	0.69	0.22	56,56,56,56	0
57	MG	DA	3122	1/1	0.69	0.19	60,60,60,60	0
57	MG	BA	3652	1/1	0.69	0.09	58,58,58,58	0
57	MG	DA	3199	1/1	0.69	0.25	62,62,62,62	0
57	MG	BA	3655	1/1	0.69	0.13	55,55,55,55	0
57	MG	DA	3545	1/1	0.70	0.12	62,62,62,62	0
57	MG	BA	3288	1/1	0.70	0.18	44,44,44,44	0
57	MG	DA	3313	1/1	0.70	0.11	39,39,39,39	0
57	MG	BA	3727	1/1	0.71	0.24	53,53,53,53	0
57	MG	BA	3068	1/1	0.71	0.17	49,49,49,49	0
57	MG	BA	3041	1/1	0.71	0.29	63,63,63,63	0
57	MG	CA	3006	1/1	0.71	0.11	68,68,68,68	0
57	MG	BA	3712	1/1	0.71	0.22	51,51,51,51	0
57	MG	AA	1701	1/1	0.72	0.27	73,73,73,73	0
57	MG	AA	1669	1/1	0.72	0.18	69,69,69,69	0
57	MG	CA	3058	1/1	0.72	0.19	66,66,66,66	0
57	MG	BA	3667	1/1	0.72	0.24	58,58,58,58	0
57	MG	BA	3688	1/1	0.72	0.27	61,61,61,61	0
57	MG	AL	201	1/1	0.72	0.13	63,63,63,63	0
57	MG	CA	3059	1/1	0.73	0.16	75,75,75,75	0
57	MG	DA	3071	1/1	0.73	0.23	47,47,47,47	0
57	MG	BA	3176	1/1	0.73	0.26	55,55,55,55	0
57	MG	DA	3596	1/1	0.73	0.19	69,69,69,69	0
57	MG	DA	3332	1/1	0.73	0.18	46,46,46,46	0
57	MG	DA	3634	1/1	0.73	0.14	68,68,68,68	0
57	MG	DQ	3003	1/1	0.73	0.64	62,62,62,62	0
57	MG	BA	3680	1/1	0.73	0.32	42,42,42,42	0
57	MG	BA	3538	1/1	0.74	0.12	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	DA	3097	1/1	0.74	0.15	47,47,47,47	0
57	MG	DA	3376	1/1	0.74	0.11	51,51,51,51	0
57	MG	BB	3004	1/1	0.74	0.21	69,69,69,69	0
57	MG	BA	3265	1/1	0.74	0.29	72,72,72,72	0
57	MG	BA	3487	1/1	0.74	0.14	54,54,54,54	0
57	MG	AA	1686	1/1	0.75	0.14	61,61,61,61	0
57	MG	DA	3502	1/1	0.75	0.24	48,48,48,48	0
57	MG	DA	3253	1/1	0.75	0.13	54,54,54,54	0
57	MG	BB	3020	1/1	0.75	0.16	65,65,65,65	0
57	MG	CA	3130	1/1	0.75	0.28	64,64,64,64	0
57	MG	DA	3624	1/1	0.75	0.48	59,59,59,59	0
57	MG	BA	3121	1/1	0.75	0.29	42,42,42,42	0
57	MG	BA	3016	1/1	0.75	0.28	67,67,67,67	0
57	MG	AA	1684	1/1	0.75	0.13	54,54,54,54	0
57	MG	BA	3340	1/1	0.75	0.18	27,27,27,27	0
57	MG	DA	3174	1/1	0.76	0.19	52,52,52,52	0
57	MG	BA	3579	1/1	0.76	0.11	63,63,63,63	0
57	MG	CA	3154	1/1	0.76	0.18	68,68,68,68	0
57	MG	DA	3086	1/1	0.76	0.11	47,47,47,47	0
57	MG	CA	3014	1/1	0.76	0.15	62,62,62,62	0
57	MG	DA	3279	1/1	0.76	0.14	36,36,36,36	0
57	MG	DA	3032	1/1	0.76	0.21	57,57,57,57	0
57	MG	CA	3005	1/1	0.76	0.20	73,73,73,73	0
57	MG	CA	3122	1/1	0.76	0.13	69,69,69,69	0
57	MG	DA	3061	1/1	0.76	0.21	60,60,60,60	0
57	MG	DA	3400	1/1	0.76	0.14	62,62,62,62	0
57	MG	DA	3079	1/1	0.77	0.11	72,72,72,72	0
57	MG	DA	3015	1/1	0.77	0.23	60,60,60,60	0
57	MG	BA	3637	1/1	0.77	0.14	38,38,38,38	0
57	MG	BA	3015	1/1	0.77	0.18	47,47,47,47	0
57	MG	DA	3108	1/1	0.77	0.12	50,50,50,50	0
57	MG	BA	3224	1/1	0.77	0.30	59,59,59,59	0
57	MG	CA	3032	1/1	0.77	0.16	53,53,53,53	0
57	MG	DA	3066	1/1	0.77	0.10	58,58,58,58	0
57	MG	AA	1689	1/1	0.77	0.29	71,71,71,71	0
57	MG	BA	3164	1/1	0.77	0.22	46,46,46,46	0
57	MG	DA	3114	1/1	0.78	0.12	51,51,51,51	0
57	MG	DA	3041	1/1	0.78	0.18	60,60,60,60	0
57	MG	AA	1620	1/1	0.78	0.14	59,59,59,59	0
57	MG	BG	202	1/1	0.78	0.15	52,52,52,52	0
57	MG	BA	3074	1/1	0.78	0.23	69,69,69,69	0
57	MG	BA	3026	1/1	0.78	0.15	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	AA	1631	1/1	0.78	0.14	64,64,64,64	0
57	MG	BA	3676	1/1	0.78	0.17	70,70,70,70	0
57	MG	BA	3730	1/1	0.78	0.17	68,68,68,68	0
57	MG	DA	3016	1/1	0.78	0.09	66,66,66,66	0
57	MG	DA	3284	1/1	0.78	0.14	58,58,58,58	0
57	MG	BA	3369	1/1	0.78	0.28	62,62,62,62	0
57	MG	DA	3314	1/1	0.78	0.12	43,43,43,43	0
57	MG	BA	3611	1/1	0.78	0.18	59,59,59,59	0
57	MG	DA	3002	1/1	0.79	0.14	64,64,64,64	0
57	MG	AA	1610	1/1	0.79	0.18	81,81,81,81	0
57	MG	DA	3320	1/1	0.79	0.09	49,49,49,49	0
57	MG	BA	3715	1/1	0.79	0.17	52,52,52,52	0
57	MG	DA	3024	1/1	0.79	0.41	61,61,61,61	0
57	MG	CA	3019	1/1	0.79	0.16	68,68,68,68	0
57	MG	BA	3229	1/1	0.79	0.24	52,52,52,52	0
57	MG	BA	3231	1/1	0.79	0.17	57,57,57,57	0
57	MG	DA	3052	1/1	0.79	0.10	49,49,49,49	0
57	MG	DA	3191	1/1	0.79	0.30	54,54,54,54	0
57	MG	DA	3520	1/1	0.79	0.11	57,57,57,57	0
57	MG	DA	3542	1/1	0.79	0.17	60,60,60,60	0
57	MG	BA	3498	1/1	0.79	0.21	45,45,45,45	0
57	MG	BA	3759	1/1	0.79	0.13	70,70,70,70	0
57	MG	AA	1655	1/1	0.79	0.12	53,53,53,53	0
57	MG	AA	1711	1/1	0.79	0.13	51,51,51,51	0
57	MG	BA	3160	1/1	0.79	0.20	49,49,49,49	0
57	MG	DA	3657	1/1	0.79	0.45	54,54,54,54	0
57	MG	DB	3007	1/1	0.79	0.12	67,67,67,67	0
57	MG	AA	1625	1/1	0.79	0.17	73,73,73,73	0
57	MG	BA	3006	1/1	0.79	0.24	54,54,54,54	0
57	MG	BA	3713	1/1	0.80	0.28	33,33,33,33	0
57	MG	AA	1622	1/1	0.80	0.21	69,69,69,69	0
57	MG	CA	3061	1/1	0.80	0.21	66,66,66,66	0
57	MG	DA	3089	1/1	0.80	0.18	52,52,52,52	0
57	MG	BA	3721	1/1	0.80	0.10	47,47,47,47	0
57	MG	CA	3091	1/1	0.80	0.15	69,69,69,69	0
57	MG	BA	3696	1/1	0.80	0.10	46,46,46,46	0
57	MG	BA	3700	1/1	0.80	0.24	36,36,36,36	0
57	MG	DA	3612	1/1	0.80	0.08	58,58,58,58	0
57	MG	DA	3056	1/1	0.80	0.12	49,49,49,49	0
57	MG	CA	3013	1/1	0.80	0.14	67,67,67,67	0
57	MG	BA	3678	1/1	0.80	0.10	67,67,67,67	0
57	MG	DA	3649	1/1	0.80	0.13	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	DA	3650	1/1	0.80	0.14	61,61,61,61	0
57	MG	DA	3356	1/1	0.80	0.16	39,39,39,39	0
57	MG	BA	3557	1/1	0.80	0.18	53,53,53,53	0
57	MG	AA	1604	1/1	0.80	0.12	58,58,58,58	0
57	MG	DA	3420	1/1	0.80	0.11	49,49,49,49	0
57	MG	CA	3049	1/1	0.81	0.21	65,65,65,65	0
57	MG	BA	3442	1/1	0.81	0.19	65,65,65,65	0
57	MG	BA	3453	1/1	0.81	0.28	50,50,50,50	0
57	MG	BA	3670	1/1	0.81	0.18	54,54,54,54	0
57	MG	BA	3458	1/1	0.81	0.20	59,59,59,59	0
57	MG	DA	3513	1/1	0.81	0.14	69,69,69,69	0
57	MG	BA	3475	1/1	0.81	0.09	49,49,49,49	0
57	MG	CA	3094	1/1	0.81	0.08	61,61,61,61	0
57	MG	BA	3270	1/1	0.81	0.22	56,56,56,56	0
57	MG	BA	3197	1/1	0.81	0.24	58,58,58,58	0
57	MG	DA	3591	1/1	0.81	0.06	66,66,66,66	0
57	MG	BA	3281	1/1	0.81	0.28	50,50,50,50	0
57	MG	DA	3301	1/1	0.81	0.11	63,63,63,63	0
57	MG	AA	1710	1/1	0.81	0.15	64,64,64,64	0
57	MG	DA	3625	1/1	0.81	0.10	60,60,60,60	0
57	MG	AA	1697	1/1	0.81	0.11	65,65,65,65	0
57	MG	AA	1623	1/1	0.81	0.24	65,65,65,65	0
57	MG	DA	3648	1/1	0.81	0.07	62,62,62,62	0
57	MG	BA	3257	1/1	0.81	0.18	43,43,43,43	0
57	MG	BA	3411	1/1	0.81	0.24	50,50,50,50	0
57	MG	DA	3351	1/1	0.81	0.08	56,56,56,56	0
57	MG	BA	3644	1/1	0.81	0.18	64,64,64,64	0
57	MG	AA	1741	1/1	0.81	0.12	86,86,86,86	0
57	MG	DA	3395	1/1	0.81	0.17	58,58,58,58	0
57	MG	CA	3146	1/1	0.82	0.18	72,72,72,72	0
57	MG	AA	1660	1/1	0.82	0.24	51,51,51,51	0
57	MG	DA	3101	1/1	0.82	0.13	56,56,56,56	0
57	MG	CA	3162	1/1	0.82	0.07	79,79,79,79	0
57	MG	BA	3717	1/1	0.82	0.15	72,72,72,72	0
57	MG	AX	3016	1/1	0.82	0.61	86,86,86,86	0
57	MG	DA	3468	1/1	0.82	0.14	62,62,62,62	0
57	MG	BA	3058	1/1	0.82	0.19	54,54,54,54	0
57	MG	DA	3497	1/1	0.82	0.19	58,58,58,58	0
57	MG	BA	3343	1/1	0.82	0.18	54,54,54,54	0
57	MG	DA	3143	1/1	0.82	0.14	62,62,62,62	0
57	MG	DA	3514	1/1	0.82	0.14	47,47,47,47	0
57	MG	BA	3347	1/1	0.82	0.19	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	BA	3755	1/1	0.82	0.24	43,43,43,43	0
57	MG	DA	3530	1/1	0.82	0.14	55,55,55,55	0
57	MG	AA	1644	1/1	0.82	0.12	56,56,56,56	0
57	MG	DA	3035	1/1	0.82	0.12	37,37,37,37	0
57	MG	DA	3549	1/1	0.82	0.20	49,49,49,49	0
57	MG	DA	3560	1/1	0.82	0.15	60,60,60,60	0
57	MG	DA	3205	1/1	0.82	0.16	62,62,62,62	0
57	MG	DA	3592	1/1	0.82	0.14	67,67,67,67	0
57	MG	DA	3233	1/1	0.82	0.13	65,65,65,65	0
57	MG	DA	3607	1/1	0.82	0.14	64,64,64,64	0
57	MG	CA	3050	1/1	0.82	0.19	73,73,73,73	0
57	MG	DA	3619	1/1	0.82	0.15	40,40,40,40	0
57	MG	BA	3807	1/1	0.82	0.24	66,66,66,66	0
57	MG	DA	3257	1/1	0.82	0.20	44,44,44,44	0
57	MG	DA	3627	1/1	0.82	0.14	57,57,57,57	0
57	MG	BB	3001	1/1	0.82	0.29	68,68,68,68	0
57	MG	BA	3183	1/1	0.82	0.48	49,49,49,49	0
57	MG	AA	1810	1/1	0.82	0.09	86,86,86,86	0
57	MG	BE	301	1/1	0.82	0.20	31,31,31,31	0
57	MG	BF	310	1/1	0.82	0.23	56,56,56,56	0
57	MG	CA	3102	1/1	0.82	0.16	71,71,71,71	0
57	MG	DB	3003	1/1	0.82	0.10	78,78,78,78	0
57	MG	AA	1616	1/1	0.82	0.09	73,73,73,73	0
57	MG	BN	3002	1/1	0.82	0.20	51,51,51,51	0
57	MG	BZ	301	1/1	0.82	0.18	49,49,49,49	0
57	MG	AA	1766	1/1	0.83	0.19	71,71,71,71	0
57	MG	CE	201	1/1	0.83	0.18	65,65,65,65	0
57	MG	CA	3012	1/1	0.83	0.32	64,64,64,64	0
57	MG	BA	3233	1/1	0.83	0.28	40,40,40,40	0
57	MG	BA	3738	1/1	0.83	0.13	41,41,41,41	0
57	MG	CA	3016	1/1	0.83	0.13	48,48,48,48	0
57	MG	CA	3017	1/1	0.83	0.15	54,54,54,54	0
57	MG	BA	3235	1/1	0.83	0.20	44,44,44,44	0
57	MG	DA	3227	1/1	0.83	0.20	56,56,56,56	0
57	MG	CA	3031	1/1	0.83	0.14	58,58,58,58	0
57	MG	DA	3238	1/1	0.83	0.15	48,48,48,48	0
57	MG	BA	3240	1/1	0.83	0.18	53,53,53,53	0
57	MG	BA	3060	1/1	0.83	0.22	51,51,51,51	0
57	MG	BA	3593	1/1	0.83	0.20	55,55,55,55	0
57	MG	BA	3600	1/1	0.83	0.28	44,44,44,44	0
57	MG	BB	3019	1/1	0.83	0.20	70,70,70,70	0
57	MG	DA	3606	1/1	0.83	0.20	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	3608	1/1	0.83	0.29	58,58,58,58	0
57	MG	CA	3070	1/1	0.83	0.15	69,69,69,69	0
57	MG	DA	3618	1/1	0.83	0.10	46,46,46,46	0
57	MG	BA	3423	1/1	0.83	0.16	69,69,69,69	0
57	MG	CA	3090	1/1	0.83	0.17	76,76,76,76	0
57	MG	AW	3001	1/1	0.83	0.11	59,59,59,59	0
57	MG	AA	1650	1/1	0.83	0.15	74,74,74,74	0
57	MG	BA	3111	1/1	0.83	0.32	53,53,53,53	0
57	MG	BA	3200	1/1	0.83	0.25	48,48,48,48	0
57	MG	DA	3369	1/1	0.83	0.12	55,55,55,55	0
57	MG	CA	3002	1/1	0.83	0.14	77,77,77,77	0
57	MG	DA	3394	1/1	0.83	0.05	60,60,60,60	0
57	MG	AA	1664	1/1	0.83	0.22	62,62,62,62	0
57	MG	DB	3001	1/1	0.83	0.17	63,63,63,63	0
57	MG	DA	3397	1/1	0.83	0.15	42,42,42,42	0
57	MG	CA	3143	1/1	0.83	0.20	74,74,74,74	0
57	MG	DB	3010	1/1	0.83	0.13	75,75,75,75	0
57	MG	CA	3004	1/1	0.83	0.09	69,69,69,69	0
57	MG	BA	3002	1/1	0.83	0.28	53,53,53,53	0
57	MG	BA	3809	1/1	0.84	0.37	61,61,61,61	0
57	MG	BA	3598	1/1	0.84	0.15	33,33,33,33	0
57	MG	CA	3009	1/1	0.84	0.12	73,73,73,73	0
57	MG	BA	3145	1/1	0.84	0.25	48,48,48,48	0
57	MG	DA	3568	1/1	0.84	0.14	43,43,43,43	0
57	MG	DA	3123	1/1	0.84	0.16	54,54,54,54	0
57	MG	AA	1695	1/1	0.84	0.20	59,59,59,59	0
57	MG	DA	3140	1/1	0.84	0.10	64,64,64,64	0
57	MG	DA	3604	1/1	0.84	0.15	61,61,61,61	0
57	MG	BA	3687	1/1	0.84	0.18	64,64,64,64	0
57	MG	DA	3379	1/1	0.84	0.09	46,46,46,46	0
57	MG	CA	3108	1/1	0.84	0.11	72,72,72,72	0
57	MG	CA	3112	1/1	0.84	0.10	72,72,72,72	0
57	MG	BA	3155	1/1	0.84	0.19	40,40,40,40	0
57	MG	BA	3505	1/1	0.84	0.22	53,53,53,53	0
57	MG	DA	3411	1/1	0.84	0.18	37,37,37,37	0
57	MG	DA	3065	1/1	0.84	0.10	56,56,56,56	0
57	MG	DA	3426	1/1	0.84	0.12	49,49,49,49	0
57	MG	DA	3456	1/1	0.84	0.21	38,38,38,38	0
57	MG	AX	3005	1/1	0.84	0.11	65,65,65,65	0
57	MG	AA	1723	1/1	0.84	0.15	63,63,63,63	0
57	MG	AA	1696	1/1	0.84	0.10	83,83,83,83	0
57	MG	CA	3039	1/1	0.84	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	B7	104	1/1	0.84	0.27	62,62,62,62	0
57	MG	DA	3087	1/1	0.84	0.18	55,55,55,55	0
57	MG	CA	3001	1/1	0.84	0.14	59,59,59,59	0
57	MG	AA	1613	1/1	0.84	0.18	75,75,75,75	0
57	MG	DF	302	1/1	0.84	0.14	53,53,53,53	0
57	MG	DF	303	1/1	0.84	0.15	42,42,42,42	0
57	MG	BA	3778	1/1	0.84	0.08	40,40,40,40	0
57	MG	BA	3049	1/1	0.84	0.19	46,46,46,46	0
57	MG	AA	1663	1/1	0.85	0.12	50,50,50,50	0
57	MG	AA	1601	1/1	0.85	0.12	81,81,81,81	0
57	MG	AA	1787	1/1	0.85	0.15	49,49,49,49	0
57	MG	DA	3111	1/1	0.85	0.13	56,56,56,56	0
57	MG	DA	3462	1/1	0.85	0.22	50,50,50,50	0
57	MG	CA	3125	1/1	0.85	0.21	64,64,64,64	0
57	MG	BA	3570	1/1	0.85	0.21	31,31,31,31	0
57	MG	CA	3139	1/1	0.85	0.36	81,81,81,81	0
57	MG	DA	3491	1/1	0.85	0.25	43,43,43,43	0
57	MG	BA	3571	1/1	0.85	0.24	28,28,28,28	0
57	MG	AA	1789	1/1	0.85	0.15	60,60,60,60	0
57	MG	CA	3011	1/1	0.85	0.25	66,66,66,66	0
57	MG	CA	3161	1/1	0.85	0.13	76,76,76,76	0
57	MG	DA	3173	1/1	0.85	0.15	62,62,62,62	0
57	MG	BA	3283	1/1	0.85	0.40	57,57,57,57	0
57	MG	CA	3164	1/1	0.85	0.33	76,76,76,76	0
57	MG	DA	3196	1/1	0.85	0.16	54,54,54,54	0
57	MG	AA	1667	1/1	0.85	0.19	55,55,55,55	0
57	MG	AA	1602	1/1	0.85	0.10	68,68,68,68	0
57	MG	BA	3175	1/1	0.85	0.29	57,57,57,57	0
57	MG	DA	3008	1/1	0.85	0.12	45,45,45,45	0
57	MG	DA	3574	1/1	0.85	0.07	61,61,61,61	0
57	MG	AA	1612	1/1	0.85	0.16	63,63,63,63	0
57	MG	DA	3234	1/1	0.85	0.15	54,54,54,54	0
57	MG	BA	3632	1/1	0.85	0.26	55,55,55,55	0
57	MG	BA	3056	1/1	0.85	0.31	46,46,46,46	0
57	MG	BA	3057	1/1	0.85	0.18	48,48,48,48	0
57	MG	AA	1682	1/1	0.85	0.26	59,59,59,59	0
57	MG	CA	3041	1/1	0.85	0.11	57,57,57,57	0
57	MG	DA	3280	1/1	0.85	0.09	48,48,48,48	0
57	MG	DA	3281	1/1	0.85	0.11	36,36,36,36	0
57	MG	DA	3620	1/1	0.85	0.12	53,53,53,53	0
57	MG	AA	1699	1/1	0.85	0.32	58,58,58,58	0
57	MG	DA	3046	1/1	0.85	0.14	56,56,56,56	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	0.85	0.17	45,45,45,45	0
57	MG	BA	3225	1/1	0.85	0.13	46,46,46,46	0
57	MG	DA	3317	1/1	0.85	0.10	54,54,54,54	0
57	MG	DA	3636	1/1	0.85	0.16	62,62,62,62	0
57	MG	DA	3637	1/1	0.85	0.14	72,72,72,72	0
57	MG	BA	3062	1/1	0.85	0.30	59,59,59,59	0
57	MG	AX	3012	1/1	0.85	0.18	52,52,52,52	0
57	MG	CA	3068	1/1	0.85	0.16	58,58,58,58	0
57	MG	AX	3013	1/1	0.85	0.20	70,70,70,70	0
57	MG	BA	3078	1/1	0.85	0.32	54,54,54,54	0
57	MG	BA	3477	1/1	0.85	0.16	68,68,68,68	0
57	MG	BA	3485	1/1	0.85	0.24	26,26,26,26	0
57	MG	BA	3103	1/1	0.85	0.35	63,63,63,63	0
57	MG	AA	1764	1/1	0.85	0.10	66,66,66,66	0
57	MG	CA	3107	1/1	0.85	0.12	68,68,68,68	0
57	MG	DA	3092	1/1	0.85	0.16	57,57,57,57	0
57	MG	D8	5001	1/1	0.85	0.22	44,44,44,44	0
57	MG	BA	3263	1/1	0.85	0.28	60,60,60,60	0
57	MG	BA	3250	1/1	0.86	0.21	68,68,68,68	0
57	MG	DA	3333	1/1	0.86	0.17	47,47,47,47	0
57	MG	BA	3253	1/1	0.86	0.20	31,31,31,31	0
57	MG	BA	3052	1/1	0.86	0.27	50,50,50,50	0
57	MG	AA	1812	1/1	0.86	0.13	63,63,63,63	0
57	MG	AA	1738	1/1	0.86	0.22	68,68,68,68	0
57	MG	BA	3005	1/1	0.86	0.19	44,44,44,44	0
57	MG	DA	3390	1/1	0.86	0.10	58,58,58,58	0
57	MG	BA	3523	1/1	0.86	0.21	41,41,41,41	0
57	MG	BA	3525	1/1	0.86	0.16	43,43,43,43	0
57	MG	CA	3052	1/1	0.86	0.12	71,71,71,71	0
57	MG	BA	3530	1/1	0.86	0.25	33,33,33,33	0
57	MG	DA	3088	1/1	0.86	0.26	50,50,50,50	0
57	MG	DA	3415	1/1	0.86	0.18	43,43,43,43	0
57	MG	DA	3417	1/1	0.86	0.13	52,52,52,52	0
57	MG	DA	3418	1/1	0.86	0.07	47,47,47,47	0
57	MG	BA	3723	1/1	0.86	0.18	30,30,30,30	0
57	MG	DA	3424	1/1	0.86	0.18	41,41,41,41	0
57	MG	BA	3726	1/1	0.86	0.20	31,31,31,31	0
57	MG	DA	3435	1/1	0.86	0.12	44,44,44,44	0
57	MG	BA	3271	1/1	0.86	0.18	60,60,60,60	0
57	MG	AA	1777	1/1	0.86	0.09	71,71,71,71	0
57	MG	AX	3003	1/1	0.86	0.23	56,56,56,56	0
57	MG	AA	1628	1/1	0.86	0.10	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	3747	1/1	0.86	0.24	55,55,55,55	0
57	MG	DA	3488	1/1	0.86	0.10	53,53,53,53	0
57	MG	DA	3112	1/1	0.86	0.13	56,56,56,56	0
57	MG	BA	3286	1/1	0.86	0.17	44,44,44,44	0
57	MG	BA	3577	1/1	0.86	0.17	58,58,58,58	0
57	MG	DA	3512	1/1	0.86	0.12	37,37,37,37	0
57	MG	DA	3118	1/1	0.86	0.16	39,39,39,39	0
57	MG	BA	3018	1/1	0.86	0.40	39,39,39,39	0
57	MG	BA	3592	1/1	0.86	0.09	65,65,65,65	0
57	MG	DA	3519	1/1	0.86	0.14	58,58,58,58	0
57	MG	DA	3130	1/1	0.86	0.15	52,52,52,52	0
57	MG	CA	3109	1/1	0.86	0.15	74,74,74,74	0
57	MG	DA	3538	1/1	0.86	0.12	60,60,60,60	0
57	MG	DA	3136	1/1	0.86	0.18	48,48,48,48	0
57	MG	BA	3318	1/1	0.86	0.16	54,54,54,54	0
57	MG	DA	3141	1/1	0.86	0.13	51,51,51,51	0
57	MG	AA	1658	1/1	0.86	0.14	64,64,64,64	0
57	MG	DA	3153	1/1	0.86	0.15	44,44,44,44	0
57	MG	DA	3161	1/1	0.86	0.17	50,50,50,50	0
57	MG	DA	3170	1/1	0.86	0.10	35,35,35,35	0
57	MG	DA	3172	1/1	0.86	0.21	61,61,61,61	0
57	MG	BA	3338	1/1	0.86	0.18	55,55,55,55	0
57	MG	BA	3094	1/1	0.86	0.19	52,52,52,52	0
57	MG	BA	3099	1/1	0.86	0.24	61,61,61,61	0
57	MG	BA	3614	1/1	0.86	0.17	53,53,53,53	0
57	MG	DA	3611	1/1	0.86	0.10	53,53,53,53	0
57	MG	BA	3346	1/1	0.86	0.10	39,39,39,39	0
57	MG	DA	3617	1/1	0.86	0.25	51,51,51,51	0
57	MG	BA	3633	1/1	0.86	0.18	57,57,57,57	0
57	MG	BA	3102	1/1	0.86	0.31	57,57,57,57	0
57	MG	CA	3157	1/1	0.86	0.12	60,60,60,60	0
57	MG	BW	3001	1/1	0.86	0.35	44,44,44,44	0
57	MG	BA	3360	1/1	0.86	0.23	37,37,37,37	0
57	MG	DA	3235	1/1	0.86	0.13	48,48,48,48	0
57	MG	BA	3365	1/1	0.86	0.13	51,51,51,51	0
57	MG	B8	5002	1/1	0.86	0.31	53,53,53,53	0
57	MG	BA	3029	1/1	0.86	0.27	36,36,36,36	0
57	MG	BA	3377	1/1	0.86	0.21	51,51,51,51	0
57	MG	DA	3275	1/1	0.86	0.14	65,65,65,65	0
57	MG	BA	3107	1/1	0.86	0.33	57,57,57,57	0
57	MG	BA	3668	1/1	0.86	0.15	75,75,75,75	0
57	MG	DA	3653	1/1	0.86	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3416	1/1	0.86	0.26	60,60,60,60	0
57	MG	BA	3232	1/1	0.86	0.24	49,49,49,49	0
57	MG	DA	3286	1/1	0.86	0.09	55,55,55,55	0
57	MG	BA	3109	1/1	0.86	0.13	56,56,56,56	0
57	MG	AA	1763	1/1	0.86	0.07	79,79,79,79	0
57	MG	BA	3681	1/1	0.86	0.23	61,61,61,61	0
57	MG	AA	1606	1/1	0.86	0.14	54,54,54,54	0
57	MG	DG	3001	1/1	0.86	0.14	66,66,66,66	0
57	MG	BA	3456	1/1	0.86	0.30	37,37,37,37	0
57	MG	BA	3243	1/1	0.86	0.67	44,44,44,44	0
57	MG	DA	3330	1/1	0.86	0.17	36,36,36,36	0
57	MG	DA	3192	1/1	0.87	0.32	34,34,34,34	0
57	MG	AA	1629	1/1	0.87	0.35	68,68,68,68	0
57	MG	BA	3149	1/1	0.87	0.19	42,42,42,42	0
57	MG	DA	3493	1/1	0.87	0.08	51,51,51,51	0
57	MG	CA	3045	1/1	0.87	0.22	62,62,62,62	0
57	MG	DA	3500	1/1	0.87	0.35	55,55,55,55	0
57	MG	BA	3504	1/1	0.87	0.20	56,56,56,56	0
57	MG	BA	3653	1/1	0.87	0.21	57,57,57,57	0
57	MG	DA	3042	1/1	0.87	0.29	49,49,49,49	0
57	MG	CA	3051	1/1	0.87	0.11	77,77,77,77	0
57	MG	BA	3792	1/1	0.87	0.19	52,52,52,52	0
57	MG	BA	3805	1/1	0.87	0.13	48,48,48,48	0
57	MG	BA	3239	1/1	0.87	0.22	47,47,47,47	0
57	MG	BA	3510	1/1	0.87	0.16	45,45,45,45	0
57	MG	BA	3660	1/1	0.87	0.19	60,60,60,60	0
57	MG	AA	1630	1/1	0.87	0.14	53,53,53,53	0
57	MG	DA	3067	1/1	0.87	0.14	63,63,63,63	0
57	MG	BA	3024	1/1	0.87	0.23	58,58,58,58	0
57	MG	CA	3087	1/1	0.87	0.07	57,57,57,57	0
57	MG	BA	3245	1/1	0.87	0.32	59,59,59,59	0
57	MG	AA	1771	1/1	0.87	0.15	75,75,75,75	0
57	MG	BA	3549	1/1	0.87	0.11	66,66,66,66	0
57	MG	AA	1666	1/1	0.87	0.33	63,63,63,63	0
57	MG	BA	3561	1/1	0.87	0.26	34,34,34,34	0
57	MG	DA	3600	1/1	0.87	0.13	72,72,72,72	0
57	MG	DA	3603	1/1	0.87	0.06	65,65,65,65	0
57	MG	BA	3564	1/1	0.87	0.09	44,44,44,44	0
57	MG	AA	1651	1/1	0.87	0.25	58,58,58,58	0
57	MG	CA	3110	1/1	0.87	0.12	63,63,63,63	0
57	MG	CA	3111	1/1	0.87	0.15	72,72,72,72	0
57	MG	DA	3106	1/1	0.87	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	B2	3001	1/1	0.87	0.25	53,53,53,53	0
57	MG	DA	3338	1/1	0.87	0.07	44,44,44,44	0
57	MG	AA	1614	1/1	0.87	0.19	75,75,75,75	0
57	MG	AA	1788	1/1	0.87	0.09	75,75,75,75	0
57	MG	DA	3623	1/1	0.87	0.10	45,45,45,45	0
57	MG	BA	3106	1/1	0.87	0.25	52,52,52,52	0
57	MG	AA	1632	1/1	0.87	0.11	48,48,48,48	0
57	MG	DA	3626	1/1	0.87	0.11	81,81,81,81	0
57	MG	BA	3588	1/1	0.87	0.09	43,43,43,43	0
57	MG	BA	3441	1/1	0.87	0.20	39,39,39,39	0
57	MG	BA	3212	1/1	0.87	0.21	57,57,57,57	0
57	MG	BA	3597	1/1	0.87	0.20	55,55,55,55	0
57	MG	AA	1680	1/1	0.87	0.17	51,51,51,51	0
57	MG	AA	1755	1/1	0.87	0.09	80,80,80,80	0
57	MG	BA	3604	1/1	0.87	0.20	43,43,43,43	0
57	MG	AA	1634	1/1	0.87	0.15	64,64,64,64	0
57	MG	BA	3230	1/1	0.87	0.33	58,58,58,58	0
57	MG	DA	3150	1/1	0.87	0.16	50,50,50,50	0
57	MG	BA	3127	1/1	0.87	0.30	45,45,45,45	0
57	MG	BA	3732	1/1	0.87	0.24	33,33,33,33	0
57	MG	BA	3484	1/1	0.87	0.13	40,40,40,40	0
57	MG	DA	3010	1/1	0.87	0.10	41,41,41,41	0
57	MG	DD	302	1/1	0.87	0.14	49,49,49,49	0
57	MG	DA	3442	1/1	0.87	0.15	64,64,64,64	0
57	MG	DA	3452	1/1	0.87	0.11	45,45,45,45	0
57	MG	BA	3140	1/1	0.87	0.12	58,58,58,58	0
57	MG	DP	201	1/1	0.87	0.21	69,69,69,69	0
57	MG	BA	3745	1/1	0.87	0.24	61,61,61,61	0
57	MG	DA	3190	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	3023	1/1	0.87	0.14	58,58,58,58	0
60	K	AX	3001	1/1	0.87	0.13	77,77,77,77	0
57	MG	DA	3445	1/1	0.88	0.13	52,52,52,52	0
57	MG	AN	503	1/1	0.88	0.18	52,52,52,52	0
57	MG	DA	3455	1/1	0.88	0.09	64,64,64,64	0
57	MG	BA	3638	1/1	0.88	0.17	65,65,65,65	0
57	MG	BA	3642	1/1	0.88	0.18	64,64,64,64	0
57	MG	DA	3194	1/1	0.88	0.16	48,48,48,48	0
57	MG	BA	3129	1/1	0.88	0.16	54,54,54,54	0
57	MG	BA	3763	1/1	0.88	0.15	44,44,44,44	0
57	MG	DA	3200	1/1	0.88	0.16	41,41,41,41	0
57	MG	DA	3201	1/1	0.88	0.10	52,52,52,52	0
57	MG	BA	3767	1/1	0.88	0.23	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	DA	3494	1/1	0.88	0.12	45,45,45,45	0
57	MG	BA	3131	1/1	0.88	0.19	44,44,44,44	0
57	MG	DA	3208	1/1	0.88	0.16	54,54,54,54	0
57	MG	DA	3218	1/1	0.88	0.17	52,52,52,52	0
57	MG	DA	3508	1/1	0.88	0.18	57,57,57,57	0
57	MG	BA	3506	1/1	0.88	0.22	61,61,61,61	0
57	MG	DA	3051	1/1	0.88	0.13	44,44,44,44	0
57	MG	BA	3794	1/1	0.88	0.13	37,37,37,37	0
57	MG	BA	3508	1/1	0.88	0.21	20,20,20,20	0
57	MG	BA	3139	1/1	0.88	0.22	44,44,44,44	0
57	MG	DA	3250	1/1	0.88	0.08	50,50,50,50	0
57	MG	DA	3522	1/1	0.88	0.11	51,51,51,51	0
57	MG	BA	3515	1/1	0.88	0.17	27,27,27,27	0
57	MG	BA	3666	1/1	0.88	0.26	74,74,74,74	0
57	MG	DA	3541	1/1	0.88	0.10	59,59,59,59	0
57	MG	BA	3014	1/1	0.88	0.14	35,35,35,35	0
57	MG	DA	3271	1/1	0.88	0.16	30,30,30,30	0
57	MG	BB	3006	1/1	0.88	0.14	62,62,62,62	0
57	MG	BA	3065	1/1	0.88	0.31	50,50,50,50	0
57	MG	AA	1704	1/1	0.88	0.13	57,57,57,57	0
57	MG	BA	3359	1/1	0.88	0.06	60,60,60,60	0
57	MG	DA	3577	1/1	0.88	0.07	60,60,60,60	0
57	MG	DA	3578	1/1	0.88	0.14	43,43,43,43	0
57	MG	DA	3580	1/1	0.88	0.21	62,62,62,62	0
57	MG	BA	3073	1/1	0.88	0.16	32,32,32,32	0
57	MG	AA	1707	1/1	0.88	0.12	57,57,57,57	0
57	MG	DA	3289	1/1	0.88	0.16	52,52,52,52	0
57	MG	AA	1747	1/1	0.88	0.15	55,55,55,55	0
57	MG	DA	3306	1/1	0.88	0.28	65,65,65,65	0
57	MG	DA	3311	1/1	0.88	0.14	46,46,46,46	0
57	MG	BA	3088	1/1	0.88	0.17	43,43,43,43	0
57	MG	BA	3381	1/1	0.88	0.11	49,49,49,49	0
57	MG	B0	3002	1/1	0.88	0.21	63,63,63,63	0
57	MG	BA	3383	1/1	0.88	0.16	37,37,37,37	0
57	MG	BA	3254	1/1	0.88	0.16	33,33,33,33	0
57	MG	DA	3324	1/1	0.88	0.10	54,54,54,54	0
57	MG	BA	3255	1/1	0.88	0.21	55,55,55,55	0
57	MG	BA	3418	1/1	0.88	0.21	38,38,38,38	0
57	MG	AA	1633	1/1	0.88	0.27	59,59,59,59	0
57	MG	CA	3129	1/1	0.88	0.13	69,69,69,69	0
57	MG	DA	3341	1/1	0.88	0.12	55,55,55,55	0
57	MG	DA	3347	1/1	0.88	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	AX	3008	1/1	0.88	0.15	76,76,76,76	0
57	MG	AX	3010	1/1	0.88	0.40	68,68,68,68	0
57	MG	DA	3633	1/1	0.88	0.10	58,58,58,58	0
57	MG	BA	3594	1/1	0.88	0.14	45,45,45,45	0
57	MG	DA	3375	1/1	0.88	0.10	57,57,57,57	0
57	MG	AA	1621	1/1	0.88	0.14	44,44,44,44	0
57	MG	CA	3153	1/1	0.88	0.11	69,69,69,69	0
57	MG	DA	3384	1/1	0.88	0.10	38,38,38,38	0
57	MG	CA	3007	1/1	0.88	0.12	51,51,51,51	0
57	MG	AA	1640	1/1	0.88	0.22	54,54,54,54	0
57	MG	BA	3203	1/1	0.88	0.34	61,61,61,61	0
57	MG	DA	3663	1/1	0.88	0.15	73,73,73,73	0
57	MG	BA	3275	1/1	0.88	0.16	66,66,66,66	0
57	MG	AA	1603	1/1	0.88	0.15	64,64,64,64	0
57	MG	DB	3005	1/1	0.88	0.12	68,68,68,68	0
57	MG	AY	3001	1/1	0.88	0.32	63,63,63,63	0
57	MG	AF	3001	1/1	0.88	0.18	50,50,50,50	0
57	MG	DB	3012	1/1	0.88	0.24	66,66,66,66	0
57	MG	AA	1605	1/1	0.88	0.15	50,50,50,50	0
57	MG	BA	3313	1/1	0.88	0.19	38,38,38,38	0
57	MG	CA	3020	1/1	0.88	0.20	45,45,45,45	0
57	MG	CA	3022	1/1	0.88	0.23	76,76,76,76	0
57	MG	CA	3030	1/1	0.88	0.07	74,74,74,74	0
57	MG	DA	3427	1/1	0.88	0.15	47,47,47,47	0
57	MG	DU	201	1/1	0.88	0.57	58,58,58,58	0
57	MG	DV	201	1/1	0.88	0.51	58,58,58,58	0
57	MG	DA	3017	1/1	0.88	0.12	59,59,59,59	0
57	MG	DA	3187	1/1	0.88	0.20	47,47,47,47	0
57	MG	DA	3444	1/1	0.88	0.21	44,44,44,44	0
57	MG	BA	3325	1/1	0.89	0.15	45,45,45,45	0
57	MG	BA	3248	1/1	0.89	0.15	67,67,67,67	0
57	MG	DA	3471	1/1	0.89	0.31	54,54,54,54	0
57	MG	DA	3480	1/1	0.89	0.12	58,58,58,58	0
57	MG	DA	3486	1/1	0.89	0.13	57,57,57,57	0
57	MG	BA	3329	1/1	0.89	0.10	60,60,60,60	0
57	MG	DA	3021	1/1	0.89	0.17	50,50,50,50	0
57	MG	CA	3023	1/1	0.89	0.10	39,39,39,39	0
57	MG	DA	3212	1/1	0.89	0.23	62,62,62,62	0
57	MG	CA	3029	1/1	0.89	0.11	50,50,50,50	0
57	MG	DA	3219	1/1	0.89	0.16	50,50,50,50	0
57	MG	BA	3735	1/1	0.89	0.23	50,50,50,50	0
57	MG	DA	3232	1/1	0.89	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AM	3002	1/1	0.89	0.12	68,68,68,68	0
57	MG	BA	3609	1/1	0.89	0.20	56,56,56,56	0
57	MG	CA	3034	1/1	0.89	0.23	66,66,66,66	0
57	MG	DA	3237	1/1	0.89	0.12	59,59,59,59	0
57	MG	DA	3515	1/1	0.89	0.13	55,55,55,55	0
57	MG	AA	1708	1/1	0.89	0.19	60,60,60,60	0
57	MG	DA	3239	1/1	0.89	0.14	49,49,49,49	0
57	MG	BA	3079	1/1	0.89	0.37	58,58,58,58	0
57	MG	BA	3622	1/1	0.89	0.21	43,43,43,43	0
57	MG	BA	3491	1/1	0.89	0.22	56,56,56,56	0
57	MG	BA	3766	1/1	0.89	0.16	47,47,47,47	0
57	MG	BA	3138	1/1	0.89	0.16	43,43,43,43	0
57	MG	BA	3501	1/1	0.89	0.14	42,42,42,42	0
57	MG	DA	3064	1/1	0.89	0.11	46,46,46,46	0
57	MG	BA	3222	1/1	0.89	0.14	42,42,42,42	0
57	MG	DA	3552	1/1	0.89	0.13	34,34,34,34	0
57	MG	DA	3558	1/1	0.89	0.11	48,48,48,48	0
57	MG	AY	3003	1/1	0.89	0.15	79,79,79,79	0
57	MG	AA	1662	1/1	0.89	0.20	58,58,58,58	0
57	MG	DA	3068	1/1	0.89	0.19	53,53,53,53	0
57	MG	CA	3063	1/1	0.89	0.23	65,65,65,65	0
57	MG	DA	3291	1/1	0.89	0.16	36,36,36,36	0
57	MG	CA	3065	1/1	0.89	0.14	59,59,59,59	0
57	MG	BA	3646	1/1	0.89	0.17	50,50,50,50	0
57	MG	BA	3266	1/1	0.89	0.10	44,44,44,44	0
57	MG	CA	3077	1/1	0.89	0.21	60,60,60,60	0
57	MG	BA	3367	1/1	0.89	0.22	52,52,52,52	0
57	MG	DA	3601	1/1	0.89	0.10	55,55,55,55	0
57	MG	BA	3513	1/1	0.89	0.34	50,50,50,50	0
57	MG	AA	1652	1/1	0.89	0.23	62,62,62,62	0
57	MG	DA	3095	1/1	0.89	0.16	60,60,60,60	0
57	MG	BA	3522	1/1	0.89	0.16	44,44,44,44	0
57	MG	AA	1712	1/1	0.89	0.21	69,69,69,69	0
57	MG	BA	3379	1/1	0.89	0.18	35,35,35,35	0
57	MG	BA	3529	1/1	0.89	0.25	24,24,24,24	0
57	MG	AA	1759	1/1	0.89	0.15	55,55,55,55	0
57	MG	BA	3536	1/1	0.89	0.14	32,32,32,32	0
57	MG	BP	3002	1/1	0.89	0.14	60,60,60,60	0
57	MG	BA	3274	1/1	0.89	0.27	66,66,66,66	0
57	MG	BA	3389	1/1	0.89	0.21	37,37,37,37	0
57	MG	DA	3358	1/1	0.89	0.19	50,50,50,50	0
57	MG	BA	3554	1/1	0.89	0.09	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	CA	3119	1/1	0.89	0.12	59,59,59,59	0
57	MG	BA	3390	1/1	0.89	0.10	31,31,31,31	0
57	MG	DA	3377	1/1	0.89	0.11	50,50,50,50	0
57	MG	DA	3125	1/1	0.89	0.14	56,56,56,56	0
57	MG	DA	3129	1/1	0.89	0.20	56,56,56,56	0
57	MG	BA	3558	1/1	0.89	0.13	51,51,51,51	0
57	MG	DA	3645	1/1	0.89	0.11	64,64,64,64	0
57	MG	DA	3393	1/1	0.89	0.16	37,37,37,37	0
57	MG	DA	3132	1/1	0.89	0.13	43,43,43,43	0
57	MG	BA	3689	1/1	0.89	0.19	59,59,59,59	0
57	MG	BA	3406	1/1	0.89	0.10	56,56,56,56	0
57	MG	CA	3137	1/1	0.89	0.15	78,78,78,78	0
57	MG	BA	3407	1/1	0.89	0.17	32,32,32,32	0
57	MG	AA	1693	1/1	0.89	0.20	76,76,76,76	0
57	MG	AA	1626	1/1	0.89	0.21	59,59,59,59	0
57	MG	CA	3148	1/1	0.89	0.15	68,68,68,68	0
57	MG	BA	3705	1/1	0.89	0.14	59,59,59,59	0
57	MG	DA	3422	1/1	0.89	0.24	62,62,62,62	0
57	MG	DB	3011	1/1	0.89	0.26	67,67,67,67	0
57	MG	AA	1671	1/1	0.89	0.10	60,60,60,60	0
57	MG	BA	3574	1/1	0.89	0.15	42,42,42,42	0
57	MG	CA	3008	1/1	0.89	0.32	47,47,47,47	0
57	MG	AA	1739	1/1	0.89	0.22	72,72,72,72	0
57	MG	AX	3015	1/1	0.89	0.29	51,51,51,51	0
57	MG	BA	3295	1/1	0.89	0.22	23,23,23,23	0
57	MG	DP	202	1/1	0.89	0.09	49,49,49,49	0
57	MG	BA	3299	1/1	0.89	0.21	60,60,60,60	0
57	MG	DA	3451	1/1	0.89	0.08	55,55,55,55	0
57	MG	CW	3001	1/1	0.89	0.19	66,66,66,66	0
57	MG	BA	3443	1/1	0.89	0.18	59,59,59,59	0
57	MG	BA	3125	1/1	0.89	0.25	38,38,38,38	0
57	MG	BA	3194	1/1	0.89	0.25	39,39,39,39	0
57	MG	DA	3482	1/1	0.90	0.15	60,60,60,60	0
57	MG	DA	3485	1/1	0.90	0.09	56,56,56,56	0
57	MG	BA	3264	1/1	0.90	0.23	51,51,51,51	0
57	MG	DA	3063	1/1	0.90	0.11	47,47,47,47	0
57	MG	CA	3089	1/1	0.90	0.23	74,74,74,74	0
57	MG	BV	204	1/1	0.90	0.26	39,39,39,39	0
57	MG	DA	3243	1/1	0.90	0.12	48,48,48,48	0
57	MG	DA	3244	1/1	0.90	0.27	55,55,55,55	0
57	MG	BA	3414	1/1	0.90	0.20	54,54,54,54	0
57	MG	BA	3704	1/1	0.90	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	3099	1/1	0.90	0.09	64,64,64,64	0
57	MG	DA	3505	1/1	0.90	0.08	51,51,51,51	0
57	MG	BA	3518	1/1	0.90	0.20	46,46,46,46	0
57	MG	BA	3333	1/1	0.90	0.14	57,57,57,57	0
57	MG	DA	3072	1/1	0.90	0.16	47,47,47,47	0
57	MG	DA	3078	1/1	0.90	0.09	47,47,47,47	0
57	MG	BA	3115	1/1	0.90	0.23	33,33,33,33	0
57	MG	BA	3117	1/1	0.90	0.64	38,38,38,38	0
57	MG	BA	3619	1/1	0.90	0.14	28,28,28,28	0
57	MG	BA	3526	1/1	0.90	0.26	41,41,41,41	0
57	MG	BA	3625	1/1	0.90	0.14	33,33,33,33	0
57	MG	DA	3523	1/1	0.90	0.14	39,39,39,39	0
57	MG	DA	3091	1/1	0.90	0.20	54,54,54,54	0
57	MG	DA	3532	1/1	0.90	0.13	48,48,48,48	0
57	MG	DA	3533	1/1	0.90	0.14	56,56,56,56	0
57	MG	DA	3296	1/1	0.90	0.10	60,60,60,60	0
57	MG	BA	3631	1/1	0.90	0.26	46,46,46,46	0
57	MG	BA	3429	1/1	0.90	0.26	50,50,50,50	0
57	MG	CA	3121	1/1	0.90	0.13	67,67,67,67	0
57	MG	AA	1635	1/1	0.90	0.15	65,65,65,65	0
57	MG	CA	3123	1/1	0.90	0.32	61,61,61,61	0
57	MG	DA	3556	1/1	0.90	0.13	55,55,55,55	0
57	MG	BA	3636	1/1	0.90	0.19	66,66,66,66	0
57	MG	CA	3126	1/1	0.90	0.09	45,45,45,45	0
57	MG	DA	3110	1/1	0.90	0.10	49,49,49,49	0
57	MG	DA	3570	1/1	0.90	0.16	43,43,43,43	0
57	MG	DA	3572	1/1	0.90	0.19	65,65,65,65	0
57	MG	BA	3532	1/1	0.90	0.14	55,55,55,55	0
57	MG	BA	3166	1/1	0.90	0.19	33,33,33,33	0
57	MG	CA	3131	1/1	0.90	0.24	69,69,69,69	0
57	MG	CA	3135	1/1	0.90	0.06	59,59,59,59	0
57	MG	DA	3590	1/1	0.90	0.22	51,51,51,51	0
57	MG	DA	3336	1/1	0.90	0.09	49,49,49,49	0
57	MG	BA	3171	1/1	0.90	0.32	35,35,35,35	0
57	MG	BA	3546	1/1	0.90	0.14	68,68,68,68	0
57	MG	CA	3141	1/1	0.90	0.14	62,62,62,62	0
57	MG	BA	3273	1/1	0.90	0.21	45,45,45,45	0
57	MG	BA	3063	1/1	0.90	0.33	47,47,47,47	0
57	MG	BA	3096	1/1	0.90	0.18	60,60,60,60	0
57	MG	AA	1816	1/1	0.90	0.20	59,59,59,59	0
57	MG	BA	3761	1/1	0.90	0.10	36,36,36,36	0
57	MG	AA	1619	1/1	0.90	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3765	1/1	0.90	0.24	49,49,49,49	0
57	MG	BA	3658	1/1	0.90	0.12	61,61,61,61	0
57	MG	CA	3026	1/1	0.90	0.21	66,66,66,66	0
57	MG	DA	3388	1/1	0.90	0.14	47,47,47,47	0
57	MG	CA	3027	1/1	0.90	0.19	65,65,65,65	0
57	MG	BA	3372	1/1	0.90	0.12	40,40,40,40	0
57	MG	DA	3158	1/1	0.90	0.39	56,56,56,56	0
57	MG	CJ	5001	1/1	0.90	0.18	77,77,77,77	0
57	MG	BA	3769	1/1	0.90	0.20	47,47,47,47	0
57	MG	DA	3399	1/1	0.90	0.15	59,59,59,59	0
57	MG	CX	3002	1/1	0.90	0.14	67,67,67,67	0
57	MG	DA	3406	1/1	0.90	0.17	70,70,70,70	0
57	MG	AA	1687	1/1	0.90	0.21	46,46,46,46	0
57	MG	DA	3413	1/1	0.90	0.20	62,62,62,62	0
57	MG	BA	3786	1/1	0.90	0.16	51,51,51,51	0
57	MG	DA	3416	1/1	0.90	0.14	52,52,52,52	0
57	MG	AA	1674	1/1	0.90	0.20	58,58,58,58	0
57	MG	AA	1768	1/1	0.90	0.11	53,53,53,53	0
57	MG	BA	3803	1/1	0.90	0.34	55,55,55,55	0
57	MG	DA	3651	1/1	0.90	0.12	48,48,48,48	0
57	MG	BA	3573	1/1	0.90	0.19	41,41,41,41	0
57	MG	AA	1756	1/1	0.90	0.33	45,45,45,45	0
57	MG	DA	3658	1/1	0.90	0.49	62,62,62,62	0
57	MG	BA	3497	1/1	0.90	0.17	50,50,50,50	0
57	MG	BA	3217	1/1	0.90	0.11	50,50,50,50	0
57	MG	BA	3147	1/1	0.90	0.20	36,36,36,36	0
57	MG	DA	3439	1/1	0.90	0.12	40,40,40,40	0
57	MG	BA	3404	1/1	0.90	0.34	59,59,59,59	0
57	MG	BB	3009	1/1	0.90	0.09	57,57,57,57	0
57	MG	BB	3016	1/1	0.90	0.14	34,34,34,34	0
57	MG	DA	3446	1/1	0.90	0.14	50,50,50,50	0
57	MG	DA	3448	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3110	1/1	0.90	0.18	36,36,36,36	0
57	MG	DA	3211	1/1	0.90	0.21	51,51,51,51	0
57	MG	BA	3087	1/1	0.90	0.38	43,43,43,43	0
57	MG	DA	3049	1/1	0.90	0.10	47,47,47,47	0
57	MG	DA	3459	1/1	0.90	0.14	49,49,49,49	0
57	MG	DQ	3002	1/1	0.90	0.16	47,47,47,47	0
57	MG	BA	3692	1/1	0.90	0.12	58,58,58,58	0
57	MG	BA	3408	1/1	0.90	0.17	51,51,51,51	0
57	MG	DA	3055	1/1	0.90	0.14	53,53,53,53	0
57	MG	BA	3694	1/1	0.90	0.19	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	3476	1/1	0.90	0.08	45,45,45,45	0
57	MG	BA	3410	1/1	0.90	0.16	55,55,55,55	0
57	MG	DA	3181	1/1	0.91	0.12	49,49,49,49	0
57	MG	CA	3160	1/1	0.91	0.14	73,73,73,73	0
57	MG	AA	1717	1/1	0.91	0.16	75,75,75,75	0
57	MG	BA	3728	1/1	0.91	0.16	52,52,52,52	0
57	MG	BA	3615	1/1	0.91	0.13	71,71,71,71	0
57	MG	CA	3166	1/1	0.91	0.15	55,55,55,55	0
57	MG	BA	3618	1/1	0.91	0.15	35,35,35,35	0
57	MG	DA	3197	1/1	0.91	0.20	59,59,59,59	0
57	MG	AA	1753	1/1	0.91	0.20	55,55,55,55	0
57	MG	AA	1781	1/1	0.91	0.10	59,59,59,59	0
57	MG	DA	3479	1/1	0.91	0.10	42,42,42,42	0
57	MG	BA	3737	1/1	0.91	0.17	34,34,34,34	0
57	MG	BA	3516	1/1	0.91	0.24	46,46,46,46	0
57	MG	BA	3740	1/1	0.91	0.19	65,65,65,65	0
57	MG	CA	3021	1/1	0.91	0.10	61,61,61,61	0
57	MG	BA	3517	1/1	0.91	0.23	33,33,33,33	0
57	MG	AA	1721	1/1	0.91	0.16	57,57,57,57	0
57	MG	AT	3001	1/1	0.91	0.13	63,63,63,63	0
57	MG	BA	3163	1/1	0.91	0.49	55,55,55,55	0
57	MG	BA	3524	1/1	0.91	0.21	33,33,33,33	0
57	MG	BA	3323	1/1	0.91	0.19	57,57,57,57	0
57	MG	AA	1609	1/1	0.91	0.13	63,63,63,63	0
57	MG	DA	3030	1/1	0.91	0.17	44,44,44,44	0
57	MG	DA	3031	1/1	0.91	0.14	42,42,42,42	0
57	MG	BA	3008	1/1	0.91	0.14	28,28,28,28	0
57	MG	DA	3511	1/1	0.91	0.10	44,44,44,44	0
57	MG	BA	3645	1/1	0.91	0.18	47,47,47,47	0
57	MG	DA	3034	1/1	0.91	0.10	42,42,42,42	0
57	MG	DA	3241	1/1	0.91	0.13	55,55,55,55	0
57	MG	BA	3419	1/1	0.91	0.20	25,25,25,25	0
57	MG	BA	3647	1/1	0.91	0.08	53,53,53,53	0
57	MG	CA	3042	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3781	1/1	0.91	0.16	56,56,56,56	0
57	MG	BA	3531	1/1	0.91	0.14	60,60,60,60	0
57	MG	BA	3420	1/1	0.91	0.18	25,25,25,25	0
57	MG	DA	3524	1/1	0.91	0.17	52,52,52,52	0
57	MG	DA	3259	1/1	0.91	0.10	42,42,42,42	0
57	MG	DA	3260	1/1	0.91	0.17	39,39,39,39	0
57	MG	DA	3261	1/1	0.91	0.16	39,39,39,39	0
57	MG	BA	3535	1/1	0.91	0.20	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	3796	1/1	0.91	0.17	47,47,47,47	0
57	MG	CA	3055	1/1	0.91	0.18	63,63,63,63	0
57	MG	BA	3802	1/1	0.91	0.23	46,46,46,46	0
57	MG	AA	1729	1/1	0.91	0.15	35,35,35,35	0
57	MG	DA	3550	1/1	0.91	0.04	60,60,60,60	0
57	MG	AX	3004	1/1	0.91	0.13	61,61,61,61	0
57	MG	DA	3554	1/1	0.91	0.09	50,50,50,50	0
57	MG	BA	3545	1/1	0.91	0.18	28,28,28,28	0
57	MG	DA	3557	1/1	0.91	0.19	57,57,57,57	0
57	MG	BA	3435	1/1	0.91	0.22	53,53,53,53	0
57	MG	BA	3814	1/1	0.91	0.28	39,39,39,39	0
57	MG	DA	3565	1/1	0.91	0.04	52,52,52,52	0
57	MG	DA	3292	1/1	0.91	0.11	29,29,29,29	0
57	MG	BA	3252	1/1	0.91	0.19	36,36,36,36	0
57	MG	CA	3076	1/1	0.91	0.20	77,77,77,77	0
57	MG	DA	3069	1/1	0.91	0.08	43,43,43,43	0
57	MG	DA	3308	1/1	0.91	0.21	62,62,62,62	0
57	MG	BA	3553	1/1	0.91	0.19	45,45,45,45	0
57	MG	CA	3081	1/1	0.91	0.16	44,44,44,44	0
57	MG	CA	3082	1/1	0.91	0.13	66,66,66,66	0
57	MG	AA	1705	1/1	0.91	0.23	70,70,70,70	0
57	MG	BA	3122	1/1	0.91	0.15	35,35,35,35	0
57	MG	DA	3593	1/1	0.91	0.08	60,60,60,60	0
57	MG	DA	3081	1/1	0.91	0.11	51,51,51,51	0
57	MG	DA	3084	1/1	0.91	0.17	44,44,44,44	0
57	MG	DA	3327	1/1	0.91	0.15	45,45,45,45	0
57	MG	DA	3328	1/1	0.91	0.21	42,42,42,42	0
57	MG	BB	3013	1/1	0.91	0.21	39,39,39,39	0
57	MG	BA	3191	1/1	0.91	0.19	40,40,40,40	0
57	MG	BB	3017	1/1	0.91	0.16	81,81,81,81	0
57	MG	BA	3446	1/1	0.91	0.09	59,59,59,59	0
57	MG	CA	3095	1/1	0.91	0.13	71,71,71,71	0
57	MG	DA	3614	1/1	0.91	0.14	55,55,55,55	0
57	MG	BA	3452	1/1	0.91	0.15	56,56,56,56	0
57	MG	DA	3344	1/1	0.91	0.14	38,38,38,38	0
57	MG	CA	3100	1/1	0.91	0.15	59,59,59,59	0
57	MG	BD	3003	1/1	0.91	0.30	37,37,37,37	0
57	MG	CA	3103	1/1	0.91	0.15	73,73,73,73	0
57	MG	BA	3685	1/1	0.91	0.20	61,61,61,61	0
57	MG	DA	3361	1/1	0.91	0.08	33,33,33,33	0
57	MG	DA	3368	1/1	0.91	0.09	67,67,67,67	0
57	MG	BF	306	1/1	0.91	0.33	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3107	1/1	0.91	0.11	61,61,61,61	0
57	MG	AA	1798	1/1	0.91	0.11	62,62,62,62	0
57	MG	BA	3358	1/1	0.91	0.18	52,52,52,52	0
57	MG	BN	3001	1/1	0.91	0.15	48,48,48,48	0
57	MG	BA	3126	1/1	0.91	0.23	36,36,36,36	0
57	MG	DA	3639	1/1	0.91	0.18	59,59,59,59	0
57	MG	BA	3470	1/1	0.91	0.11	57,57,57,57	0
57	MG	BA	3019	1/1	0.91	0.28	54,54,54,54	0
57	MG	BA	3128	1/1	0.91	0.19	42,42,42,42	0
57	MG	BW	3004	1/1	0.91	0.20	45,45,45,45	0
57	MG	BX	3001	1/1	0.91	0.35	44,44,44,44	0
57	MG	BY	502	1/1	0.91	0.24	46,46,46,46	0
57	MG	DA	3127	1/1	0.91	0.10	52,52,52,52	0
57	MG	BA	3207	1/1	0.91	0.18	36,36,36,36	0
57	MG	DA	3403	1/1	0.91	0.09	49,49,49,49	0
57	MG	BA	3209	1/1	0.91	0.24	48,48,48,48	0
57	MG	DA	3409	1/1	0.91	0.12	54,54,54,54	0
57	MG	AA	1801	1/1	0.91	0.09	71,71,71,71	0
57	MG	B7	103	1/1	0.91	0.30	40,40,40,40	0
57	MG	AA	1643	1/1	0.91	0.21	58,58,58,58	0
57	MG	BA	3378	1/1	0.91	0.24	39,39,39,39	0
57	MG	BA	3132	1/1	0.91	0.18	50,50,50,50	0
57	MG	AA	1639	1/1	0.91	0.07	54,54,54,54	0
57	MG	BA	3036	1/1	0.91	0.12	56,56,56,56	0
57	MG	BA	3388	1/1	0.91	0.20	25,25,25,25	0
57	MG	DA	3154	1/1	0.91	0.08	51,51,51,51	0
57	MG	DO	202	1/1	0.91	0.12	60,60,60,60	0
57	MG	AA	1814	1/1	0.91	0.15	57,57,57,57	0
57	MG	DA	3159	1/1	0.91	0.11	62,62,62,62	0
57	MG	DA	3160	1/1	0.91	0.34	62,62,62,62	0
57	MG	CA	3151	1/1	0.91	0.10	64,64,64,64	0
57	MG	CA	3152	1/1	0.91	0.10	71,71,71,71	0
57	MG	BA	3507	1/1	0.91	0.26	43,43,43,43	0
57	MG	D0	101	1/1	0.91	0.13	71,71,71,71	0
57	MG	AA	1714	1/1	0.91	0.20	56,56,56,56	0
59	ZN	CN	501	1/1	0.91	0.06	100,100,100,100	0
57	MG	BA	3613	1/1	0.91	0.23	53,53,53,53	0
57	MG	DA	3179	1/1	0.91	0.06	59,59,59,59	0
57	MG	DA	3053	1/1	0.92	0.13	47,47,47,47	0
57	MG	DA	3470	1/1	0.92	0.08	61,61,61,61	0
57	MG	AA	1692	1/1	0.92	0.15	65,65,65,65	0
57	MG	BA	3563	1/1	0.92	0.12	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	DA	3478	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3134	1/1	0.92	0.19	40,40,40,40	0
57	MG	DA	3236	1/1	0.92	0.13	55,55,55,55	0
57	MG	DA	3481	1/1	0.92	0.13	40,40,40,40	0
57	MG	BA	3682	1/1	0.92	0.14	60,60,60,60	0
57	MG	BA	3460	1/1	0.92	0.11	52,52,52,52	0
57	MG	BB	3022	1/1	0.92	0.20	60,60,60,60	0
57	MG	BA	3137	1/1	0.92	0.25	52,52,52,52	0
57	MG	DA	3242	1/1	0.92	0.09	52,52,52,52	0
57	MG	BA	3364	1/1	0.92	0.15	47,47,47,47	0
57	MG	BA	3268	1/1	0.92	0.22	54,54,54,54	0
57	MG	BF	307	1/1	0.92	0.13	34,34,34,34	0
57	MG	BA	3483	1/1	0.92	0.17	44,44,44,44	0
57	MG	BF	311	1/1	0.92	0.12	52,52,52,52	0
57	MG	DA	3256	1/1	0.92	0.16	51,51,51,51	0
57	MG	BA	3001	1/1	0.92	0.15	43,43,43,43	0
57	MG	DA	3506	1/1	0.92	0.08	55,55,55,55	0
57	MG	BA	3051	1/1	0.92	0.23	37,37,37,37	0
57	MG	DA	3075	1/1	0.92	0.14	55,55,55,55	0
57	MG	DA	3077	1/1	0.92	0.14	38,38,38,38	0
57	MG	BA	3587	1/1	0.92	0.11	46,46,46,46	0
57	MG	BA	3219	1/1	0.92	0.50	58,58,58,58	0
57	MG	DA	3080	1/1	0.92	0.10	49,49,49,49	0
57	MG	BA	3375	1/1	0.92	0.22	39,39,39,39	0
57	MG	AA	1799	1/1	0.92	0.11	78,78,78,78	0
57	MG	BA	3141	1/1	0.92	0.32	38,38,38,38	0
57	MG	BA	3500	1/1	0.92	0.20	57,57,57,57	0
57	MG	AW	3002	1/1	0.92	0.14	79,79,79,79	0
57	MG	AA	1754	1/1	0.92	0.15	58,58,58,58	0
57	MG	DA	3528	1/1	0.92	0.14	36,36,36,36	0
57	MG	DA	3090	1/1	0.92	0.31	50,50,50,50	0
57	MG	CA	3113	1/1	0.92	0.16	47,47,47,47	0
57	MG	DA	3298	1/1	0.92	0.20	55,55,55,55	0
57	MG	BZ	302	1/1	0.92	0.17	60,60,60,60	0
57	MG	DA	3094	1/1	0.92	0.06	39,39,39,39	0
57	MG	AA	1688	1/1	0.92	0.21	66,66,66,66	0
57	MG	DA	3543	1/1	0.92	0.14	64,64,64,64	0
57	MG	DA	3310	1/1	0.92	0.13	35,35,35,35	0
57	MG	DA	3096	1/1	0.92	0.19	68,68,68,68	0
57	MG	BA	3010	1/1	0.92	0.18	53,53,53,53	0
57	MG	B4	502	1/1	0.92	0.09	70,70,70,70	0
57	MG	DA	3553	1/1	0.92	0.07	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3100	1/1	0.92	0.09	47,47,47,47	0
57	MG	AA	1778	1/1	0.92	0.09	51,51,51,51	0
57	MG	BA	3290	1/1	0.92	0.21	57,57,57,57	0
57	MG	BA	3400	1/1	0.92	0.24	39,39,39,39	0
57	MG	DA	3559	1/1	0.92	0.15	67,67,67,67	0
57	MG	BA	3512	1/1	0.92	0.21	23,23,23,23	0
57	MG	DA	3561	1/1	0.92	0.16	52,52,52,52	0
57	MG	BA	3156	1/1	0.92	0.23	35,35,35,35	0
57	MG	DA	3566	1/1	0.92	0.18	37,37,37,37	0
57	MG	BA	3729	1/1	0.92	0.14	46,46,46,46	0
57	MG	DA	3569	1/1	0.92	0.24	45,45,45,45	0
57	MG	BA	3296	1/1	0.92	0.16	55,55,55,55	0
57	MG	AA	1694	1/1	0.92	0.08	47,47,47,47	0
57	MG	BA	3300	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3575	1/1	0.92	0.08	56,56,56,56	0
57	MG	DA	3576	1/1	0.92	0.16	67,67,67,67	0
57	MG	BA	3623	1/1	0.92	0.17	43,43,43,43	0
57	MG	DA	3339	1/1	0.92	0.20	52,52,52,52	0
57	MG	DA	3119	1/1	0.92	0.26	50,50,50,50	0
57	MG	DA	3582	1/1	0.92	0.05	53,53,53,53	0
57	MG	BA	3305	1/1	0.92	0.15	46,46,46,46	0
57	MG	BA	3626	1/1	0.92	0.19	50,50,50,50	0
57	MG	BA	3309	1/1	0.92	0.17	65,65,65,65	0
57	MG	DA	3352	1/1	0.92	0.09	34,34,34,34	0
57	MG	BA	3741	1/1	0.92	0.11	57,57,57,57	0
57	MG	DA	3357	1/1	0.92	0.13	33,33,33,33	0
57	MG	AA	1815	1/1	0.92	0.14	47,47,47,47	0
57	MG	BA	3314	1/1	0.92	0.18	39,39,39,39	0
57	MG	DA	3362	1/1	0.92	0.24	42,42,42,42	0
57	MG	DA	3363	1/1	0.92	0.09	50,50,50,50	0
57	MG	DA	3366	1/1	0.92	0.12	44,44,44,44	0
57	MG	AA	1648	1/1	0.92	0.19	56,56,56,56	0
57	MG	AA	1691	1/1	0.92	0.27	62,62,62,62	0
57	MG	DA	3374	1/1	0.92	0.22	62,62,62,62	0
57	MG	BA	3528	1/1	0.92	0.20	36,36,36,36	0
57	MG	BA	3640	1/1	0.92	0.17	57,57,57,57	0
57	MG	BA	3641	1/1	0.92	0.18	68,68,68,68	0
57	MG	BA	3170	1/1	0.92	0.17	38,38,38,38	0
57	MG	DA	3146	1/1	0.92	0.14	54,54,54,54	0
57	MG	AA	1745	1/1	0.92	0.16	36,36,36,36	0
57	MG	DA	3151	1/1	0.92	0.13	37,37,37,37	0
57	MG	BA	3768	1/1	0.92	0.13	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	3426	1/1	0.92	0.15	46,46,46,46	0
57	MG	DA	3155	1/1	0.92	0.24	53,53,53,53	0
57	MG	DA	3630	1/1	0.92	0.14	69,69,69,69	0
57	MG	DA	3156	1/1	0.92	0.16	52,52,52,52	0
57	MG	BA	3773	1/1	0.92	0.21	32,32,32,32	0
57	MG	CT	3001	1/1	0.92	0.17	60,60,60,60	0
57	MG	BA	3124	1/1	0.92	0.28	57,57,57,57	0
57	MG	DA	3405	1/1	0.92	0.07	47,47,47,47	0
57	MG	DA	3643	1/1	0.92	0.07	54,54,54,54	0
57	MG	BA	3431	1/1	0.92	0.28	57,57,57,57	0
57	MG	DA	3407	1/1	0.92	0.08	58,58,58,58	0
57	MG	DA	3001	1/1	0.92	0.14	57,57,57,57	0
57	MG	BA	3025	1/1	0.92	0.18	43,43,43,43	0
57	MG	BA	3789	1/1	0.92	0.14	47,47,47,47	0
57	MG	CA	3035	1/1	0.92	0.11	53,53,53,53	0
57	MG	CA	3036	1/1	0.92	0.16	73,73,73,73	0
57	MG	BA	3790	1/1	0.92	0.54	66,66,66,66	0
57	MG	DA	3662	1/1	0.92	0.22	50,50,50,50	0
57	MG	DA	3186	1/1	0.92	0.15	49,49,49,49	0
57	MG	BA	3436	1/1	0.92	0.15	57,57,57,57	0
57	MG	DA	3189	1/1	0.92	0.23	47,47,47,47	0
57	MG	BA	3541	1/1	0.92	0.20	38,38,38,38	0
57	MG	DA	3425	1/1	0.92	0.16	51,51,51,51	0
57	MG	DA	3022	1/1	0.92	0.45	60,60,60,60	0
57	MG	BA	3542	1/1	0.92	0.16	44,44,44,44	0
57	MG	DA	3431	1/1	0.92	0.23	42,42,42,42	0
57	MG	AL	202	1/1	0.92	0.26	56,56,56,56	0
57	MG	DE	3005	1/1	0.92	0.14	35,35,35,35	0
57	MG	DF	301	1/1	0.92	0.31	48,48,48,48	0
57	MG	DA	3028	1/1	0.92	0.13	39,39,39,39	0
57	MG	BA	3086	1/1	0.92	0.33	42,42,42,42	0
57	MG	BA	3662	1/1	0.92	0.22	62,62,62,62	0
57	MG	BA	3806	1/1	0.92	0.17	43,43,43,43	0
57	MG	BA	3663	1/1	0.92	0.20	50,50,50,50	0
57	MG	AA	1726	1/1	0.92	0.16	58,58,58,58	0
57	MG	DQ	3001	1/1	0.92	0.08	50,50,50,50	0
57	MG	AA	1797	1/1	0.92	0.17	59,59,59,59	0
57	MG	BA	3091	1/1	0.92	0.40	42,42,42,42	0
57	MG	DR	3001	1/1	0.92	0.13	49,49,49,49	0
57	MG	DA	3454	1/1	0.92	0.12	43,43,43,43	0
57	MG	CA	3062	1/1	0.92	0.11	64,64,64,64	0
57	MG	BA	3348	1/1	0.92	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3458	1/1	0.92	0.10	41,41,41,41	0
57	MG	CA	3064	1/1	0.92	0.21	55,55,55,55	0
57	MG	BA	3672	1/1	0.92	0.25	44,44,44,44	0
57	MG	BA	3349	1/1	0.92	0.18	34,34,34,34	0
57	MG	DA	3464	1/1	0.93	0.30	54,54,54,54	0
57	MG	DA	3466	1/1	0.93	0.11	48,48,48,48	0
57	MG	AA	1790	1/1	0.93	0.08	81,81,81,81	0
57	MG	DA	3026	1/1	0.93	0.72	50,50,50,50	0
57	MG	DA	3222	1/1	0.93	0.23	58,58,58,58	0
57	MG	BA	3757	1/1	0.93	0.18	43,43,43,43	0
57	MG	BA	3066	1/1	0.93	0.24	58,58,58,58	0
57	MG	BA	3195	1/1	0.93	0.18	36,36,36,36	0
57	MG	AA	1791	1/1	0.93	0.08	54,54,54,54	0
57	MG	AA	1645	1/1	0.93	0.15	61,61,61,61	0
57	MG	AA	1675	1/1	0.93	0.24	61,61,61,61	0
57	MG	BA	3279	1/1	0.93	0.32	52,52,52,52	0
57	MG	AA	1765	1/1	0.93	0.13	65,65,65,65	0
57	MG	BA	3282	1/1	0.93	0.24	57,57,57,57	0
57	MG	BA	3403	1/1	0.93	0.29	33,33,33,33	0
57	MG	DA	3048	1/1	0.93	0.12	59,59,59,59	0
57	MG	BA	3775	1/1	0.93	0.33	39,39,39,39	0
57	MG	AA	1800	1/1	0.93	0.13	59,59,59,59	0
57	MG	DA	3249	1/1	0.93	0.08	65,65,65,65	0
57	MG	DA	3499	1/1	0.93	0.14	52,52,52,52	0
57	MG	BA	3081	1/1	0.93	0.30	48,48,48,48	0
57	MG	BA	3785	1/1	0.93	0.14	56,56,56,56	0
57	MG	DA	3504	1/1	0.93	0.09	52,52,52,52	0
57	MG	BA	3527	1/1	0.93	0.19	24,24,24,24	0
57	MG	AA	1690	1/1	0.93	0.42	52,52,52,52	0
57	MG	CA	3054	1/1	0.93	0.33	69,69,69,69	0
57	MG	BA	3649	1/1	0.93	0.14	55,55,55,55	0
57	MG	BA	3651	1/1	0.93	0.14	66,66,66,66	0
57	MG	BA	3289	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3218	1/1	0.93	0.15	45,45,45,45	0
57	MG	DA	3273	1/1	0.93	0.12	62,62,62,62	0
57	MG	BA	3798	1/1	0.93	0.24	22,22,22,22	0
57	MG	AA	1802	1/1	0.93	0.10	54,54,54,54	0
57	MG	BA	3220	1/1	0.93	0.16	35,35,35,35	0
57	MG	BA	3657	1/1	0.93	0.11	38,38,38,38	0
57	MG	DA	3282	1/1	0.93	0.10	55,55,55,55	0
57	MG	BA	3415	1/1	0.93	0.23	35,35,35,35	0
57	MG	BA	3659	1/1	0.93	0.11	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	CA	3071	1/1	0.93	0.19	56,56,56,56	0
57	MG	CA	3073	1/1	0.93	0.20	55,55,55,55	0
57	MG	AA	1654	1/1	0.93	0.23	65,65,65,65	0
57	MG	DA	3536	1/1	0.93	0.08	52,52,52,52	0
57	MG	BA	3661	1/1	0.93	0.24	25,25,25,25	0
57	MG	DA	3539	1/1	0.93	0.08	55,55,55,55	0
57	MG	CA	3078	1/1	0.93	0.16	65,65,65,65	0
57	MG	AX	3011	1/1	0.93	0.13	60,60,60,60	0
57	MG	DA	3305	1/1	0.93	0.12	53,53,53,53	0
57	MG	BA	3540	1/1	0.93	0.16	31,31,31,31	0
57	MG	DA	3083	1/1	0.93	0.26	41,41,41,41	0
57	MG	BB	3005	1/1	0.93	0.28	51,51,51,51	0
57	MG	BA	3301	1/1	0.93	0.18	62,62,62,62	0
57	MG	BA	3302	1/1	0.93	0.15	49,49,49,49	0
57	MG	BA	3543	1/1	0.93	0.23	52,52,52,52	0
57	MG	DA	3315	1/1	0.93	0.13	44,44,44,44	0
57	MG	BA	3303	1/1	0.93	0.23	26,26,26,26	0
57	MG	BA	3304	1/1	0.93	0.18	39,39,39,39	0
57	MG	BA	3673	1/1	0.93	0.28	61,61,61,61	0
57	MG	CA	3098	1/1	0.93	0.11	54,54,54,54	0
57	MG	BA	3428	1/1	0.93	0.16	51,51,51,51	0
57	MG	DA	3563	1/1	0.93	0.10	70,70,70,70	0
57	MG	BA	3552	1/1	0.93	0.15	55,55,55,55	0
57	MG	CA	3101	1/1	0.93	0.11	65,65,65,65	0
57	MG	BA	3092	1/1	0.93	0.29	40,40,40,40	0
57	MG	AA	1641	1/1	0.93	0.17	65,65,65,65	0
57	MG	DA	3335	1/1	0.93	0.25	49,49,49,49	0
57	MG	DA	3571	1/1	0.93	0.28	45,45,45,45	0
57	MG	BE	304	1/1	0.93	0.23	23,23,23,23	0
57	MG	BA	3432	1/1	0.93	0.22	32,32,32,32	0
57	MG	DA	3104	1/1	0.93	0.11	57,57,57,57	0
57	MG	DA	3105	1/1	0.93	0.22	45,45,45,45	0
57	MG	DA	3342	1/1	0.93	0.10	53,53,53,53	0
57	MG	BA	3684	1/1	0.93	0.22	51,51,51,51	0
57	MG	DA	3579	1/1	0.93	0.16	62,62,62,62	0
57	MG	AA	1751	1/1	0.93	0.23	53,53,53,53	0
57	MG	BA	3686	1/1	0.93	0.19	27,27,27,27	0
57	MG	DA	3587	1/1	0.93	0.12	51,51,51,51	0
57	MG	AX	3014	1/1	0.93	0.24	61,61,61,61	0
57	MG	BA	3148	1/1	0.93	0.28	38,38,38,38	0
57	MG	BA	3321	1/1	0.93	0.13	53,53,53,53	0
57	MG	CA	3117	1/1	0.93	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3595	1/1	0.93	0.13	57,57,57,57	0
57	MG	BN	3003	1/1	0.93	0.21	38,38,38,38	0
57	MG	CA	3120	1/1	0.93	0.12	68,68,68,68	0
57	MG	BA	3690	1/1	0.93	0.13	39,39,39,39	0
57	MG	BR	5001	1/1	0.93	0.20	50,50,50,50	0
57	MG	DA	3367	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3322	1/1	0.93	0.16	38,38,38,38	0
57	MG	CA	3124	1/1	0.93	0.22	69,69,69,69	0
57	MG	DA	3371	1/1	0.93	0.17	34,34,34,34	0
57	MG	BA	3101	1/1	0.93	0.24	37,37,37,37	0
57	MG	DA	3613	1/1	0.93	0.11	56,56,56,56	0
57	MG	BA	3150	1/1	0.93	0.17	39,39,39,39	0
57	MG	CA	3127	1/1	0.93	0.08	59,59,59,59	0
57	MG	DA	3131	1/1	0.93	0.25	49,49,49,49	0
57	MG	BA	3449	1/1	0.93	0.23	62,62,62,62	0
57	MG	DA	3133	1/1	0.93	0.18	60,60,60,60	0
57	MG	DA	3622	1/1	0.93	0.10	49,49,49,49	0
57	MG	BA	3697	1/1	0.93	0.18	41,41,41,41	0
57	MG	BA	3699	1/1	0.93	0.20	67,67,67,67	0
57	MG	DA	3391	1/1	0.93	0.16	45,45,45,45	0
57	MG	BA	3237	1/1	0.93	0.17	44,44,44,44	0
57	MG	B0	3001	1/1	0.93	0.19	47,47,47,47	0
57	MG	BA	3047	1/1	0.93	0.22	43,43,43,43	0
57	MG	DA	3396	1/1	0.93	0.17	46,46,46,46	0
57	MG	BA	3330	1/1	0.93	0.15	27,27,27,27	0
57	MG	AA	1752	1/1	0.93	0.14	48,48,48,48	0
57	MG	B5	102	1/1	0.93	0.19	43,43,43,43	0
57	MG	B6	101	1/1	0.93	0.32	60,60,60,60	0
57	MG	CA	3150	1/1	0.93	0.15	65,65,65,65	0
57	MG	B6	103	1/1	0.93	0.15	52,52,52,52	0
57	MG	DA	3644	1/1	0.93	0.24	58,58,58,58	0
57	MG	BA	3337	1/1	0.93	0.25	44,44,44,44	0
57	MG	DA	3646	1/1	0.93	0.15	56,56,56,56	0
57	MG	BA	3462	1/1	0.93	0.11	53,53,53,53	0
57	MG	AA	1656	1/1	0.93	0.16	63,63,63,63	0
57	MG	AA	1782	1/1	0.93	0.14	54,54,54,54	0
57	MG	DA	3414	1/1	0.93	0.15	42,42,42,42	0
57	MG	CA	3159	1/1	0.93	0.13	62,62,62,62	0
57	MG	BA	3247	1/1	0.93	0.17	29,29,29,29	0
57	MG	BA	3161	1/1	0.93	0.29	44,44,44,44	0
57	MG	BA	3599	1/1	0.93	0.16	60,60,60,60	0
57	MG	BA	3055	1/1	0.93	0.23	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3421	1/1	0.93	0.12	56,56,56,56	0
57	MG	DA	3177	1/1	0.93	0.13	58,58,58,58	0
57	MG	CA	3165	1/1	0.93	0.09	42,42,42,42	0
57	MG	AY	3002	1/1	0.93	0.31	52,52,52,52	0
57	MG	AK	3101	1/1	0.93	0.17	69,69,69,69	0
57	MG	AA	1657	1/1	0.93	0.12	64,64,64,64	0
57	MG	AA	1607	1/1	0.93	0.13	55,55,55,55	0
57	MG	DA	3433	1/1	0.93	0.17	59,59,59,59	0
57	MG	DD	303	1/1	0.93	0.34	51,51,51,51	0
57	MG	AA	1737	1/1	0.93	0.09	60,60,60,60	0
57	MG	AA	1638	1/1	0.93	0.23	60,60,60,60	0
57	MG	DA	3441	1/1	0.93	0.20	58,58,58,58	0
57	MG	BA	3177	1/1	0.93	0.23	46,46,46,46	0
57	MG	DF	305	1/1	0.93	0.59	45,45,45,45	0
57	MG	BA	3366	1/1	0.93	0.16	52,52,52,52	0
57	MG	CA	3015	1/1	0.93	0.19	64,64,64,64	0
57	MG	DA	3006	1/1	0.93	0.11	41,41,41,41	0
57	MG	BA	3179	1/1	0.93	0.23	43,43,43,43	0
57	MG	DA	3449	1/1	0.93	0.13	34,34,34,34	0
57	MG	BA	3181	1/1	0.93	0.10	40,40,40,40	0
57	MG	BA	3123	1/1	0.93	0.09	43,43,43,43	0
57	MG	BA	3624	1/1	0.93	0.13	38,38,38,38	0
57	MG	BA	3746	1/1	0.93	0.14	78,78,78,78	0
57	MG	DA	3207	1/1	0.93	0.14	48,48,48,48	0
57	MG	DY	502	1/1	0.93	0.17	55,55,55,55	0
57	MG	BA	3269	1/1	0.93	0.25	45,45,45,45	0
57	MG	DA	3210	1/1	0.93	0.08	52,52,52,52	0
57	MG	DA	3461	1/1	0.93	0.13	51,51,51,51	0
57	MG	BA	3754	1/1	0.93	0.14	42,42,42,42	0
57	MG	CA	3025	1/1	0.93	0.24	53,53,53,53	0
57	MG	BA	3242	1/1	0.94	0.69	55,55,55,55	0
57	MG	AA	1659	1/1	0.94	0.19	65,65,65,65	0
57	MG	DA	3134	1/1	0.94	0.21	52,52,52,52	0
57	MG	BA	3244	1/1	0.94	0.26	31,31,31,31	0
57	MG	CA	3106	1/1	0.94	0.13	58,58,58,58	0
57	MG	DA	3138	1/1	0.94	0.14	54,54,54,54	0
57	MG	DA	3139	1/1	0.94	0.11	44,44,44,44	0
57	MG	BA	3027	1/1	0.94	0.41	64,64,64,64	0
57	MG	BB	3003	1/1	0.94	0.18	30,30,30,30	0
57	MG	DA	3142	1/1	0.94	0.13	51,51,51,51	0
57	MG	DA	3438	1/1	0.94	0.08	42,42,42,42	0
57	MG	BA	3351	1/1	0.94	0.19	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	3353	1/1	0.94	0.12	55,55,55,55	0
57	MG	DA	3148	1/1	0.94	0.21	49,49,49,49	0
57	MG	BA	3246	1/1	0.94	0.31	55,55,55,55	0
57	MG	BA	3509	1/1	0.94	0.18	50,50,50,50	0
57	MG	BB	3010	1/1	0.94	0.18	53,53,53,53	0
57	MG	CA	3114	1/1	0.94	0.14	71,71,71,71	0
57	MG	BB	3012	1/1	0.94	0.19	56,56,56,56	0
57	MG	BA	3028	1/1	0.94	0.20	37,37,37,37	0
57	MG	AA	1728	1/1	0.94	0.25	49,49,49,49	0
57	MG	BA	3030	1/1	0.94	0.24	39,39,39,39	0
57	MG	BA	3095	1/1	0.94	0.23	53,53,53,53	0
57	MG	AA	1676	1/1	0.94	0.16	58,58,58,58	0
57	MG	DA	3164	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3166	1/1	0.94	0.16	55,55,55,55	0
57	MG	DA	3460	1/1	0.94	0.18	37,37,37,37	0
57	MG	DA	3167	1/1	0.94	0.21	40,40,40,40	0
57	MG	BA	3097	1/1	0.94	0.12	41,41,41,41	0
57	MG	BA	3098	1/1	0.94	0.22	23,23,23,23	0
57	MG	BA	3519	1/1	0.94	0.19	45,45,45,45	0
57	MG	DA	3465	1/1	0.94	0.17	42,42,42,42	0
57	MG	BE	303	1/1	0.94	0.15	43,43,43,43	0
57	MG	DA	3467	1/1	0.94	0.24	52,52,52,52	0
57	MG	DA	3176	1/1	0.94	0.24	38,38,38,38	0
57	MG	BA	3038	1/1	0.94	0.23	20,20,20,20	0
57	MG	BE	306	1/1	0.94	0.10	38,38,38,38	0
57	MG	DA	3475	1/1	0.94	0.18	56,56,56,56	0
57	MG	BF	301	1/1	0.94	0.25	40,40,40,40	0
57	MG	DA	3185	1/1	0.94	0.15	51,51,51,51	0
57	MG	BF	302	1/1	0.94	0.31	30,30,30,30	0
57	MG	BA	3373	1/1	0.94	0.22	34,34,34,34	0
57	MG	CA	3136	1/1	0.94	0.14	48,48,48,48	0
57	MG	BA	3165	1/1	0.94	0.31	52,52,52,52	0
57	MG	DA	3483	1/1	0.94	0.09	53,53,53,53	0
57	MG	BA	3100	1/1	0.94	0.25	61,61,61,61	0
57	MG	BA	3040	1/1	0.94	0.27	33,33,33,33	0
57	MG	AA	1785	1/1	0.94	0.11	72,72,72,72	0
57	MG	CA	3144	1/1	0.94	0.13	82,82,82,82	0
57	MG	BA	3044	1/1	0.94	0.35	43,43,43,43	0
57	MG	CA	3147	1/1	0.94	0.10	70,70,70,70	0
57	MG	BA	3675	1/1	0.94	0.26	56,56,56,56	0
57	MG	BA	3105	1/1	0.94	0.12	46,46,46,46	0
57	MG	DA	3202	1/1	0.94	0.20	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	BO	5001	1/1	0.94	0.13	61,61,61,61	0
57	MG	BA	3677	1/1	0.94	0.10	44,44,44,44	0
57	MG	DA	3206	1/1	0.94	0.08	50,50,50,50	0
57	MG	BA	3384	1/1	0.94	0.11	45,45,45,45	0
57	MG	BR	5002	1/1	0.94	0.14	50,50,50,50	0
57	MG	BU	201	1/1	0.94	0.36	43,43,43,43	0
57	MG	BV	201	1/1	0.94	0.36	31,31,31,31	0
57	MG	BA	3679	1/1	0.94	0.22	52,52,52,52	0
57	MG	BA	3386	1/1	0.94	0.14	28,28,28,28	0
57	MG	BW	3002	1/1	0.94	0.27	58,58,58,58	0
57	MG	DA	3220	1/1	0.94	0.32	50,50,50,50	0
57	MG	AB	3001	1/1	0.94	0.13	77,77,77,77	0
57	MG	DA	3517	1/1	0.94	0.12	48,48,48,48	0
57	MG	DA	3223	1/1	0.94	0.19	39,39,39,39	0
57	MG	DA	3226	1/1	0.94	0.18	57,57,57,57	0
57	MG	BA	3048	1/1	0.94	0.22	29,29,29,29	0
57	MG	DA	3230	1/1	0.94	0.14	46,46,46,46	0
57	MG	AA	1731	1/1	0.94	0.18	56,56,56,56	0
57	MG	DA	3526	1/1	0.94	0.12	52,52,52,52	0
57	MG	CA	3169	1/1	0.94	0.18	62,62,62,62	0
57	MG	DA	3529	1/1	0.94	0.07	76,76,76,76	0
57	MG	BA	3394	1/1	0.94	0.28	40,40,40,40	0
57	MG	DA	3531	1/1	0.94	0.07	48,48,48,48	0
57	MG	BA	3395	1/1	0.94	0.20	30,30,30,30	0
57	MG	BA	3399	1/1	0.94	0.20	41,41,41,41	0
57	MG	DA	3534	1/1	0.94	0.10	46,46,46,46	0
57	MG	DA	3535	1/1	0.94	0.19	44,44,44,44	0
57	MG	AA	1733	1/1	0.94	0.12	50,50,50,50	0
57	MG	BA	3187	1/1	0.94	0.22	38,38,38,38	0
57	MG	AA	1617	1/1	0.94	0.10	58,58,58,58	0
57	MG	DA	3540	1/1	0.94	0.06	50,50,50,50	0
57	MG	DA	3240	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3192	1/1	0.94	0.20	19,19,19,19	0
57	MG	BA	3280	1/1	0.94	0.21	25,25,25,25	0
57	MG	DA	3004	1/1	0.94	0.20	53,53,53,53	0
57	MG	DA	3548	1/1	0.94	0.10	66,66,66,66	0
57	MG	BA	3193	1/1	0.94	0.13	37,37,37,37	0
57	MG	DA	3247	1/1	0.94	0.16	49,49,49,49	0
57	MG	DA	3551	1/1	0.94	0.17	49,49,49,49	0
57	MG	BA	3695	1/1	0.94	0.15	40,40,40,40	0
57	MG	DA	3009	1/1	0.94	0.17	61,61,61,61	0
57	MG	DA	3251	1/1	0.94	0.15	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	3112	1/1	0.94	0.26	41,41,41,41	0
57	MG	DA	3012	1/1	0.94	0.11	43,43,43,43	0
57	MG	DA	3255	1/1	0.94	0.24	47,47,47,47	0
57	MG	B8	5001	1/1	0.94	0.20	42,42,42,42	0
57	MG	BA	3113	1/1	0.94	0.14	50,50,50,50	0
57	MG	BA	3555	1/1	0.94	0.19	50,50,50,50	0
57	MG	DA	3018	1/1	0.94	0.10	31,31,31,31	0
57	MG	DA	3564	1/1	0.94	0.17	53,53,53,53	0
57	MG	DA	3019	1/1	0.94	0.08	42,42,42,42	0
57	MG	DA	3268	1/1	0.94	0.12	41,41,41,41	0
57	MG	DA	3567	1/1	0.94	0.26	44,44,44,44	0
57	MG	BA	3556	1/1	0.94	0.07	46,46,46,46	0
57	MG	DA	3272	1/1	0.94	0.19	49,49,49,49	0
57	MG	AA	1698	1/1	0.94	0.23	58,58,58,58	0
57	MG	BA	3703	1/1	0.94	0.33	28,28,28,28	0
57	MG	DA	3277	1/1	0.94	0.13	50,50,50,50	0
57	MG	BA	3198	1/1	0.94	0.16	44,44,44,44	0
57	MG	AM	3001	1/1	0.94	0.09	66,66,66,66	0
57	MG	BA	3706	1/1	0.94	0.16	47,47,47,47	0
57	MG	BA	3562	1/1	0.94	0.16	55,55,55,55	0
57	MG	DA	3283	1/1	0.94	0.07	27,27,27,27	0
57	MG	BA	3202	1/1	0.94	0.15	62,62,62,62	0
57	MG	DA	3285	1/1	0.94	0.12	50,50,50,50	0
57	MG	BA	3292	1/1	0.94	0.24	26,26,26,26	0
57	MG	DA	3585	1/1	0.94	0.25	55,55,55,55	0
57	MG	DA	3288	1/1	0.94	0.16	39,39,39,39	0
57	MG	BA	3714	1/1	0.94	0.12	46,46,46,46	0
57	MG	BA	3294	1/1	0.94	0.16	43,43,43,43	0
57	MG	BA	3422	1/1	0.94	0.16	36,36,36,36	0
57	MG	AA	1646	1/1	0.94	0.23	58,58,58,58	0
57	MG	BA	3722	1/1	0.94	0.19	64,64,64,64	0
57	MG	BA	3206	1/1	0.94	0.16	34,34,34,34	0
57	MG	DA	3047	1/1	0.94	0.16	45,45,45,45	0
57	MG	CA	3018	1/1	0.94	0.13	63,63,63,63	0
57	MG	DA	3602	1/1	0.94	0.26	62,62,62,62	0
57	MG	BA	3427	1/1	0.94	0.17	33,33,33,33	0
57	MG	BA	3298	1/1	0.94	0.15	27,27,27,27	0
57	MG	DA	3605	1/1	0.94	0.12	45,45,45,45	0
57	MG	AA	1636	1/1	0.94	0.31	52,52,52,52	0
57	MG	BA	3581	1/1	0.94	0.12	59,59,59,59	0
57	MG	DA	3608	1/1	0.94	0.09	57,57,57,57	0
57	MG	DA	3609	1/1	0.94	0.10	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	3584	1/1	0.94	0.12	55,55,55,55	0
57	MG	CA	3024	1/1	0.94	0.16	67,67,67,67	0
57	MG	BA	3059	1/1	0.94	0.14	36,36,36,36	0
57	MG	DA	3060	1/1	0.94	0.28	60,60,60,60	0
57	MG	DA	3616	1/1	0.94	0.20	63,63,63,63	0
57	MG	BA	3733	1/1	0.94	0.15	42,42,42,42	0
57	MG	BA	3210	1/1	0.94	0.25	41,41,41,41	0
57	MG	BA	3589	1/1	0.94	0.23	59,59,59,59	0
57	MG	BA	3211	1/1	0.94	0.18	43,43,43,43	0
57	MG	DA	3621	1/1	0.94	0.49	52,52,52,52	0
57	MG	AA	1715	1/1	0.94	0.23	45,45,45,45	0
57	MG	BA	3437	1/1	0.94	0.23	62,62,62,62	0
57	MG	BA	3596	1/1	0.94	0.17	59,59,59,59	0
57	MG	BA	3743	1/1	0.94	0.59	47,47,47,47	0
57	MG	BA	3744	1/1	0.94	0.18	55,55,55,55	0
57	MG	CA	3037	1/1	0.94	0.21	53,53,53,53	0
57	MG	AA	1683	1/1	0.94	0.13	62,62,62,62	0
57	MG	DA	3074	1/1	0.94	0.08	59,59,59,59	0
57	MG	DA	3631	1/1	0.94	0.12	49,49,49,49	0
57	MG	BA	3009	1/1	0.94	0.17	31,31,31,31	0
57	MG	BA	3064	1/1	0.94	0.23	45,45,45,45	0
57	MG	DA	3635	1/1	0.94	0.11	43,43,43,43	0
57	MG	AA	1673	1/1	0.94	0.13	48,48,48,48	0
57	MG	CA	3046	1/1	0.94	0.18	61,61,61,61	0
57	MG	BA	3601	1/1	0.94	0.32	40,40,40,40	0
57	MG	DA	3642	1/1	0.94	0.21	62,62,62,62	0
57	MG	BA	3445	1/1	0.94	0.23	54,54,54,54	0
57	MG	BA	3758	1/1	0.94	0.12	41,41,41,41	0
57	MG	BA	3012	1/1	0.94	0.17	25,25,25,25	0
57	MG	BA	3317	1/1	0.94	0.21	43,43,43,43	0
57	MG	BA	3450	1/1	0.94	0.25	54,54,54,54	0
57	MG	CA	3056	1/1	0.94	0.10	64,64,64,64	0
57	MG	AX	3002	1/1	0.94	0.30	71,71,71,71	0
57	MG	BA	3320	1/1	0.94	0.16	55,55,55,55	0
57	MG	CA	3060	1/1	0.94	0.08	71,71,71,71	0
57	MG	BA	3069	1/1	0.94	0.34	48,48,48,48	0
57	MG	BA	3616	1/1	0.94	0.20	59,59,59,59	0
57	MG	DA	3659	1/1	0.94	0.14	41,41,41,41	0
57	MG	DA	3660	1/1	0.94	0.52	46,46,46,46	0
57	MG	DA	3372	1/1	0.94	0.13	53,53,53,53	0
57	MG	BA	3070	1/1	0.94	0.24	41,41,41,41	0
57	MG	BA	3771	1/1	0.94	0.11	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	DB	3002	1/1	0.94	0.26	63,63,63,63	0
57	MG	BA	3135	1/1	0.94	0.45	56,56,56,56	0
57	MG	DB	3004	1/1	0.94	0.21	63,63,63,63	0
57	MG	BA	3620	1/1	0.94	0.14	29,29,29,29	0
57	MG	DB	3006	1/1	0.94	0.14	55,55,55,55	0
57	MG	CA	3069	1/1	0.94	0.22	58,58,58,58	0
57	MG	DB	3009	1/1	0.94	0.14	58,58,58,58	0
57	MG	AA	1749	1/1	0.94	0.19	50,50,50,50	0
57	MG	AA	1649	1/1	0.94	0.18	28,28,28,28	0
57	MG	CA	3072	1/1	0.94	0.14	62,62,62,62	0
57	MG	BA	3784	1/1	0.94	0.18	52,52,52,52	0
57	MG	CA	3075	1/1	0.94	0.24	65,65,65,65	0
57	MG	DE	3003	1/1	0.94	0.12	43,43,43,43	0
57	MG	BA	3474	1/1	0.94	0.27	33,33,33,33	0
57	MG	AA	1805	1/1	0.94	0.07	48,48,48,48	0
57	MG	BA	3788	1/1	0.94	0.24	44,44,44,44	0
57	MG	AA	1806	1/1	0.94	0.18	74,74,74,74	0
57	MG	DA	3113	1/1	0.94	0.13	35,35,35,35	0
57	MG	BA	3480	1/1	0.94	0.18	47,47,47,47	0
57	MG	DA	3401	1/1	0.94	0.06	69,69,69,69	0
57	MG	DA	3402	1/1	0.94	0.09	48,48,48,48	0
57	MG	BA	3332	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3236	1/1	0.94	0.13	52,52,52,52	0
57	MG	BA	3334	1/1	0.94	0.21	56,56,56,56	0
57	MG	AA	1808	1/1	0.94	0.14	49,49,49,49	0
57	MG	BA	3799	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3489	1/1	0.94	0.25	50,50,50,50	0
57	MG	DA	3126	1/1	0.94	0.15	59,59,59,59	0
57	MG	BA	3084	1/1	0.94	0.18	42,42,42,42	0
57	MG	DA	3128	1/1	0.94	0.28	56,56,56,56	0
57	MG	D3	3001	1/1	0.94	0.27	63,63,63,63	0
57	MG	BA	3804	1/1	0.94	0.16	36,36,36,36	0
59	ZN	B4	501	1/1	0.94	0.10	118,118,118,118	0
57	MG	AA	1780	1/1	0.94	0.11	69,69,69,69	0
57	MG	BA	3241	1/1	0.94	0.16	56,56,56,56	0
57	MG	DA	3419	1/1	0.94	0.14	50,50,50,50	0
57	MG	DA	3076	1/1	0.95	0.18	52,52,52,52	0
57	MG	CA	3088	1/1	0.95	0.12	43,43,43,43	0
57	MG	DA	3490	1/1	0.95	0.13	33,33,33,33	0
57	MG	BE	305	1/1	0.95	0.07	48,48,48,48	0
57	MG	BA	3578	1/1	0.95	0.35	39,39,39,39	0
57	MG	BA	3276	1/1	0.95	0.40	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	3496	1/1	0.95	0.17	56,56,56,56	0
57	MG	DA	3266	1/1	0.95	0.12	37,37,37,37	0
57	MG	DA	3498	1/1	0.95	0.17	35,35,35,35	0
57	MG	CA	3093	1/1	0.95	0.20	55,55,55,55	0
57	MG	DA	3269	1/1	0.95	0.11	50,50,50,50	0
57	MG	DA	3082	1/1	0.95	0.22	47,47,47,47	0
57	MG	BA	3580	1/1	0.95	0.15	48,48,48,48	0
57	MG	BA	3465	1/1	0.95	0.09	48,48,48,48	0
57	MG	CA	3097	1/1	0.95	0.27	60,60,60,60	0
57	MG	BA	3469	1/1	0.95	0.16	61,61,61,61	0
57	MG	DA	3509	1/1	0.95	0.06	49,49,49,49	0
57	MG	DA	3510	1/1	0.95	0.26	64,64,64,64	0
57	MG	DA	3278	1/1	0.95	0.10	39,39,39,39	0
57	MG	BA	3363	1/1	0.95	0.17	52,52,52,52	0
57	MG	BA	3471	1/1	0.95	0.19	27,27,27,27	0
57	MG	BA	3277	1/1	0.95	0.43	52,52,52,52	0
57	MG	BA	3153	1/1	0.95	0.15	45,45,45,45	0
57	MG	BA	3708	1/1	0.95	0.21	33,33,33,33	0
57	MG	BA	3709	1/1	0.95	0.34	48,48,48,48	0
57	MG	BA	3037	1/1	0.95	0.28	42,42,42,42	0
57	MG	BA	3478	1/1	0.95	0.15	54,54,54,54	0
57	MG	DA	3287	1/1	0.95	0.21	52,52,52,52	0
57	MG	BQ	3002	1/1	0.95	0.28	46,46,46,46	0
57	MG	BA	3479	1/1	0.95	0.06	53,53,53,53	0
57	MG	BA	3071	1/1	0.95	0.31	59,59,59,59	0
57	MG	DA	3527	1/1	0.95	0.13	52,52,52,52	0
57	MG	BA	3481	1/1	0.95	0.12	54,54,54,54	0
57	MG	DA	3295	1/1	0.95	0.19	67,67,67,67	0
57	MG	DA	3102	1/1	0.95	0.32	40,40,40,40	0
57	MG	BU	202	1/1	0.95	0.15	40,40,40,40	0
57	MG	DA	3299	1/1	0.95	0.09	46,46,46,46	0
57	MG	BA	3716	1/1	0.95	0.25	45,45,45,45	0
57	MG	BV	202	1/1	0.95	0.26	32,32,32,32	0
57	MG	CA	3116	1/1	0.95	0.20	57,57,57,57	0
57	MG	AA	1769	1/1	0.95	0.19	50,50,50,50	0
57	MG	BA	3158	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3284	1/1	0.95	0.10	57,57,57,57	0
57	MG	DA	3312	1/1	0.95	0.12	42,42,42,42	0
57	MG	BW	3003	1/1	0.95	0.15	35,35,35,35	0
57	MG	BA	3223	1/1	0.95	0.18	41,41,41,41	0
57	MG	BA	3607	1/1	0.95	0.17	36,36,36,36	0
57	MG	DA	3115	1/1	0.95	0.29	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1615	1/1	0.95	0.21	51,51,51,51	0
57	MG	AA	1774	1/1	0.95	0.17	51,51,51,51	0
57	MG	DA	3322	1/1	0.95	0.16	42,42,42,42	0
57	MG	BA	3495	1/1	0.95	0.16	43,43,43,43	0
57	MG	DA	3325	1/1	0.95	0.23	45,45,45,45	0
57	MG	BA	3228	1/1	0.95	0.10	65,65,65,65	0
57	MG	BA	3116	1/1	0.95	0.35	46,46,46,46	0
57	MG	DA	3555	1/1	0.95	0.21	46,46,46,46	0
57	MG	DA	3329	1/1	0.95	0.10	47,47,47,47	0
57	MG	DA	3124	1/1	0.95	0.17	43,43,43,43	0
57	MG	DA	3331	1/1	0.95	0.15	47,47,47,47	0
57	MG	BA	3293	1/1	0.95	0.11	58,58,58,58	0
57	MG	BA	3042	1/1	0.95	0.13	37,37,37,37	0
57	MG	CA	3134	1/1	0.95	0.12	64,64,64,64	0
57	MG	BA	3617	1/1	0.95	0.10	42,42,42,42	0
57	MG	DA	3337	1/1	0.95	0.06	48,48,48,48	0
57	MG	BA	3118	1/1	0.95	0.21	35,35,35,35	0
57	MG	BA	3120	1/1	0.95	0.18	45,45,45,45	0
57	MG	B7	101	1/1	0.95	0.12	41,41,41,41	0
57	MG	BA	3297	1/1	0.95	0.22	42,42,42,42	0
57	MG	CA	3142	1/1	0.95	0.18	50,50,50,50	0
57	MG	DA	3346	1/1	0.95	0.14	49,49,49,49	0
57	MG	BA	3168	1/1	0.95	0.24	45,45,45,45	0
57	MG	BA	3169	1/1	0.95	0.24	50,50,50,50	0
57	MG	BA	3080	1/1	0.95	0.14	31,31,31,31	0
57	MG	BA	3043	1/1	0.95	0.17	31,31,31,31	0
57	MG	BA	3511	1/1	0.95	0.18	50,50,50,50	0
57	MG	BA	3629	1/1	0.95	0.25	58,58,58,58	0
57	MG	DA	3359	1/1	0.95	0.16	40,40,40,40	0
57	MG	BA	3748	1/1	0.95	0.17	61,61,61,61	0
57	MG	BA	3752	1/1	0.95	0.12	34,34,34,34	0
57	MG	BA	3753	1/1	0.95	0.19	68,68,68,68	0
57	MG	DA	3583	1/1	0.95	0.12	52,52,52,52	0
57	MG	DA	3364	1/1	0.95	0.10	45,45,45,45	0
57	MG	DA	3586	1/1	0.95	0.08	50,50,50,50	0
57	MG	DA	3145	1/1	0.95	0.32	48,48,48,48	0
57	MG	DA	3588	1/1	0.95	0.15	59,59,59,59	0
57	MG	DA	3589	1/1	0.95	0.08	29,29,29,29	0
57	MG	BA	3238	1/1	0.95	0.48	44,44,44,44	0
57	MG	DA	3147	1/1	0.95	0.14	44,44,44,44	0
57	MG	BA	3401	1/1	0.95	0.25	26,26,26,26	0
57	MG	DA	3149	1/1	0.95	0.08	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	DA	3594	1/1	0.95	0.09	58,58,58,58	0
57	MG	AX	3006	1/1	0.95	0.15	68,68,68,68	0
57	MG	AA	1775	1/1	0.95	0.11	73,73,73,73	0
57	MG	AA	1776	1/1	0.95	0.16	73,73,73,73	0
57	MG	BA	3178	1/1	0.95	0.17	32,32,32,32	0
57	MG	AX	3009	1/1	0.95	0.37	65,65,65,65	0
57	MG	DA	3378	1/1	0.95	0.14	52,52,52,52	0
57	MG	BA	3520	1/1	0.95	0.25	29,29,29,29	0
57	MG	DA	3382	1/1	0.95	0.12	41,41,41,41	0
57	MG	AA	1794	1/1	0.95	0.16	58,58,58,58	0
57	MG	DA	3385	1/1	0.95	0.07	60,60,60,60	0
57	MG	CA	3168	1/1	0.95	0.20	41,41,41,41	0
57	MG	DA	3389	1/1	0.95	0.19	59,59,59,59	0
57	MG	DA	3610	1/1	0.95	0.09	47,47,47,47	0
57	MG	AA	1757	1/1	0.95	0.25	68,68,68,68	0
57	MG	CD	502	1/1	0.95	0.27	53,53,53,53	0
57	MG	BA	3093	1/1	0.95	0.24	41,41,41,41	0
57	MG	DA	3165	1/1	0.95	0.21	55,55,55,55	0
57	MG	BA	3188	1/1	0.95	0.19	32,32,32,32	0
57	MG	BA	3017	1/1	0.95	0.28	65,65,65,65	0
57	MG	AA	1750	1/1	0.95	0.14	49,49,49,49	0
57	MG	DA	3171	1/1	0.95	0.17	40,40,40,40	0
57	MG	BA	3774	1/1	0.95	0.32	27,27,27,27	0
57	MG	CX	3001	1/1	0.95	0.18	57,57,57,57	0
57	MG	BA	3251	1/1	0.95	0.25	43,43,43,43	0
57	MG	DA	3175	1/1	0.95	0.14	41,41,41,41	0
57	MG	DA	3404	1/1	0.95	0.08	43,43,43,43	0
57	MG	BA	3324	1/1	0.95	0.15	60,60,60,60	0
57	MG	BA	3780	1/1	0.95	0.13	42,42,42,42	0
57	MG	DA	3003	1/1	0.95	0.23	36,36,36,36	0
57	MG	BA	3421	1/1	0.95	0.26	62,62,62,62	0
57	MG	DA	3410	1/1	0.95	0.22	40,40,40,40	0
57	MG	DA	3184	1/1	0.95	0.12	52,52,52,52	0
57	MG	AA	1742	1/1	0.95	0.14	52,52,52,52	0
57	MG	BA	3023	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3328	1/1	0.95	0.19	27,27,27,27	0
57	MG	AA	1670	1/1	0.95	0.17	67,67,67,67	0
57	MG	BA	3537	1/1	0.95	0.08	43,43,43,43	0
57	MG	CA	3033	1/1	0.95	0.10	54,54,54,54	0
57	MG	DA	3641	1/1	0.95	0.07	46,46,46,46	0
57	MG	AA	1709	1/1	0.95	0.26	55,55,55,55	0
57	MG	DA	3193	1/1	0.95	0.15	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	3061	1/1	0.95	0.30	25,25,25,25	0
57	MG	BA	3258	1/1	0.95	0.35	44,44,44,44	0
57	MG	DA	3423	1/1	0.95	0.20	37,37,37,37	0
57	MG	BA	3261	1/1	0.95	0.21	18,18,18,18	0
57	MG	BA	3664	1/1	0.95	0.21	69,69,69,69	0
57	MG	CA	3040	1/1	0.95	0.12	56,56,56,56	0
57	MG	BA	3433	1/1	0.95	0.20	27,27,27,27	0
57	MG	DA	3429	1/1	0.95	0.15	36,36,36,36	0
57	MG	DA	3656	1/1	0.95	0.25	41,41,41,41	0
57	MG	BA	3801	1/1	0.95	0.16	71,71,71,71	0
57	MG	BA	3335	1/1	0.95	0.15	40,40,40,40	0
57	MG	DA	3434	1/1	0.95	0.07	60,60,60,60	0
57	MG	BA	3199	1/1	0.95	0.30	64,64,64,64	0
57	MG	AA	1783	1/1	0.95	0.17	35,35,35,35	0
57	MG	BA	3671	1/1	0.95	0.19	24,24,24,24	0
57	MG	BA	3550	1/1	0.95	0.16	50,50,50,50	0
57	MG	AA	1804	1/1	0.95	0.12	70,70,70,70	0
57	MG	DA	3443	1/1	0.95	0.19	51,51,51,51	0
57	MG	CA	3053	1/1	0.95	0.12	41,41,41,41	0
57	MG	BA	3143	1/1	0.95	0.10	41,41,41,41	0
57	MG	DA	3038	1/1	0.95	0.14	56,56,56,56	0
57	MG	BA	3812	1/1	0.95	0.12	42,42,42,42	0
57	MG	DB	3008	1/1	0.95	0.17	56,56,56,56	0
57	MG	AA	1746	1/1	0.95	0.10	56,56,56,56	0
57	MG	DA	3043	1/1	0.95	0.19	53,53,53,53	0
57	MG	CA	3057	1/1	0.95	0.14	84,84,84,84	0
57	MG	DA	3224	1/1	0.95	0.08	39,39,39,39	0
57	MG	DD	301	1/1	0.95	0.22	44,44,44,44	0
57	MG	DA	3225	1/1	0.95	0.10	55,55,55,55	0
57	MG	AA	1700	1/1	0.95	0.08	71,71,71,71	0
57	MG	DE	3002	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3444	1/1	0.95	0.15	48,48,48,48	0
57	MG	BA	3208	1/1	0.95	0.11	43,43,43,43	0
57	MG	AA	1807	1/1	0.95	0.07	68,68,68,68	0
57	MG	BA	3350	1/1	0.95	0.12	34,34,34,34	0
57	MG	BB	3008	1/1	0.95	0.36	59,59,59,59	0
57	MG	BA	3032	1/1	0.95	0.21	33,33,33,33	0
57	MG	BA	3451	1/1	0.95	0.25	44,44,44,44	0
57	MG	DN	5001	1/1	0.95	0.11	63,63,63,63	0
57	MG	AA	1786	1/1	0.95	0.14	69,69,69,69	0
57	MG	BA	3567	1/1	0.95	0.25	32,32,32,32	0
57	MG	BB	3014	1/1	0.95	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3354	1/1	0.95	0.12	47,47,47,47	0
57	MG	BA	3455	1/1	0.95	0.14	52,52,52,52	0
57	MG	BB	3018	1/1	0.95	0.06	54,54,54,54	0
57	MG	DA	3474	1/1	0.95	0.09	53,53,53,53	0
57	MG	CA	3074	1/1	0.95	0.14	60,60,60,60	0
57	MG	BA	3355	1/1	0.95	0.15	35,35,35,35	0
57	MG	BA	3572	1/1	0.95	0.26	39,39,39,39	0
57	MG	BA	3691	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3152	1/1	0.95	0.26	23,23,23,23	0
57	MG	BD	3007	1/1	0.95	0.30	46,46,46,46	0
59	ZN	BY	501	1/1	0.95	0.18	68,68,68,68	0
57	MG	DA	3252	1/1	0.95	0.07	50,50,50,50	0
57	MG	BA	3459	1/1	0.95	0.15	31,31,31,31	0
57	MG	BA	3575	1/1	0.95	0.12	50,50,50,50	0
57	MG	BA	3213	1/1	0.95	0.15	43,43,43,43	0
57	MG	BA	3756	1/1	0.96	0.19	18,18,18,18	0
57	MG	DA	3117	1/1	0.96	0.09	56,56,56,56	0
57	MG	B7	105	1/1	0.96	0.20	28,28,28,28	0
57	MG	CA	3138	1/1	0.96	0.10	65,65,65,65	0
57	MG	DA	3121	1/1	0.96	0.10	40,40,40,40	0
57	MG	BA	3046	1/1	0.96	0.15	43,43,43,43	0
57	MG	CA	3140	1/1	0.96	0.16	57,57,57,57	0
57	MG	DA	3309	1/1	0.96	0.12	48,48,48,48	0
57	MG	BA	3521	1/1	0.96	0.22	40,40,40,40	0
57	MG	B9	502	1/1	0.96	0.34	46,46,46,46	0
57	MG	AA	1744	1/1	0.96	0.17	44,44,44,44	0
57	MG	BA	3082	1/1	0.96	0.18	28,28,28,28	0
57	MG	BA	3762	1/1	0.96	0.18	20,20,20,20	0
57	MG	BA	3643	1/1	0.96	0.12	52,52,52,52	0
57	MG	BA	3764	1/1	0.96	0.20	66,66,66,66	0
57	MG	DA	3525	1/1	0.96	0.15	28,28,28,28	0
57	MG	CA	3149	1/1	0.96	0.12	54,54,54,54	0
57	MG	BA	3159	1/1	0.96	0.18	27,27,27,27	0
57	MG	BA	3119	1/1	0.96	0.15	46,46,46,46	0
57	MG	BA	3214	1/1	0.96	0.50	43,43,43,43	0
57	MG	BA	3336	1/1	0.96	0.17	20,20,20,20	0
57	MG	BA	3648	1/1	0.96	0.22	58,58,58,58	0
57	MG	DA	3137	1/1	0.96	0.17	52,52,52,52	0
57	MG	CA	3155	1/1	0.96	0.15	57,57,57,57	0
57	MG	CA	3156	1/1	0.96	0.08	59,59,59,59	0
57	MG	BA	3215	1/1	0.96	0.42	37,37,37,37	0
57	MG	BA	3216	1/1	0.96	0.28	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	3430	1/1	0.96	0.24	34,34,34,34	0
57	MG	AE	3001	1/1	0.96	0.07	63,63,63,63	0
57	MG	BA	3654	1/1	0.96	0.11	59,59,59,59	0
57	MG	AA	1706	1/1	0.96	0.22	60,60,60,60	0
57	MG	BA	3050	1/1	0.96	0.15	32,32,32,32	0
57	MG	BA	3783	1/1	0.96	0.15	37,37,37,37	0
57	MG	AA	1719	1/1	0.96	0.16	63,63,63,63	0
57	MG	BA	3090	1/1	0.96	0.26	38,38,38,38	0
57	MG	DA	3343	1/1	0.96	0.15	34,34,34,34	0
57	MG	BA	3278	1/1	0.96	0.78	54,54,54,54	0
57	MG	DA	3152	1/1	0.96	0.17	45,45,45,45	0
57	MG	BA	3787	1/1	0.96	0.14	45,45,45,45	0
57	MG	DA	3349	1/1	0.96	0.16	34,34,34,34	0
57	MG	DA	3350	1/1	0.96	0.18	31,31,31,31	0
57	MG	BA	3438	1/1	0.96	0.20	35,35,35,35	0
57	MG	CF	3001	1/1	0.96	0.12	51,51,51,51	0
57	MG	DA	3354	1/1	0.96	0.11	41,41,41,41	0
57	MG	BA	3167	1/1	0.96	0.18	45,45,45,45	0
57	MG	DA	3157	1/1	0.96	0.13	34,34,34,34	0
57	MG	CK	5001	1/1	0.96	0.05	61,61,61,61	0
57	MG	BA	3440	1/1	0.96	0.20	35,35,35,35	0
57	MG	DA	3360	1/1	0.96	0.09	31,31,31,31	0
57	MG	BA	3791	1/1	0.96	0.38	49,49,49,49	0
57	MG	CA	3028	1/1	0.96	0.27	48,48,48,48	0
57	MG	DA	3162	1/1	0.96	0.14	57,57,57,57	0
57	MG	BA	3022	1/1	0.96	0.11	25,25,25,25	0
57	MG	DA	3365	1/1	0.96	0.14	19,19,19,19	0
57	MG	BA	3352	1/1	0.96	0.16	68,68,68,68	0
57	MG	BA	3795	1/1	0.96	0.25	19,19,19,19	0
57	MG	AA	1779	1/1	0.96	0.14	59,59,59,59	0
57	MG	BA	3797	1/1	0.96	0.32	51,51,51,51	0
57	MG	DA	3573	1/1	0.96	0.05	61,61,61,61	0
57	MG	BA	3226	1/1	0.96	0.22	25,25,25,25	0
57	MG	AA	1760	1/1	0.96	0.15	65,65,65,65	0
57	MG	AA	1734	1/1	0.96	0.12	43,43,43,43	0
57	MG	BA	3447	1/1	0.96	0.32	52,52,52,52	0
57	MG	DA	3011	1/1	0.96	0.07	35,35,35,35	0
57	MG	CA	3038	1/1	0.96	0.09	57,57,57,57	0
57	MG	BA	3285	1/1	0.96	0.15	58,58,58,58	0
57	MG	BA	3172	1/1	0.96	0.26	40,40,40,40	0
57	MG	DA	3380	1/1	0.96	0.04	66,66,66,66	0
57	MG	BA	3361	1/1	0.96	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3183	1/1	0.96	0.17	41,41,41,41	0
57	MG	AA	1748	1/1	0.96	0.16	64,64,64,64	0
57	MG	DA	3387	1/1	0.96	0.10	59,59,59,59	0
57	MG	BA	3130	1/1	0.96	0.46	48,48,48,48	0
57	MG	BA	3808	1/1	0.96	0.15	38,38,38,38	0
57	MG	BA	3454	1/1	0.96	0.17	46,46,46,46	0
57	MG	AA	1736	1/1	0.96	0.10	49,49,49,49	0
57	MG	BA	3291	1/1	0.96	0.26	53,53,53,53	0
57	MG	BA	3234	1/1	0.96	0.12	52,52,52,52	0
57	MG	BA	3565	1/1	0.96	0.14	61,61,61,61	0
57	MG	DA	3029	1/1	0.96	0.57	45,45,45,45	0
57	MG	DA	3598	1/1	0.96	0.10	55,55,55,55	0
57	MG	AA	1637	1/1	0.96	0.10	61,61,61,61	0
57	MG	BA	3568	1/1	0.96	0.23	24,24,24,24	0
57	MG	AA	1767	1/1	0.96	0.11	67,67,67,67	0
57	MG	AA	1685	1/1	0.96	0.21	62,62,62,62	0
57	MG	BA	3464	1/1	0.96	0.13	44,44,44,44	0
57	MG	BA	3374	1/1	0.96	0.19	50,50,50,50	0
57	MG	BA	3466	1/1	0.96	0.17	51,51,51,51	0
57	MG	BA	3468	1/1	0.96	0.19	45,45,45,45	0
57	MG	BA	3031	1/1	0.96	0.27	36,36,36,36	0
57	MG	BB	3015	1/1	0.96	0.26	45,45,45,45	0
57	MG	DA	3044	1/1	0.96	0.19	53,53,53,53	0
57	MG	BA	3376	1/1	0.96	0.19	29,29,29,29	0
57	MG	AA	1725	1/1	0.96	0.22	51,51,51,51	0
57	MG	CA	3066	1/1	0.96	0.14	48,48,48,48	0
57	MG	BA	3034	1/1	0.96	0.23	35,35,35,35	0
57	MG	DA	3214	1/1	0.96	0.08	51,51,51,51	0
57	MG	DA	3215	1/1	0.96	0.18	40,40,40,40	0
57	MG	DA	3216	1/1	0.96	0.15	35,35,35,35	0
57	MG	BA	3035	1/1	0.96	0.27	49,49,49,49	0
57	MG	BA	3380	1/1	0.96	0.15	40,40,40,40	0
57	MG	AA	1647	1/1	0.96	0.22	44,44,44,44	0
57	MG	DA	3221	1/1	0.96	0.10	41,41,41,41	0
57	MG	BA	3585	1/1	0.96	0.16	29,29,29,29	0
57	MG	BA	3142	1/1	0.96	0.31	46,46,46,46	0
57	MG	AA	1811	1/1	0.96	0.21	49,49,49,49	0
57	MG	DA	3058	1/1	0.96	0.08	61,61,61,61	0
57	MG	DA	3059	1/1	0.96	0.10	50,50,50,50	0
57	MG	BE	302	1/1	0.96	0.16	35,35,35,35	0
57	MG	DA	3228	1/1	0.96	0.16	44,44,44,44	0
57	MG	DA	3430	1/1	0.96	0.13	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	3144	1/1	0.96	0.18	41,41,41,41	0
57	MG	DA	3432	1/1	0.96	0.17	52,52,52,52	0
57	MG	DA	3231	1/1	0.96	0.18	61,61,61,61	0
57	MG	BA	3590	1/1	0.96	0.15	33,33,33,33	0
57	MG	BA	3482	1/1	0.96	0.16	51,51,51,51	0
57	MG	DA	3638	1/1	0.96	0.09	47,47,47,47	0
57	MG	DA	3437	1/1	0.96	0.18	48,48,48,48	0
57	MG	BA	3196	1/1	0.96	0.23	56,56,56,56	0
57	MG	AA	1773	1/1	0.96	0.10	61,61,61,61	0
57	MG	CA	3083	1/1	0.96	0.16	50,50,50,50	0
57	MG	BA	3595	1/1	0.96	0.09	61,61,61,61	0
57	MG	BF	303	1/1	0.96	0.26	33,33,33,33	0
57	MG	BF	304	1/1	0.96	0.39	41,41,41,41	0
57	MG	DA	3647	1/1	0.96	0.11	52,52,52,52	0
57	MG	BA	3711	1/1	0.96	0.25	44,44,44,44	0
57	MG	BA	3306	1/1	0.96	0.17	15,15,15,15	0
57	MG	BF	308	1/1	0.96	0.08	43,43,43,43	0
57	MG	BF	309	1/1	0.96	0.18	31,31,31,31	0
57	MG	DA	3652	1/1	0.96	0.16	31,31,31,31	0
57	MG	DA	3450	1/1	0.96	0.06	50,50,50,50	0
57	MG	BA	3486	1/1	0.96	0.13	41,41,41,41	0
57	MG	DA	3246	1/1	0.96	0.06	46,46,46,46	0
57	MG	BA	3392	1/1	0.96	0.18	26,26,26,26	0
57	MG	BG	201	1/1	0.96	0.14	39,39,39,39	0
57	MG	BA	3307	1/1	0.96	0.19	28,28,28,28	0
57	MG	DA	3457	1/1	0.96	0.18	44,44,44,44	0
57	MG	BA	3308	1/1	0.96	0.23	39,39,39,39	0
57	MG	DA	3664	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3492	1/1	0.96	0.12	38,38,38,38	0
57	MG	BA	3720	1/1	0.96	0.12	38,38,38,38	0
57	MG	BA	3602	1/1	0.96	0.11	47,47,47,47	0
57	MG	BP	3001	1/1	0.96	0.14	34,34,34,34	0
57	MG	BA	3493	1/1	0.96	0.21	38,38,38,38	0
57	MG	BA	3396	1/1	0.96	0.23	25,25,25,25	0
57	MG	DA	3258	1/1	0.96	0.16	45,45,45,45	0
57	MG	BA	3724	1/1	0.96	0.18	20,20,20,20	0
57	MG	BA	3397	1/1	0.96	0.15	28,28,28,28	0
57	MG	BA	3398	1/1	0.96	0.22	32,32,32,32	0
57	MG	DA	3263	1/1	0.96	0.13	65,65,65,65	0
57	MG	DA	3265	1/1	0.96	0.16	57,57,57,57	0
57	MG	DA	3473	1/1	0.96	0.22	50,50,50,50	0
57	MG	BA	3610	1/1	0.96	0.09	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	3108	1/1	0.96	0.21	42,42,42,42	0
57	MG	BA	3249	1/1	0.96	0.23	53,53,53,53	0
57	MG	DA	3270	1/1	0.96	0.09	42,42,42,42	0
57	MG	DE	3004	1/1	0.96	0.17	31,31,31,31	0
57	MG	BA	3502	1/1	0.96	0.19	30,30,30,30	0
57	MG	DE	3007	1/1	0.96	0.11	58,58,58,58	0
57	MG	BA	3503	1/1	0.96	0.10	51,51,51,51	0
57	MG	AA	1813	1/1	0.96	0.21	38,38,38,38	0
57	MG	DA	3098	1/1	0.96	0.10	66,66,66,66	0
57	MG	DA	3276	1/1	0.96	0.16	28,28,28,28	0
57	MG	DA	3484	1/1	0.96	0.07	46,46,46,46	0
57	MG	BA	3402	1/1	0.96	0.18	27,27,27,27	0
57	MG	AA	1608	1/1	0.96	0.22	43,43,43,43	0
57	MG	BA	3201	1/1	0.96	0.21	48,48,48,48	0
57	MG	BA	3405	1/1	0.96	0.16	52,52,52,52	0
57	MG	BA	3319	1/1	0.96	0.22	23,23,23,23	0
57	MG	BA	3013	1/1	0.96	0.20	28,28,28,28	0
57	MG	BA	3151	1/1	0.96	0.17	36,36,36,36	0
57	MG	BA	3409	1/1	0.96	0.23	22,22,22,22	0
57	MG	BA	3204	1/1	0.96	0.27	67,67,67,67	0
57	MG	DA	3109	1/1	0.96	0.13	49,49,49,49	0
57	MG	DW	3001	1/1	0.96	0.21	41,41,41,41	0
57	MG	BA	3514	1/1	0.96	0.19	43,43,43,43	0
57	MG	BA	3205	1/1	0.96	0.43	57,57,57,57	0
57	MG	BA	3076	1/1	0.96	0.38	42,42,42,42	0
57	MG	AA	1716	1/1	0.96	0.17	50,50,50,50	0
57	MG	DA	3503	1/1	0.96	0.22	38,38,38,38	0
57	MG	BA	3262	1/1	0.96	0.27	31,31,31,31	0
57	MG	DA	3293	1/1	0.96	0.15	61,61,61,61	0
57	MG	AA	1793	1/1	0.96	0.17	63,63,63,63	0
57	MG	DA	3507	1/1	0.96	0.07	59,59,59,59	0
57	MG	AA	1653	1/1	0.97	0.23	54,54,54,54	0
57	MG	DA	3334	1/1	0.97	0.22	57,57,57,57	0
57	MG	BA	3344	1/1	0.97	0.10	71,71,71,71	0
57	MG	BA	3634	1/1	0.97	0.14	55,55,55,55	0
57	MG	BA	3635	1/1	0.97	0.12	42,42,42,42	0
57	MG	DA	3169	1/1	0.97	0.28	41,41,41,41	0
57	MG	BA	3547	1/1	0.97	0.16	45,45,45,45	0
57	MG	DA	3340	1/1	0.97	0.14	27,27,27,27	0
57	MG	BA	3548	1/1	0.97	0.13	35,35,35,35	0
57	MG	DA	3027	1/1	0.97	0.53	43,43,43,43	0
57	MG	BA	3736	1/1	0.97	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3473	1/1	0.97	0.19	28,28,28,28	0
57	MG	BA	3639	1/1	0.97	0.18	49,49,49,49	0
57	MG	BA	3174	1/1	0.97	0.53	38,38,38,38	0
57	MG	DA	3348	1/1	0.97	0.21	53,53,53,53	0
57	MG	AU	101	1/1	0.97	0.12	56,56,56,56	0
57	MG	DA	3537	1/1	0.97	0.16	45,45,45,45	0
57	MG	AA	1665	1/1	0.97	0.16	55,55,55,55	0
57	MG	DA	3180	1/1	0.97	0.21	48,48,48,48	0
57	MG	AA	1703	1/1	0.97	0.29	43,43,43,43	0
57	MG	DA	3353	1/1	0.97	0.13	47,47,47,47	0
57	MG	DA	3182	1/1	0.97	0.21	52,52,52,52	0
57	MG	BA	3089	1/1	0.97	0.19	36,36,36,36	0
57	MG	DA	3544	1/1	0.97	0.12	53,53,53,53	0
57	MG	DA	3036	1/1	0.97	0.17	35,35,35,35	0
57	MG	DA	3037	1/1	0.97	0.12	26,26,26,26	0
57	MG	BH	201	1/1	0.97	0.19	56,56,56,56	0
57	MG	DA	3039	1/1	0.97	0.16	38,38,38,38	0
57	MG	DA	3040	1/1	0.97	0.14	28,28,28,28	0
57	MG	AA	1803	1/1	0.97	0.12	46,46,46,46	0
57	MG	BA	3256	1/1	0.97	0.34	34,34,34,34	0
57	MG	BA	3412	1/1	0.97	0.17	30,30,30,30	0
57	MG	BA	3749	1/1	0.97	0.16	52,52,52,52	0
57	MG	DA	3045	1/1	0.97	0.22	51,51,51,51	0
57	MG	CA	3084	1/1	0.97	0.14	56,56,56,56	0
57	MG	BA	3559	1/1	0.97	0.22	26,26,26,26	0
57	MG	DA	3198	1/1	0.97	0.16	52,52,52,52	0
57	MG	DA	3370	1/1	0.97	0.13	59,59,59,59	0
57	MG	BA	3560	1/1	0.97	0.14	63,63,63,63	0
57	MG	BQ	3001	1/1	0.97	0.26	37,37,37,37	0
57	MG	BA	3413	1/1	0.97	0.17	37,37,37,37	0
57	MG	BA	3180	1/1	0.97	0.27	46,46,46,46	0
57	MG	DA	3203	1/1	0.97	0.18	53,53,53,53	0
57	MG	AA	1624	1/1	0.97	0.25	66,66,66,66	0
57	MG	BA	3260	1/1	0.97	0.20	19,19,19,19	0
57	MG	BA	3356	1/1	0.97	0.24	31,31,31,31	0
57	MG	BU	203	1/1	0.97	0.31	34,34,34,34	0
57	MG	CA	3096	1/1	0.97	0.18	43,43,43,43	0
57	MG	BA	3566	1/1	0.97	0.21	31,31,31,31	0
57	MG	BA	3760	1/1	0.97	0.17	50,50,50,50	0
57	MG	DA	3386	1/1	0.97	0.10	44,44,44,44	0
57	MG	BV	203	1/1	0.97	0.21	23,23,23,23	0
57	MG	DA	3213	1/1	0.97	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3062	1/1	0.97	0.11	53,53,53,53	0
57	MG	BA	3357	1/1	0.97	0.07	34,34,34,34	0
57	MG	BA	3490	1/1	0.97	0.17	43,43,43,43	0
57	MG	AA	1727	1/1	0.97	0.14	50,50,50,50	0
57	MG	BA	3221	1/1	0.97	0.21	29,29,29,29	0
57	MG	CA	3105	1/1	0.97	0.11	75,75,75,75	0
57	MG	BA	3184	1/1	0.97	0.21	42,42,42,42	0
57	MG	BA	3494	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3185	1/1	0.97	0.15	33,33,33,33	0
57	MG	BA	3496	1/1	0.97	0.12	51,51,51,51	0
57	MG	BA	3424	1/1	0.97	0.29	31,31,31,31	0
57	MG	DA	3073	1/1	0.97	0.08	33,33,33,33	0
57	MG	BA	3770	1/1	0.97	0.44	49,49,49,49	0
57	MG	BA	3576	1/1	0.97	0.24	30,30,30,30	0
57	MG	DA	3229	1/1	0.97	0.12	38,38,38,38	0
57	MG	BA	3362	1/1	0.97	0.22	47,47,47,47	0
57	MG	BA	3669	1/1	0.97	0.20	28,28,28,28	0
57	MG	BA	3186	1/1	0.97	0.27	41,41,41,41	0
57	MG	B5	104	1/1	0.97	0.09	58,58,58,58	0
57	MG	BA	3776	1/1	0.97	0.22	60,60,60,60	0
57	MG	CA	3118	1/1	0.97	0.18	60,60,60,60	0
57	MG	BA	3777	1/1	0.97	0.10	41,41,41,41	0
57	MG	AA	1642	1/1	0.97	0.23	59,59,59,59	0
57	MG	B7	102	1/1	0.97	0.17	41,41,41,41	0
57	MG	AA	1668	1/1	0.97	0.10	63,63,63,63	0
57	MG	BA	3311	1/1	0.97	0.19	56,56,56,56	0
57	MG	BA	3674	1/1	0.97	0.34	48,48,48,48	0
57	MG	BA	3227	1/1	0.97	0.17	33,33,33,33	0
57	MG	BA	3190	1/1	0.97	0.28	54,54,54,54	0
57	MG	BA	3586	1/1	0.97	0.11	55,55,55,55	0
57	MG	CA	3128	1/1	0.97	0.13	52,52,52,52	0
57	MG	BA	3370	1/1	0.97	0.24	50,50,50,50	0
57	MG	DA	3248	1/1	0.97	0.11	58,58,58,58	0
57	MG	BA	3434	1/1	0.97	0.12	19,19,19,19	0
57	MG	BA	3315	1/1	0.97	0.18	40,40,40,40	0
57	MG	DA	3428	1/1	0.97	0.11	38,38,38,38	0
57	MG	CA	3132	1/1	0.97	0.14	64,64,64,64	0
57	MG	CA	3133	1/1	0.97	0.17	82,82,82,82	0
57	MG	BA	3316	1/1	0.97	0.20	54,54,54,54	0
57	MG	BA	3004	1/1	0.97	0.22	36,36,36,36	0
57	MG	BA	3683	1/1	0.97	0.21	62,62,62,62	0
57	MG	BA	3045	1/1	0.97	0.17	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	AA	1661	1/1	0.97	0.37	54,54,54,54	0
57	MG	DA	3436	1/1	0.97	0.11	35,35,35,35	0
57	MG	AA	1809	1/1	0.97	0.17	42,42,42,42	0
57	MG	BA	3007	1/1	0.97	0.23	21,21,21,21	0
57	MG	BA	3157	1/1	0.97	0.20	46,46,46,46	0
57	MG	DA	3629	1/1	0.97	0.12	57,57,57,57	0
57	MG	DA	3440	1/1	0.97	0.13	36,36,36,36	0
57	MG	BA	3072	1/1	0.97	0.24	49,49,49,49	0
57	MG	DA	3262	1/1	0.97	0.13	20,20,20,20	0
57	MG	AA	1627	1/1	0.97	0.14	54,54,54,54	0
57	MG	DA	3264	1/1	0.97	0.18	51,51,51,51	0
57	MG	AA	1611	1/1	0.97	0.19	20,20,20,20	0
57	MG	AN	502	1/1	0.97	0.29	62,62,62,62	0
57	MG	DA	3267	1/1	0.97	0.12	44,44,44,44	0
57	MG	BA	3385	1/1	0.97	0.23	30,30,30,30	0
57	MG	DA	3640	1/1	0.97	0.10	62,62,62,62	0
57	MG	BA	3603	1/1	0.97	0.28	42,42,42,42	0
57	MG	BA	3448	1/1	0.97	0.18	17,17,17,17	0
57	MG	BA	3605	1/1	0.97	0.18	47,47,47,47	0
57	MG	BA	3606	1/1	0.97	0.16	36,36,36,36	0
57	MG	BA	3698	1/1	0.97	0.11	47,47,47,47	0
57	MG	BA	3810	1/1	0.97	0.21	35,35,35,35	0
57	MG	BA	3162	1/1	0.97	0.29	41,41,41,41	0
57	MG	DA	3120	1/1	0.97	0.33	56,56,56,56	0
57	MG	BA	3387	1/1	0.97	0.20	29,29,29,29	0
57	MG	BA	3077	1/1	0.97	0.20	15,15,15,15	0
57	MG	BA	3133	1/1	0.97	0.27	37,37,37,37	0
57	MG	CA	3158	1/1	0.97	0.20	55,55,55,55	0
57	MG	BA	3331	1/1	0.97	0.20	53,53,53,53	0
57	MG	DA	3654	1/1	0.97	0.19	35,35,35,35	0
57	MG	DA	3655	1/1	0.97	0.08	38,38,38,38	0
57	MG	BA	3612	1/1	0.97	0.10	60,60,60,60	0
57	MG	BA	3391	1/1	0.97	0.15	41,41,41,41	0
57	MG	BB	3007	1/1	0.97	0.17	41,41,41,41	0
57	MG	BA	3011	1/1	0.97	0.15	30,30,30,30	0
57	MG	BA	3393	1/1	0.97	0.20	23,23,23,23	0
57	MG	DA	3661	1/1	0.97	0.10	62,62,62,62	0
57	MG	BA	3053	1/1	0.97	0.27	23,23,23,23	0
57	MG	CA	3167	1/1	0.97	0.30	57,57,57,57	0
57	MG	DA	3290	1/1	0.97	0.14	33,33,33,33	0
57	MG	BB	3011	1/1	0.97	0.20	47,47,47,47	0
57	MG	BA	3136	1/1	0.97	0.36	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3287	1/1	0.97	0.17	27,27,27,27	0
57	MG	DA	3294	1/1	0.97	0.12	40,40,40,40	0
57	MG	BA	3461	1/1	0.97	0.11	45,45,45,45	0
57	MG	BA	3054	1/1	0.97	0.22	30,30,30,30	0
57	MG	BA	3621	1/1	0.97	0.19	43,43,43,43	0
57	MG	BA	3463	1/1	0.97	0.21	56,56,56,56	0
57	MG	AA	1735	1/1	0.97	0.12	45,45,45,45	0
57	MG	DA	3302	1/1	0.97	0.23	53,53,53,53	0
57	MG	DA	3303	1/1	0.97	0.12	43,43,43,43	0
57	MG	DA	3304	1/1	0.97	0.14	42,42,42,42	0
57	MG	CA	3043	1/1	0.97	0.18	44,44,44,44	0
57	MG	BA	3033	1/1	0.97	0.40	31,31,31,31	0
57	MG	DA	3489	1/1	0.97	0.09	48,48,48,48	0
57	MG	DD	304	1/1	0.97	0.09	36,36,36,36	0
57	MG	DA	3307	1/1	0.97	0.12	51,51,51,51	0
57	MG	BA	3083	1/1	0.97	0.34	60,60,60,60	0
57	MG	DA	3492	1/1	0.97	0.07	48,48,48,48	0
57	MG	DA	3144	1/1	0.97	0.23	41,41,41,41	0
57	MG	DE	3006	1/1	0.97	0.21	38,38,38,38	0
57	MG	CA	3047	1/1	0.97	0.16	50,50,50,50	0
57	MG	DA	3495	1/1	0.97	0.05	50,50,50,50	0
57	MG	CA	3048	1/1	0.97	0.12	58,58,58,58	0
57	MG	BB	3021	1/1	0.97	0.18	41,41,41,41	0
57	MG	DF	304	1/1	0.97	0.07	51,51,51,51	0
57	MG	BA	3341	1/1	0.97	0.20	18,18,18,18	0
57	MG	BB	3023	1/1	0.97	0.16	47,47,47,47	0
57	MG	DA	3005	1/1	0.97	0.16	54,54,54,54	0
57	MG	DA	3501	1/1	0.97	0.10	49,49,49,49	0
57	MG	DA	3316	1/1	0.97	0.20	57,57,57,57	0
57	MG	BD	3001	1/1	0.97	0.14	34,34,34,34	0
57	MG	DA	3007	1/1	0.97	0.13	30,30,30,30	0
57	MG	DA	3319	1/1	0.97	0.14	33,33,33,33	0
57	MG	BA	3627	1/1	0.97	0.21	56,56,56,56	0
57	MG	DA	3321	1/1	0.97	0.15	29,29,29,29	0
57	MG	BD	3004	1/1	0.97	0.20	28,28,28,28	0
57	MG	DA	3323	1/1	0.97	0.21	49,49,49,49	0
57	MG	BD	3005	1/1	0.97	0.24	44,44,44,44	0
57	MG	BA	3628	1/1	0.97	0.28	52,52,52,52	0
57	MG	DA	3326	1/1	0.97	0.10	46,46,46,46	0
57	MG	BD	3010	1/1	0.97	0.20	46,46,46,46	0
57	MG	DA	3014	1/1	0.97	0.22	44,44,44,44	0
59	ZN	AN	501	1/1	0.97	0.16	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3725	1/1	0.97	0.18	31,31,31,31	0
57	MG	BA	3342	1/1	0.97	0.29	67,67,67,67	0
57	MG	BA	3630	1/1	0.97	0.25	39,39,39,39	0
59	ZN	DY	501	1/1	0.97	0.11	90,90,90,90	0
57	MG	DA	3518	1/1	0.97	0.10	56,56,56,56	0
59	ZN	D6	501	1/1	0.97	0.18	65,65,65,65	0
59	ZN	D9	501	1/1	0.97	0.12	64,64,64,64	0
57	MG	BA	3544	1/1	0.97	0.18	52,52,52,52	0
57	MG	BA	3719	1/1	0.98	0.20	41,41,41,41	0
57	MG	BA	3021	1/1	0.98	0.12	43,43,43,43	0
57	MG	DA	3615	1/1	0.98	0.09	62,62,62,62	0
57	MG	BA	3772	1/1	0.98	0.15	36,36,36,36	0
57	MG	AA	1740	1/1	0.98	0.17	41,41,41,41	0
57	MG	BA	3114	1/1	0.98	0.20	39,39,39,39	0
57	MG	BA	3039	1/1	0.98	0.19	36,36,36,36	0
57	MG	BA	3075	1/1	0.98	0.20	24,24,24,24	0
57	MG	BA	3591	1/1	0.98	0.39	41,41,41,41	0
57	MG	AA	1732	1/1	0.98	0.20	63,63,63,63	0
57	MG	DA	3085	1/1	0.98	0.18	28,28,28,28	0
57	MG	DA	3521	1/1	0.98	0.09	57,57,57,57	0
57	MG	DA	3245	1/1	0.98	0.08	58,58,58,58	0
57	MG	BA	3779	1/1	0.98	0.19	17,17,17,17	0
57	MG	DA	3163	1/1	0.98	0.21	34,34,34,34	0
57	MG	DA	3013	1/1	0.98	0.13	39,39,39,39	0
57	MG	BA	3467	1/1	0.98	0.13	46,46,46,46	0
57	MG	BD	3002	1/1	0.98	0.21	28,28,28,28	0
57	MG	AA	1761	1/1	0.98	0.20	70,70,70,70	0
57	MG	DA	3632	1/1	0.98	0.17	52,52,52,52	0
57	MG	DA	3168	1/1	0.98	0.12	44,44,44,44	0
57	MG	BA	3782	1/1	0.98	0.16	38,38,38,38	0
57	MG	BA	3182	1/1	0.98	0.67	52,52,52,52	0
57	MG	DA	3093	1/1	0.98	0.13	47,47,47,47	0
57	MG	AA	1762	1/1	0.98	0.21	66,66,66,66	0
57	MG	DA	3020	1/1	0.98	0.12	26,26,26,26	0
57	MG	BD	3008	1/1	0.98	0.30	45,45,45,45	0
57	MG	DA	3345	1/1	0.98	0.15	58,58,58,58	0
57	MG	BD	3009	1/1	0.98	0.16	37,37,37,37	0
57	MG	AA	1702	1/1	0.98	0.27	47,47,47,47	0
57	MG	BA	3472	1/1	0.98	0.20	24,24,24,24	0
57	MG	DA	3178	1/1	0.98	0.17	40,40,40,40	0
57	MG	DA	3025	1/1	0.98	0.45	47,47,47,47	0
57	MG	BA	3368	1/1	0.98	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3447	1/1	0.98	0.16	59,59,59,59	0
57	MG	CA	3067	1/1	0.98	0.24	46,46,46,46	0
57	MG	DA	3103	1/1	0.98	0.22	56,56,56,56	0
57	MG	DA	3546	1/1	0.98	0.04	47,47,47,47	0
57	MG	DA	3547	1/1	0.98	0.08	48,48,48,48	0
57	MG	AA	1720	1/1	0.98	0.19	55,55,55,55	0
57	MG	BA	3339	1/1	0.98	0.21	43,43,43,43	0
57	MG	BA	3371	1/1	0.98	0.10	49,49,49,49	0
57	MG	DA	3453	1/1	0.98	0.17	54,54,54,54	0
57	MG	AA	1677	1/1	0.98	0.21	43,43,43,43	0
57	MG	BA	3739	1/1	0.98	0.11	21,21,21,21	0
57	MG	DA	3188	1/1	0.98	0.24	35,35,35,35	0
57	MG	BA	3793	1/1	0.98	0.22	11,11,11,11	0
57	MG	DA	3274	1/1	0.98	0.22	40,40,40,40	0
57	MG	BA	3312	1/1	0.98	0.19	31,31,31,31	0
57	MG	BA	3259	1/1	0.98	0.18	25,25,25,25	0
57	MG	BF	305	1/1	0.98	0.14	36,36,36,36	0
57	MG	CA	3145	1/1	0.98	0.12	65,65,65,65	0
57	MG	BA	3742	1/1	0.98	0.21	48,48,48,48	0
57	MG	DA	3562	1/1	0.98	0.12	31,31,31,31	0
57	MG	DA	3195	1/1	0.98	0.13	42,42,42,42	0
57	MG	AA	1722	1/1	0.98	0.18	57,57,57,57	0
57	MG	CA	3079	1/1	0.98	0.12	49,49,49,49	0
57	MG	CA	3080	1/1	0.98	0.10	49,49,49,49	0
57	MG	AA	1718	1/1	0.98	0.11	66,66,66,66	0
57	MG	DA	3469	1/1	0.98	0.07	50,50,50,50	0
57	MG	DA	3373	1/1	0.98	0.09	31,31,31,31	0
57	MG	BA	3650	1/1	0.98	0.17	45,45,45,45	0
57	MG	BA	3345	1/1	0.98	0.19	51,51,51,51	0
57	MG	BA	3189	1/1	0.98	0.22	39,39,39,39	0
57	MG	AA	1792	1/1	0.98	0.12	47,47,47,47	0
57	MG	BA	3146	1/1	0.98	0.17	41,41,41,41	0
57	MG	DA	3477	1/1	0.98	0.11	53,53,53,53	0
57	MG	BA	3750	1/1	0.98	0.22	46,46,46,46	0
57	MG	DE	3001	1/1	0.98	0.44	31,31,31,31	0
57	MG	BA	3751	1/1	0.98	0.23	37,37,37,37	0
57	MG	DA	3381	1/1	0.98	0.15	40,40,40,40	0
57	MG	DA	3050	1/1	0.98	0.25	44,44,44,44	0
57	MG	AA	1730	1/1	0.98	0.25	27,27,27,27	0
57	MG	DA	3581	1/1	0.98	0.07	44,44,44,44	0
57	MG	BA	3488	1/1	0.98	0.13	20,20,20,20	0
57	MG	BA	3701	1/1	0.98	0.23	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	DA	3584	1/1	0.98	0.09	31,31,31,31	0
57	MG	DA	3054	1/1	0.98	0.10	27,27,27,27	0
57	MG	DA	3297	1/1	0.98	0.18	51,51,51,51	0
57	MG	BA	3382	1/1	0.98	0.12	55,55,55,55	0
57	MG	BA	3811	1/1	0.98	0.21	48,48,48,48	0
57	MG	DA	3300	1/1	0.98	0.10	38,38,38,38	0
57	MG	DO	201	1/1	0.98	0.12	49,49,49,49	0
57	MG	CA	3163	1/1	0.98	0.19	62,62,62,62	0
57	MG	BA	3067	1/1	0.98	0.21	43,43,43,43	0
57	MG	DA	3217	1/1	0.98	0.24	57,57,57,57	0
57	MG	BA	3813	1/1	0.98	0.13	29,29,29,29	0
57	MG	BA	3267	1/1	0.98	0.30	61,61,61,61	0
57	MG	AA	1724	1/1	0.98	0.17	39,39,39,39	0
57	MG	BB	3002	1/1	0.98	0.28	55,55,55,55	0
57	MG	DA	3597	1/1	0.98	0.15	48,48,48,48	0
57	MG	AA	1795	1/1	0.98	0.12	55,55,55,55	0
57	MG	DA	3599	1/1	0.98	0.09	48,48,48,48	0
57	MG	BA	3533	1/1	0.98	0.18	23,23,23,23	0
57	MG	BU	204	1/1	0.98	0.31	47,47,47,47	0
57	MG	CA	3104	1/1	0.98	0.23	37,37,37,37	0
57	MG	BA	3534	1/1	0.98	0.23	26,26,26,26	0
58	SF4	AD	501	8/8	0.98	0.15	59,68,73,79	0
58	SF4	CD	501	8/8	0.98	0.14	64,67,74,91	0
57	MG	AA	1796	1/1	0.98	0.07	64,64,64,64	0
57	MG	BA	3665	1/1	0.98	0.17	42,42,42,42	0
57	MG	DA	3408	1/1	0.98	0.23	55,55,55,55	0
57	MG	BA	3173	1/1	0.98	0.28	32,32,32,32	0
57	MG	BA	3457	1/1	0.98	0.19	48,48,48,48	0
57	MG	BA	3326	1/1	0.98	0.15	24,24,24,24	0
57	MG	BA	3539	1/1	0.98	0.14	42,42,42,42	0
57	MG	BA	3020	1/1	0.98	0.21	25,25,25,25	0
57	MG	BA	3425	1/1	0.98	0.25	48,48,48,48	0
57	MG	BA	3800	1/1	0.99	0.19	29,29,29,29	0
57	MG	DA	3383	1/1	0.99	0.13	28,28,28,28	0
57	MG	BA	3085	1/1	0.99	0.29	31,31,31,31	0
57	MG	DA	3355	1/1	0.99	0.11	43,43,43,43	0
57	MG	CA	3044	1/1	0.99	0.16	47,47,47,47	0
57	MG	BA	3707	1/1	0.99	0.19	39,39,39,39	0
57	MG	BD	3006	1/1	0.99	0.09	34,34,34,34	0
57	MG	BV	205	1/1	0.99	0.12	34,34,34,34	0
57	MG	BA	3551	1/1	0.99	0.15	44,44,44,44	0
57	MG	BA	3499	1/1	0.99	0.13	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	DA	3392	1/1	0.99	0.19	53,53,53,53	0
57	MG	AA	1758	1/1	0.99	0.09	37,37,37,37	0
57	MG	BA	3582	1/1	0.99	0.12	31,31,31,31	0
57	MG	BA	3583	1/1	0.99	0.15	33,33,33,33	0
57	MG	BA	3731	1/1	0.99	0.14	32,32,32,32	0
57	MG	BA	3476	1/1	0.99	0.16	48,48,48,48	0
57	MG	DA	3398	1/1	0.99	0.08	40,40,40,40	0
57	MG	BA	3310	1/1	0.99	0.23	26,26,26,26	0
57	MG	AA	1772	1/1	0.99	0.20	47,47,47,47	0
57	MG	BA	3104	1/1	0.99	0.19	24,24,24,24	0
57	MG	BA	3003	1/1	0.99	0.17	33,33,33,33	0
57	MG	CA	3010	1/1	0.99	0.10	49,49,49,49	0
57	MG	CA	3085	1/1	0.99	0.15	41,41,41,41	0
57	MG	BA	3718	1/1	0.99	0.17	47,47,47,47	0
57	MG	DA	3472	1/1	0.99	0.14	25,25,25,25	0
57	MG	DB	3013	1/1	0.99	0.12	66,66,66,66	0
57	MG	B5	101	1/1	0.99	0.27	30,30,30,30	0
57	MG	AA	1678	1/1	0.99	0.25	47,47,47,47	0
57	MG	AA	1681	1/1	0.99	0.12	38,38,38,38	0
59	ZN	B5	103	1/1	0.99	0.21	40,40,40,40	0
59	ZN	B6	102	1/1	0.99	0.26	50,50,50,50	0
57	MG	AA	1672	1/1	0.99	0.17	45,45,45,45	0
57	MG	DA	3209	1/1	0.99	0.09	49,49,49,49	0
57	MG	BA	3417	1/1	0.99	0.21	24,24,24,24	0
59	ZN	D5	501	1/1	0.99	0.19	57,57,57,57	0
57	MG	DA	3412	1/1	0.99	0.14	41,41,41,41	0
57	MG	CA	3092	1/1	0.99	0.24	51,51,51,51	0
57	MG	AA	1770	1/1	0.99	0.13	51,51,51,51	0
59	ZN	B9	501	1/1	1.00	0.23	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.