wwPDB X-ray Structure Validation Summary Report (i)

Mar 28, 2026 – 05:34 PM UTC

PDB ID	:	4V9R / pdb_00004v9r
Title	:	Crystal structure of antibiotic DITYROMYCIN bound to 70S ribosome
Authors	:	Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.; Gualerzi, C.O.; Steitz, T.A.
Deposited on	:	2013-12-05
Resolution	:	3.00 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:

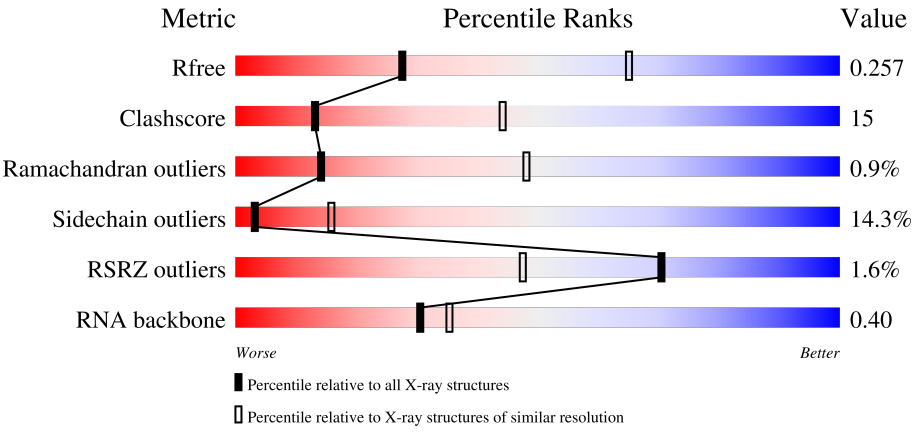
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1522	2% 32% 48% 18%
1	CA	1522	% 34% 46% 18%
2	AB	256	2% 37% 35% 17% 10%
2	CB	256	4% 31% 45% 13% 10%

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Mol	Chain	Length	Quality of chain
3	AC	239	2% 56% 26% 5% 14%
3	CC	239	3% 46% 32% 8% 14%
4	AD	209	3% 47% 44% 8%
4	CD	209	% 50% 40% 10%
5	AE	162	49% 33% 8% 9%
5	CE	162	43% 41% 8% 9%
6	AF	101	% 54% 42%
6	CF	101	63% 32%
7	AG	156	3% 61% 32% 5%
7	CG	156	3% 51% 38% 10%
8	AH	138	54% 38% 8%
8	CH	138	2% 48% 44% 7%
9	AI	128	7% 50% 41% 8%
9	CI	128	21% 46% 48% 5%
10	AJ	105	13% 49% 35% 9% 8%
10	CJ	105	13% 35% 50% 5% 9%
11	AK	129	% 63% 19% 5% 12%
11	CK	129	50% 34% 12%
12	AL	132	3% 57% 32% 8%
12	CL	132	2% 56% 31% 5% 8%
13	AM	126	6% 58% 33% 7%
13	CM	126	6% 54% 34% 8%
14	AN	61	10% 57% 26% 15%
14	CN	61	23% 41% 54%
15	AO	89	% 60% 36%

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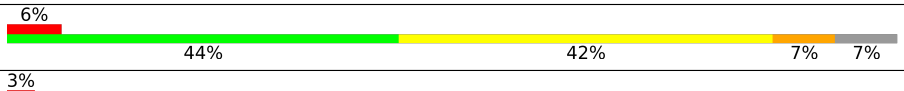
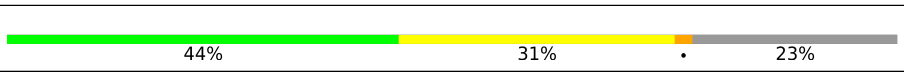
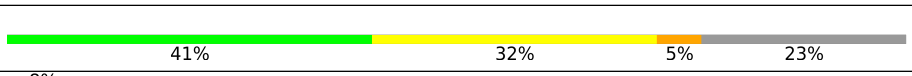
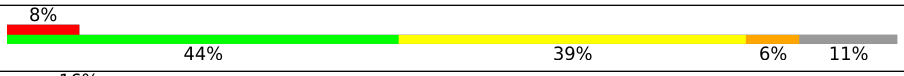
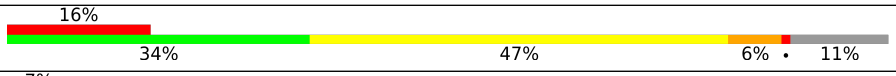
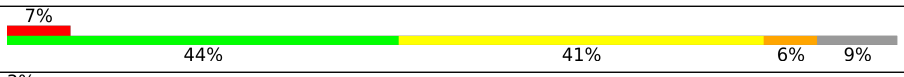
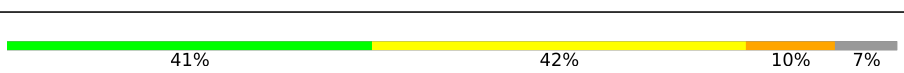
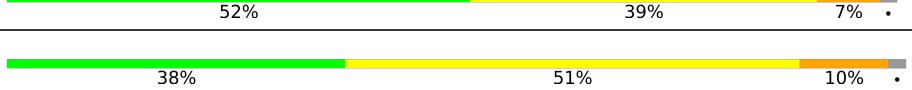
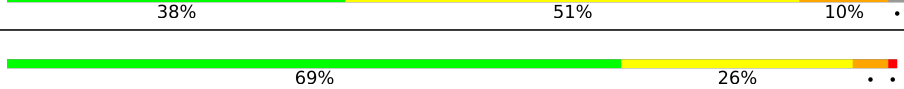
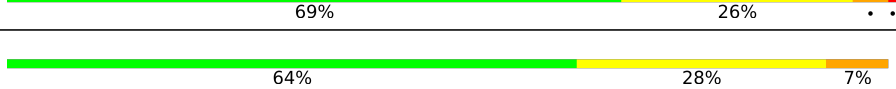
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	

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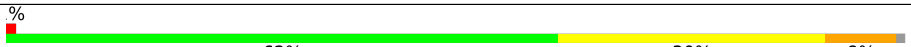
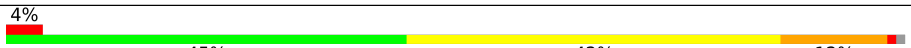
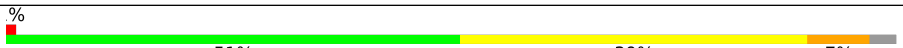
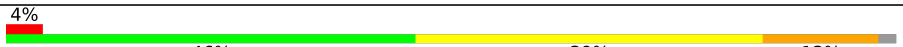
Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	

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Mol	Chain	Length	Quality of chain
40	DU	118	64% 28% 6%
41	BV	101	72% 21% 6%
41	DV	101	62% 30% 7%
42	BW	113	% 74% 19% 6%
42	DW	113	63% 31% 5%
43	BX	96	% 71% 26%
43	DX	96	69% 24% 6%
44	BY	110	3% 67% 26%
44	DY	110	3% 62% 33%
45	BZ	206	% 49% 29% 5% 17%
45	DZ	206	41% 38% 5% 16%
46	B0	85	7% 72% 20% 6%
46	D0	85	4% 60% 27% 11%
47	B1	98	67% 24% 7%
47	D1	98	% 63% 29% 7%
48	B2	72	62% 28% 7%
48	D2	72	58% 33% 6%
49	B3	60	63% 23% 10%
49	D3	60	65% 22% 12%
50	B4	71	41% 34% 20%
50	D4	71	6% 41% 37% 18%
51	B5	60	72% 23%
51	D5	60	70% 28%
52	B6	54	65% 30%
52	D6	54	63% 33%

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Mol	Chain	Length	Quality of chain
53	B7	49	73% 18% 6%
53	D7	49	2% 69% 24%
54	B8	65	52% 45%
54	D8	65	52% 46%
55	B9	37	3% 76% 22%
55	D9	37	3% 54% 41% 5%

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
56	MG	AA	3133	-	-	-	X
56	MG	CA	3028	-	-	-	X
56	MG	CA	3030	-	-	-	X
56	MG	CA	3053	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 286321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32196	14328	5966	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

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

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

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

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

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

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

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

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

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

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

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

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

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

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

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

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

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	7	Total	C	N	O	P	0	0	1
			114	49	22	37	6			
22	CV	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			
23	CX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 24 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AW	10	Total	C	N	O	0	0	0
			93	67	10	16			
24	CW	10	Total	C	N	O	0	0	0
			93	67	10	16			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2731	Total	C	N	O	P	0	0	0
			58834	26185	11020	18899	2730			
25	DA	2714	Total	C	N	O	P	0	0	0
			58458	26018	10942	18786	2712			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

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

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

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

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

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

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

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

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

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

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

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

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

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

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

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

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

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

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

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

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

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

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

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

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			551	348	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			531	338	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

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

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

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

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

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

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	222	Total	Mg	0	0
			222	222		
56	AD	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	1	Total	Mg	0	0
			1	1		
56	AL	1	Total	Mg	0	0
			1	1		
56	AM	2	Total	Mg	0	0
			2	2		
56	AN	1	Total	Mg	0	0
			1	1		
56	AS	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AX	9	Total Mg 9 9	0	0
56	BA	739	Total Mg 739 739	0	0
56	BB	18	Total Mg 18 18	0	0
56	BD	12	Total Mg 12 12	0	0
56	BE	9	Total Mg 9 9	0	0
56	BF	6	Total Mg 6 6	0	0
56	BG	4	Total Mg 4 4	0	0
56	BN	6	Total Mg 6 6	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	4	Total Mg 4 4	0	0
56	BQ	4	Total Mg 4 4	0	0
56	BR	3	Total Mg 3 3	0	0
56	BU	9	Total Mg 9 9	0	0
56	BV	3	Total Mg 3 3	0	0
56	BW	5	Total Mg 5 5	0	0
56	BX	2	Total Mg 2 2	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B0	6	Total Mg 6 6	0	0
56	B1	2	Total Mg 2 2	0	0
56	B2	1	Total Mg 1 1	0	0
56	B3	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B5	1	Total Mg 1 1	0	0
56	B7	4	Total Mg 4 4	0	0
56	B8	2	Total Mg 2 2	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	172	Total Mg 172 172	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CN	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CX	3	Total Mg 3 3	0	0
56	DA	657	Total Mg 657 657	0	0
56	DB	12	Total Mg 12 12	0	0
56	DD	5	Total Mg 5 5	0	0
56	DE	6	Total Mg 6 6	0	0
56	DF	5	Total Mg 5 5	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	1	Total Mg 1 1	0	0
56	DP	2	Total Mg 2 2	0	0
56	DQ	4	Total Mg 4 4	0	0
56	DR	1	Total Mg 1 1	0	0

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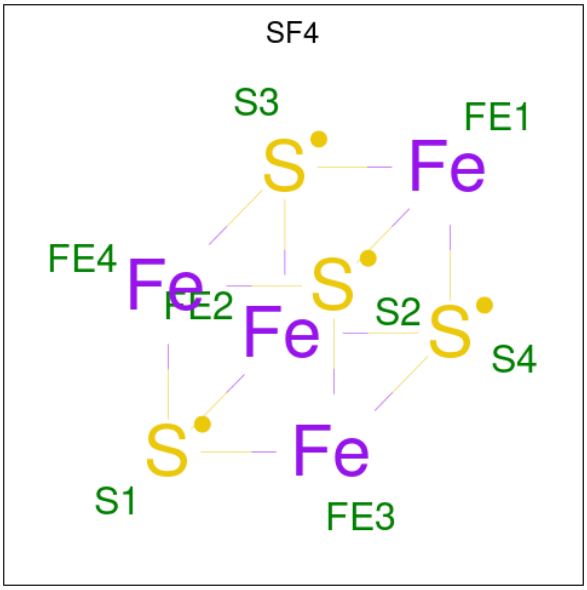
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DU	2	Total Mg 2 2	0	0
56	DV	3	Total Mg 3 3	0	0
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D5	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

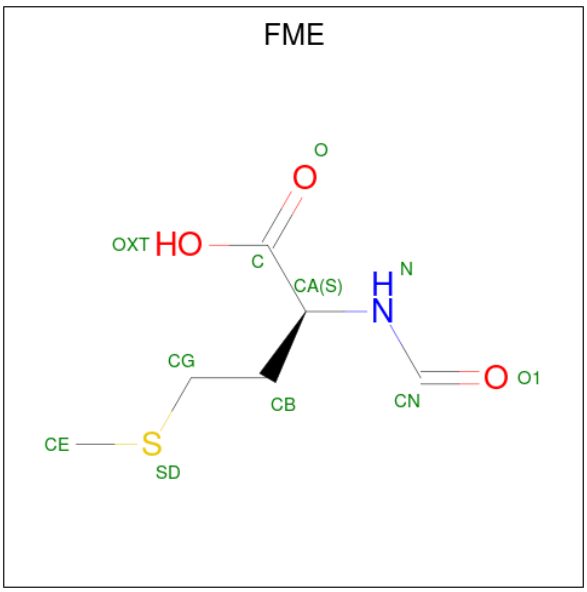


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AD	1	Total Fe S 8 4 4	0	0
57	CD	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AN	1	Total Zn 1 1	0	0
58	BY	1	Total Zn 1 1	0	0
58	B4	1	Total Zn 1 1	0	0
58	B5	1	Total Zn 1 1	0	0
58	B6	1	Total Zn 1 1	0	0
58	B9	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0
58	DY	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0
58	D5	1	Total Zn 1 1	0	0
58	D6	1	Total Zn 1 1	0	0
58	D9	1	Total Zn 1 1	0	0

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AX	1	Total C N O S 10 6 1 2 1	0	0
59	CX	1	Total C N O S 10 6 1 2 1	0	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	BA	1	Total K 1 1	0	0
60	DA	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	147	Total O 147 147	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	AO	2	Total O 2 2	0	0
61	AU	1	Total O 1 1	0	0
61	AV	2	Total O 2 2	0	0
61	AX	1	Total O 1 1	0	0
61	BA	1086	Total O 1086 1086	0	0
61	BB	26	Total O 26 26	0	0
61	BD	6	Total O 6 6	0	0
61	BE	13	Total O 13 13	0	0
61	BF	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BG	1	Total O 1 1	0	0
61	BN	3	Total O 3 3	0	0
61	BO	2	Total O 2 2	0	0
61	BP	15	Total O 15 15	0	0
61	BQ	3	Total O 3 3	0	0
61	BR	1	Total O 1 1	0	0
61	BT	2	Total O 2 2	0	0
61	BU	5	Total O 5 5	0	0
61	BV	2	Total O 2 2	0	0
61	BW	4	Total O 4 4	0	0
61	BX	4	Total O 4 4	0	0
61	B0	4	Total O 4 4	0	0
61	B1	2	Total O 2 2	0	0
61	B5	2	Total O 2 2	0	0
61	B7	1	Total O 1 1	0	0
61	B8	7	Total O 7 7	0	0
61	CA	186	Total O 186 186	0	0
61	CE	2	Total O 2 2	0	0
61	CN	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CX	2	Total O 2 2	0	0

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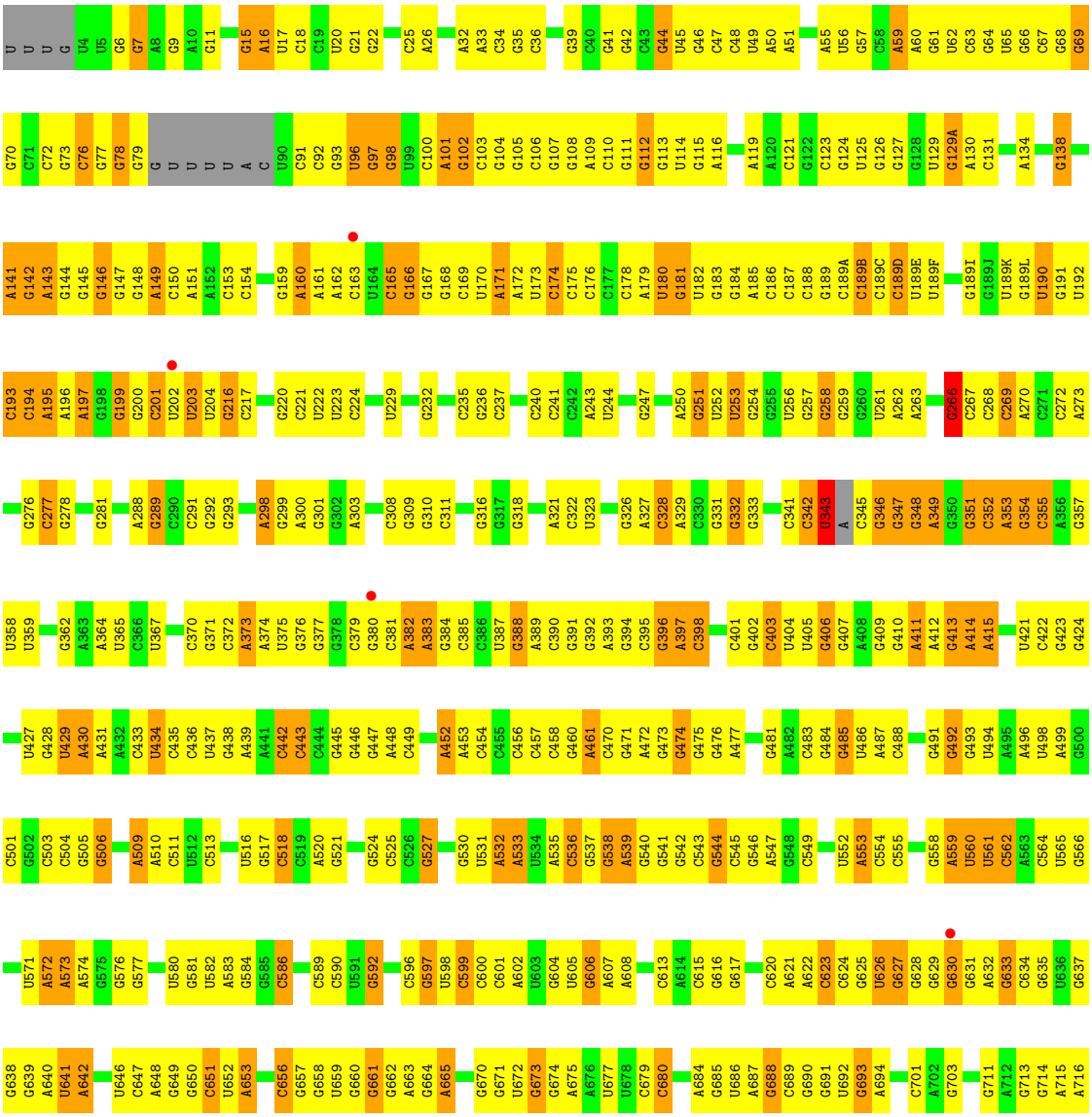
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DA	906	Total O 906 906	0	0
61	DB	7	Total O 7 7	0	0
61	DD	10	Total O 10 10	0	0
61	DE	11	Total O 11 11	0	0
61	DF	4	Total O 4 4	0	0
61	DO	1	Total O 1 1	0	0
61	DP	14	Total O 14 14	0	0
61	DQ	3	Total O 3 3	0	0
61	DR	1	Total O 1 1	0	0
61	DU	4	Total O 4 4	0	0
61	DV	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	3	Total O 3 3	0	0
61	D1	1	Total O 1 1	0	0
61	D3	1	Total O 1 1	0	0
61	D7	1	Total O 1 1	0	0
61	D8	4	Total O 4 4	0	0

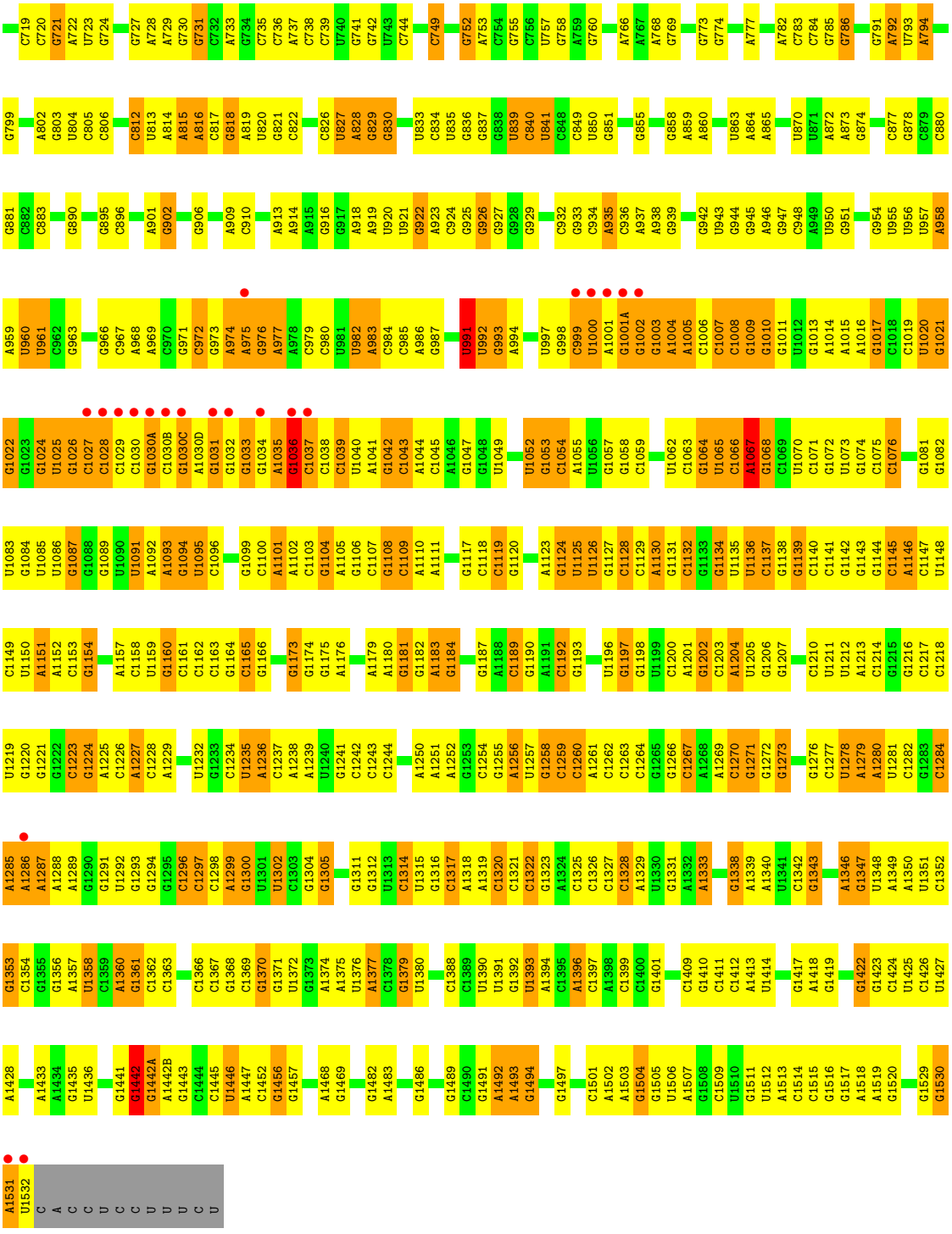
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA

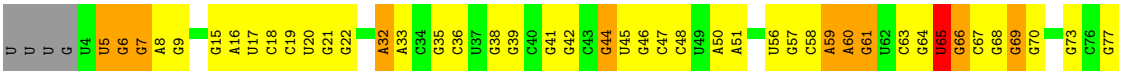
Chain AA:

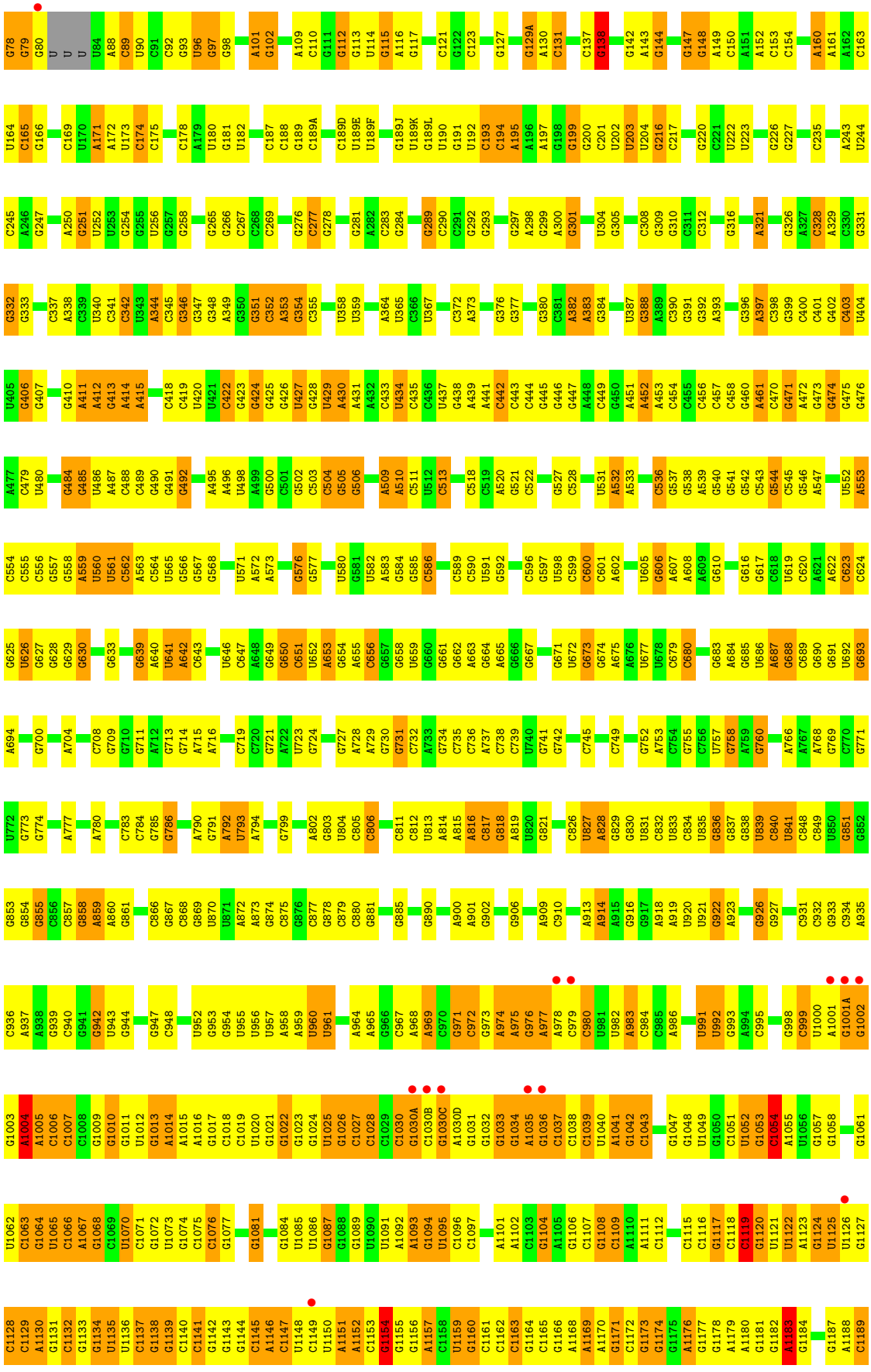




• Molecule 1: 16S Ribosomal RNA

Chain CA:




G78 G79 G80 U U U U84 A88 C89 U90 C91 C92 G93 U96 G97 G98 A101 G102 A109 C110 G111 G112 G113 U114 G115 A116 G117 C121 G122 C123 G127 G129A A130 C131 C137 G138 G142 A143 G144 G147 G148 A149 C150 A151 A152 C153 C154 A160 A161 A162 C163
U164 C165 G166 C169 U170 A171 A172 U173 C174 C175 C178 A179 U180 G181 U182 C187 C188 G189 C189A C189D U189E U189F G189J U189K G189L U190 G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U202 U203 U204 G216 C217 G220 C221 U222 U223 G226 G227 C235 A243 U244
C245 A246 G247 A250 G251 U252 U253 G254 G255 U256 G257 G258 G265 G266 C267 C268 C269 G276 C277 G278 G281 A282 C283 G284 G289 C290 C291 G292 G293 G297 A298 G299 A300 G301 U304 G305 C308 G309 G310 C311 C312 G316 A321 G326 A327 C328 A329 C330 G331
G332 G333 C337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 U358 U359 A364 U365 C366 U367 C372 A373 G376 G377 G380 C381 A382 A383 G384 U387 G388 A389 C390 G391 G392 A393 G396 A397 C398 G399 C400 C401 G402 C403 U404
U405 G406 G407 G410 A411 A412 G413 A414 A415 C418 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 A448 G449 G450 A451 A452 A453 C454 C455 C456 C457 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476
A477 C479 U480 G484 C485 U486 A487 C488 C489 G490 G491 G492 A495 A496 U498 A499 G500 C501 G502 C503 C504 G505 G506 A509 A510 C511 U512 C513 C518 C519 A520 G521 C522 G527 C528 U531 A532 A533 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 U552 A553
C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 U571 A572 A573 G576 G577 U580 G581 U582 A583 G584 G585 C586 C589 C590 U591 G592 C596 G597 U598 C599 C600 C601 A602 U605 G606 A607 A608 A609 G610 G616 G617 C618 U619 C620 A621 A622 C623 C624
G625 U626 G627 G628 G629 G630 G633 G639 A640 U641 A642 C643 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G671 U672 G673 G674 A675 A676 U677 U678 C679 G680 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693
A694 G700 A704 C708 G709 G710 G711 A712 G713 G714 A715 A716 C719 G720 G721 A722 U723 G724 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739 U740 G741 G742 C745 C749 G752 A753 C754 G755 C756 U757 G758 A759 G760 A766 A767 A768 G769 C770 G771
U772 G773 G774 A777 A780 C783 C784 G785 G786 A790 G791 A792 U793 A794 G799 A802 G803 U804 C805 C806 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852
G853 G854 G855 C856 C857 G858 A859 A860 G861 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 G885 G890 A900 A901 G902 G906 A909 C910 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 G926 G927 C931 C932 G933 C934 A935
C936 A937 A938 G939 C940 G941 G942 U943 G944 G947 C948 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 G972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 U991 U992 G993 A994 C995 G998 C999 U1000 A1001 G1001A G1002
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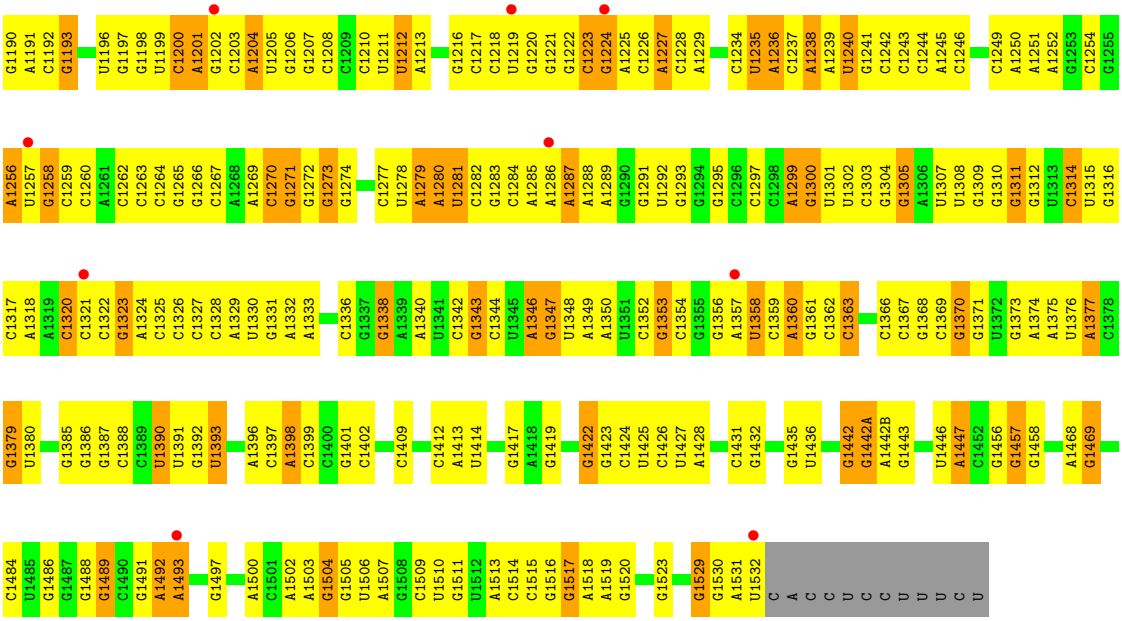
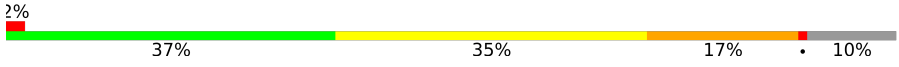
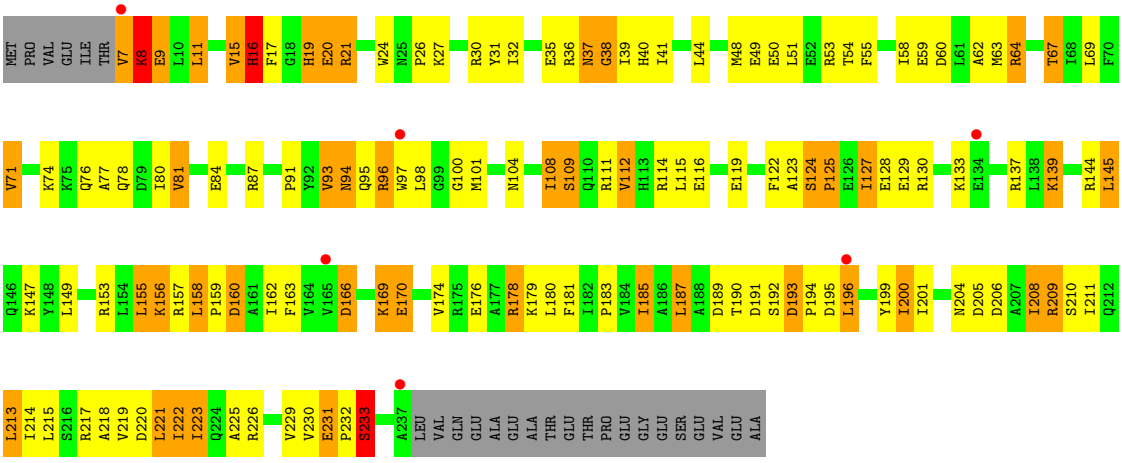
C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 G1166 A1168 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1187 A1188 C1189



• Molecule 2: 30S Ribosomal Protein S2

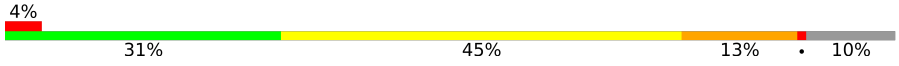
Chain AB:

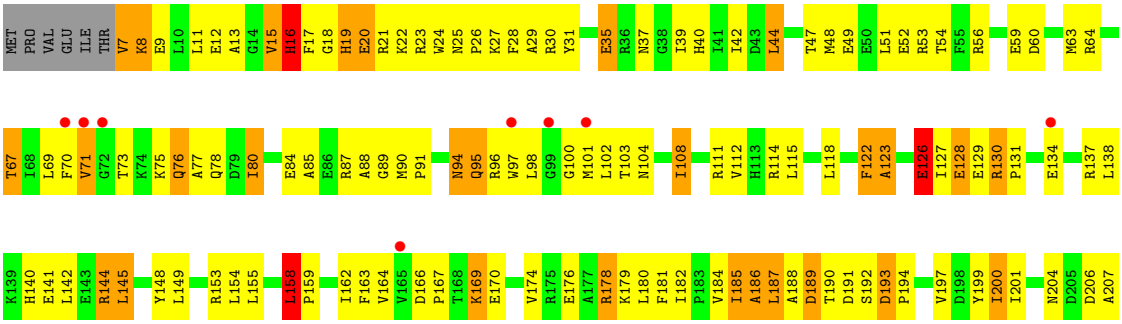




• Molecule 2: 30S Ribosomal Protein S2

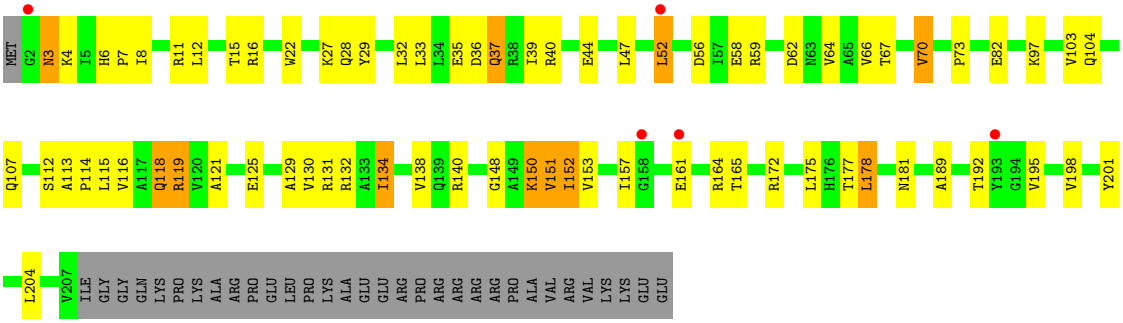
Chain CB:





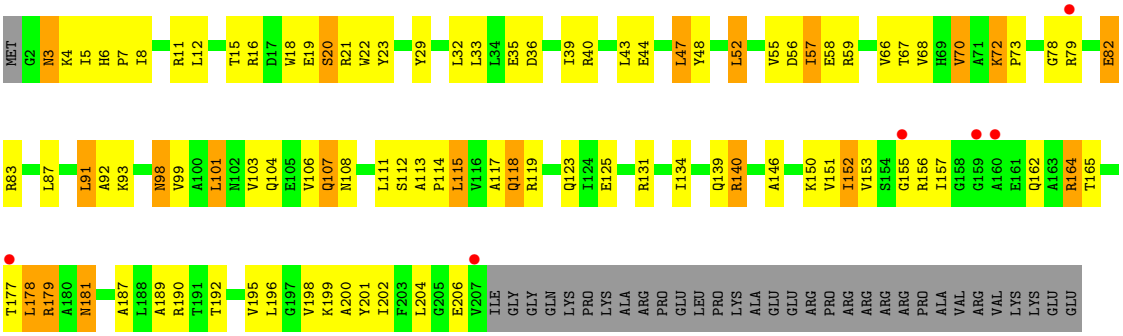
• Molecule 3: 30S Ribosomal Protein S3

Chain AC:



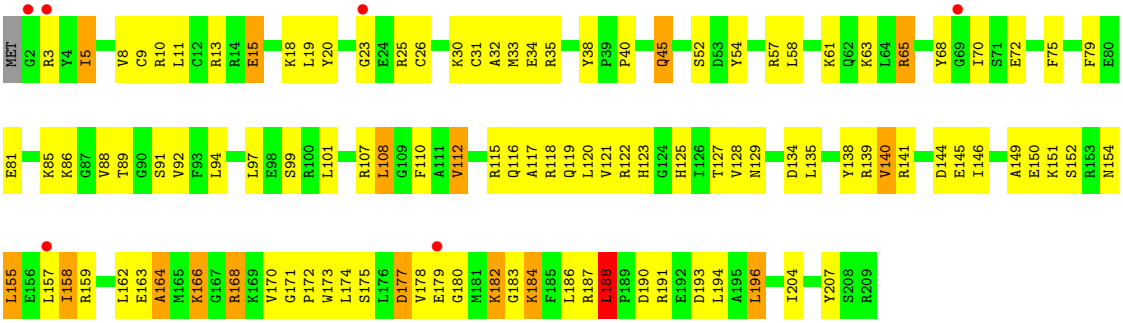
• Molecule 3: 30S Ribosomal Protein S3

Chain CC:



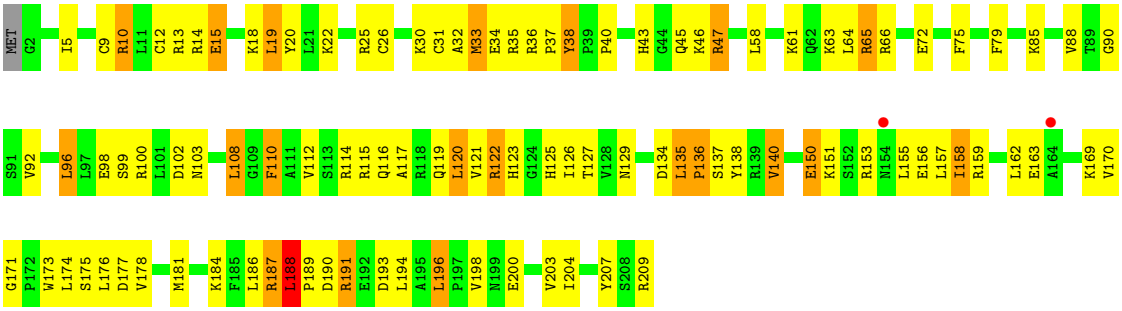
• Molecule 4: 30S Ribosomal Protein S4

Chain AD:



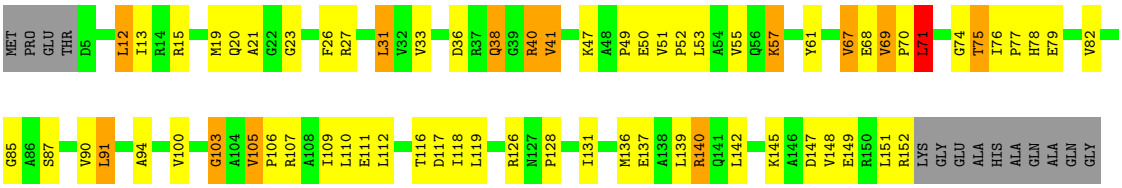
• Molecule 4: 30S Ribosomal Protein S4

Chain CD:



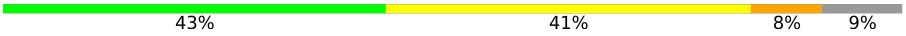
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



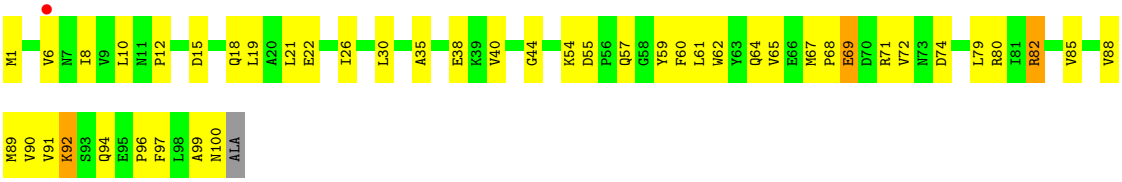
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



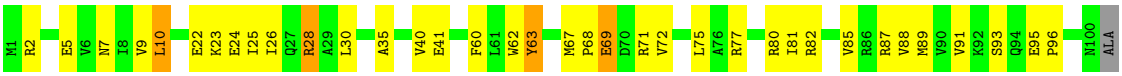
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



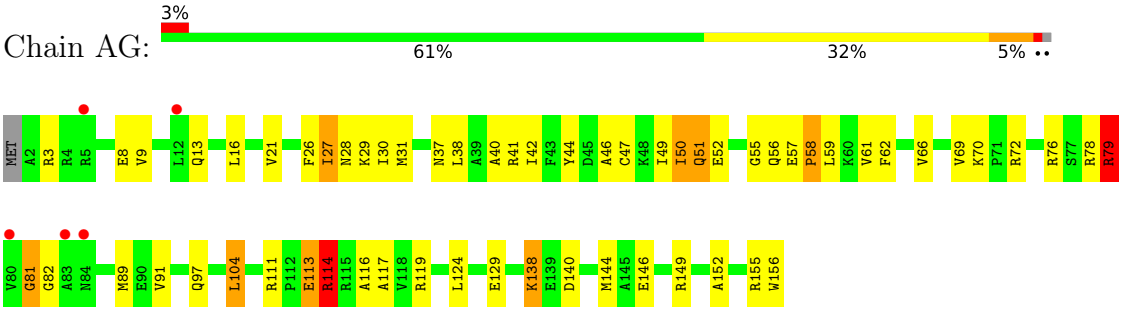
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



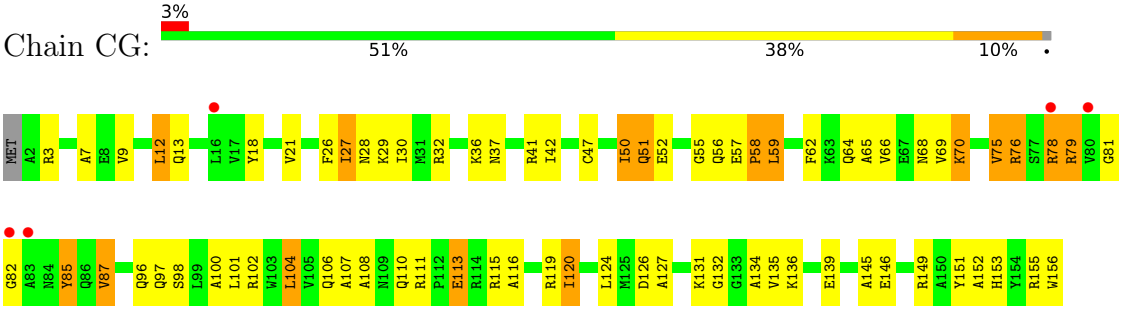
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



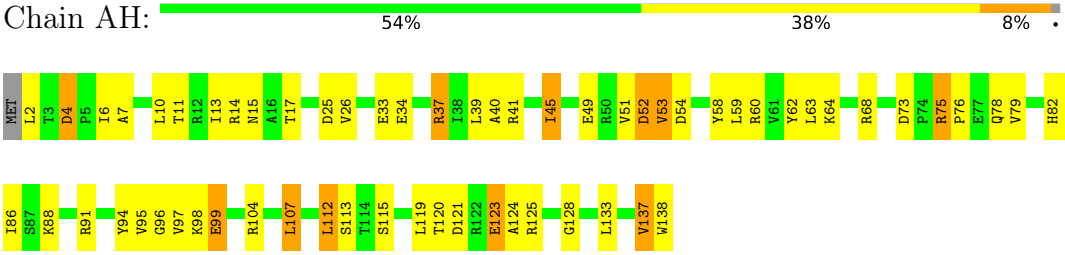
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:



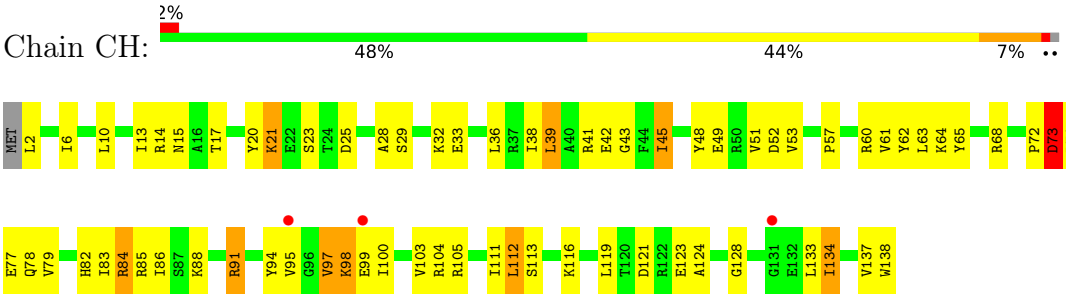
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



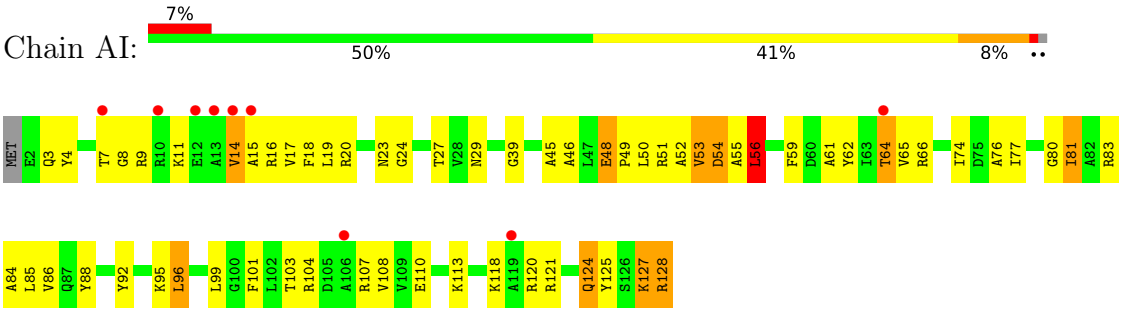
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:



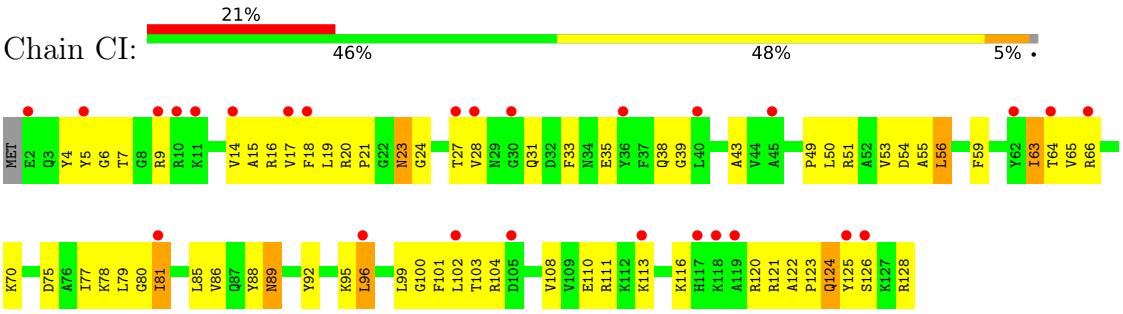
• Molecule 9: 30S Ribosomal Protein S9

Chain AI:



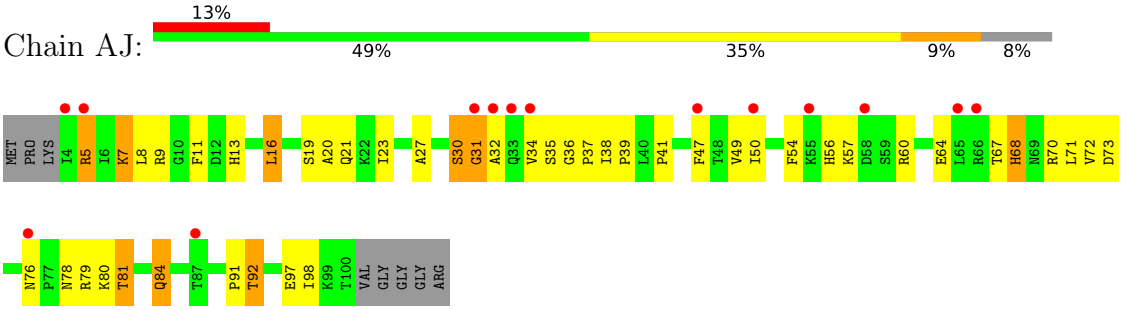
• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



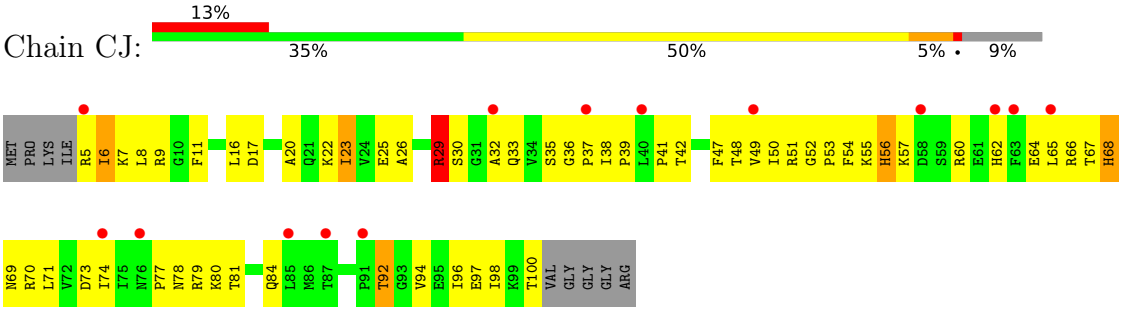
• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:



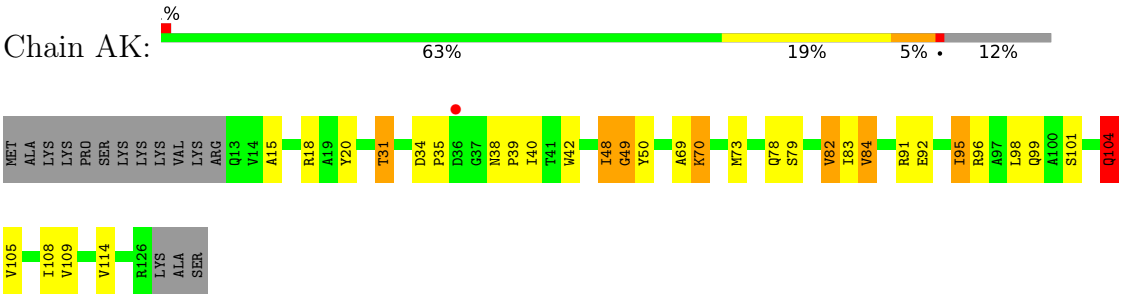
• Molecule 10: 30S Ribosomal Protein S10

Chain CJ:



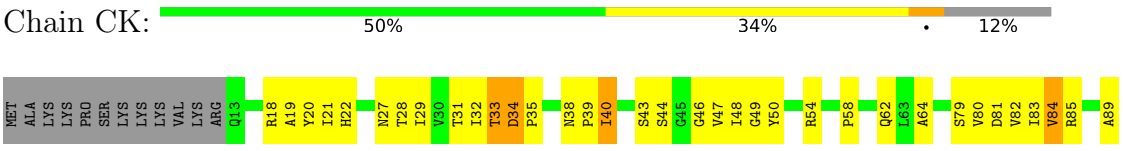
• Molecule 11: 30S Ribosomal Protein S11

Chain AK:



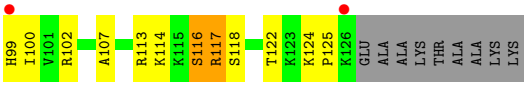
• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



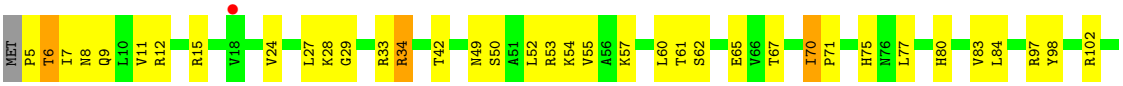
• Molecule 12: 30S Ribosomal Protein S12

Chain AL:



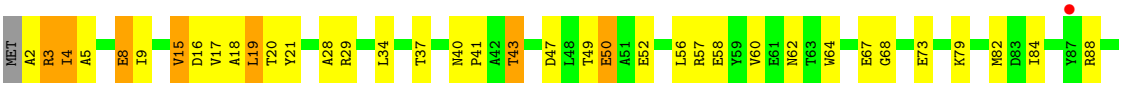
• Molecule 12: 30S Ribosomal Protein S12

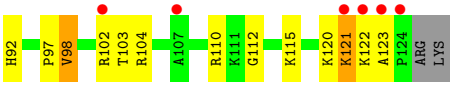
Chain CL:



• Molecule 13: 30S Ribosomal Protein S13

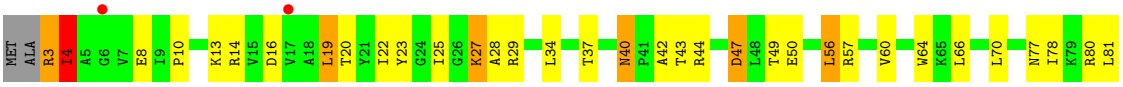
Chain AM:

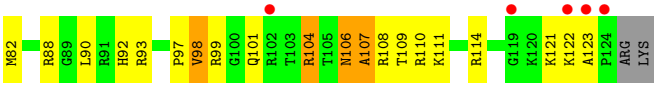




• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



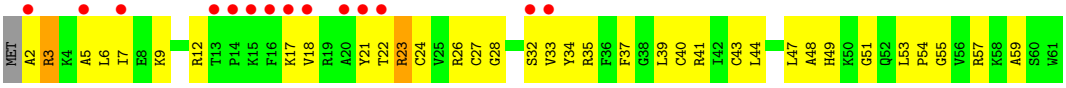


• Molecule 14: 30S Ribosomal Protein S14

Chain AN:

• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



• Molecule 15: 30S Ribosomal Protein S15

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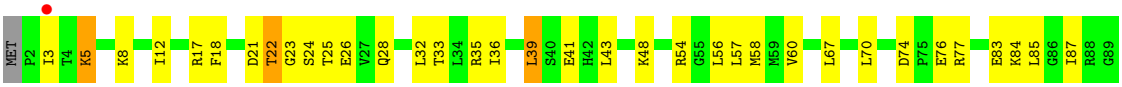

• Molecule 15: 30S Ribosomal Protein S15

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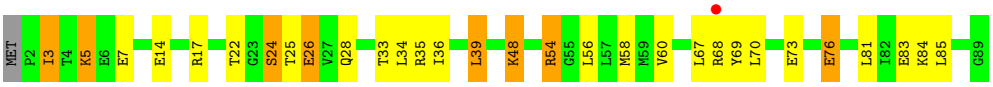
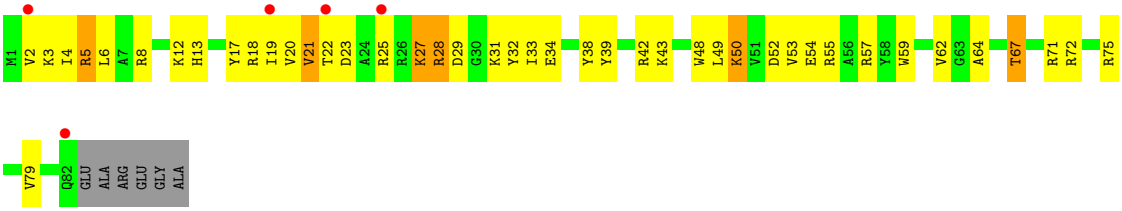


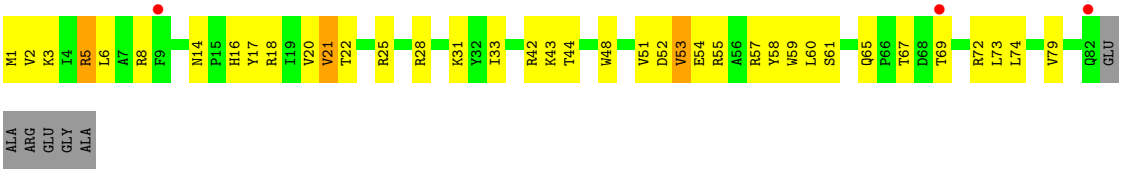
• Molecule 16: 30S Ribosomal Protein S16

Chain AP:



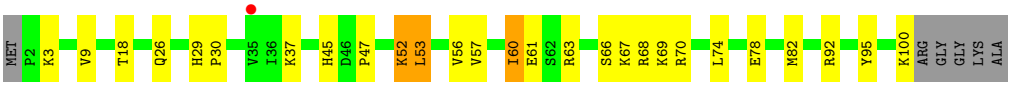
• Molecule 16: 30S Ribosomal Protein S16

Chain CP:



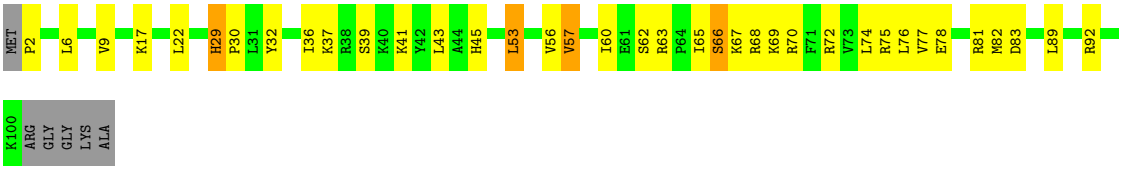
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



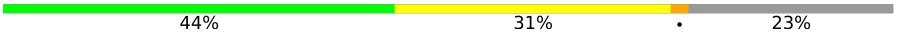
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



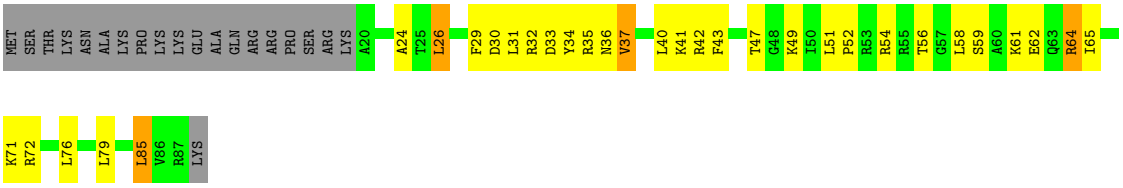
• Molecule 18: 30S Ribosomal Protein S18

Chain AR:



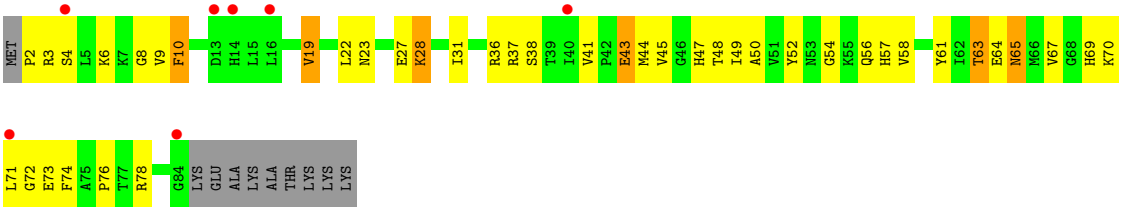
• Molecule 18: 30S Ribosomal Protein S18

Chain CR:



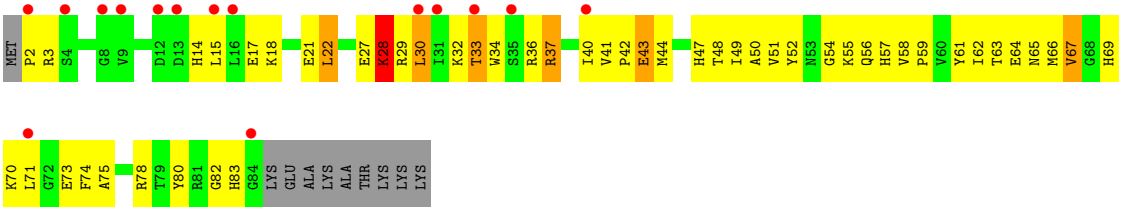
• Molecule 19: 30S Ribosomal Protein S19

Chain AS:

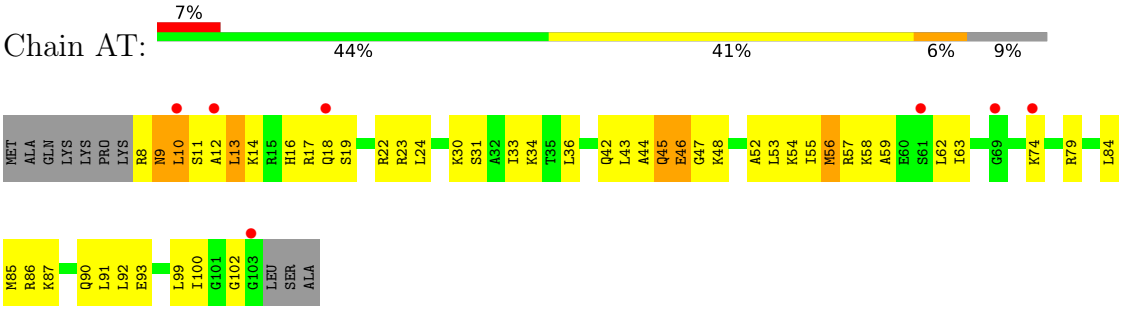


• Molecule 19: 30S Ribosomal Protein S19

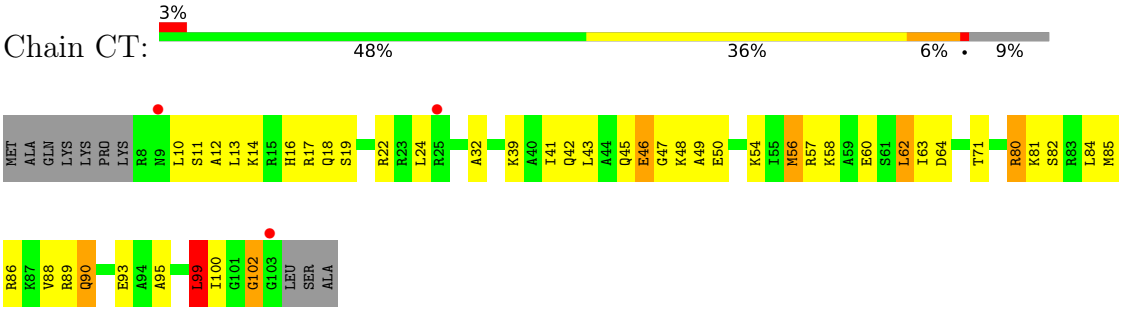
Chain CS:



• Molecule 20: 30S Ribosomal Protein S20

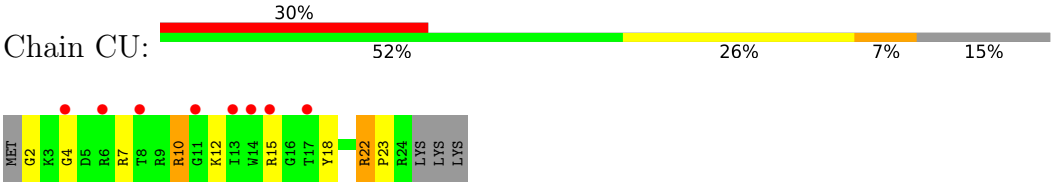


• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX

• Molecule 21: 30S Ribosomal Protein THX



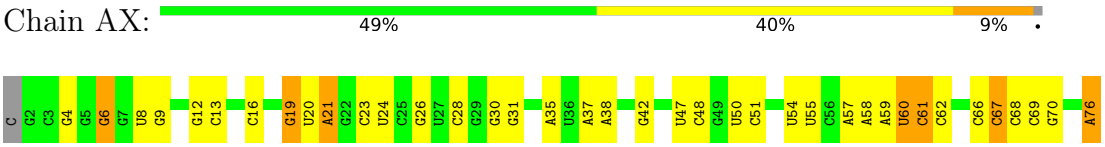
• Molecule 22: mRNA

• Molecule 22: mRNA

Chain CV:

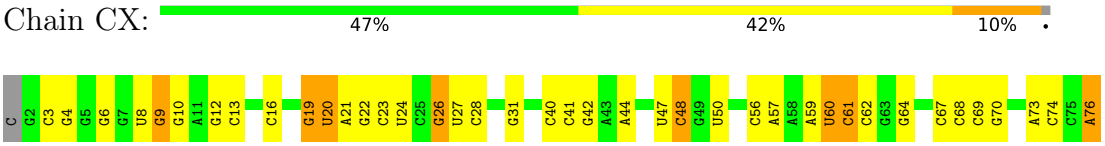
• Molecule 23: P-site tRNA

Chain AX:



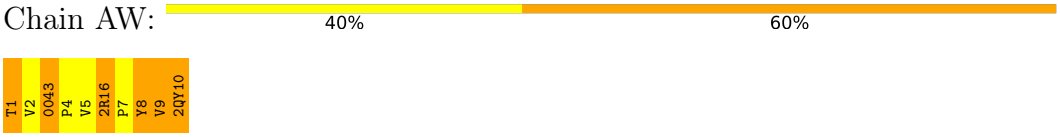
• Molecule 23: P-site tRNA

Chain CX:



• Molecule 24: Dityromycin

Chain AW:

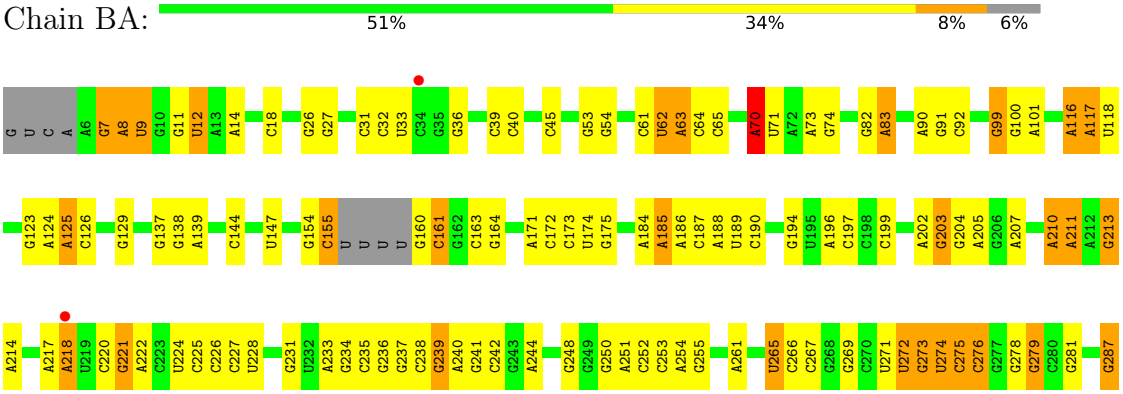


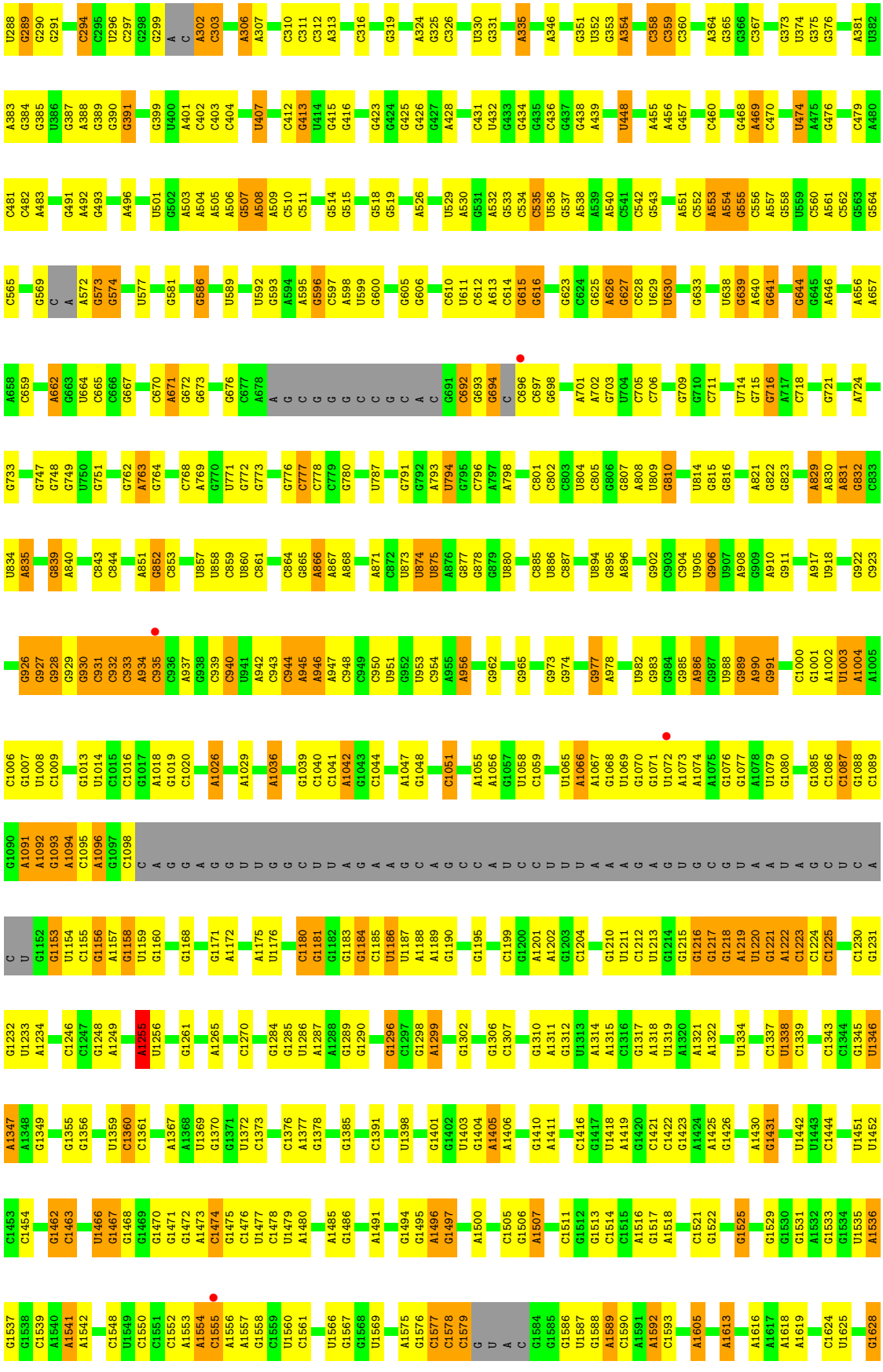
• Molecule 24: Dityromycin

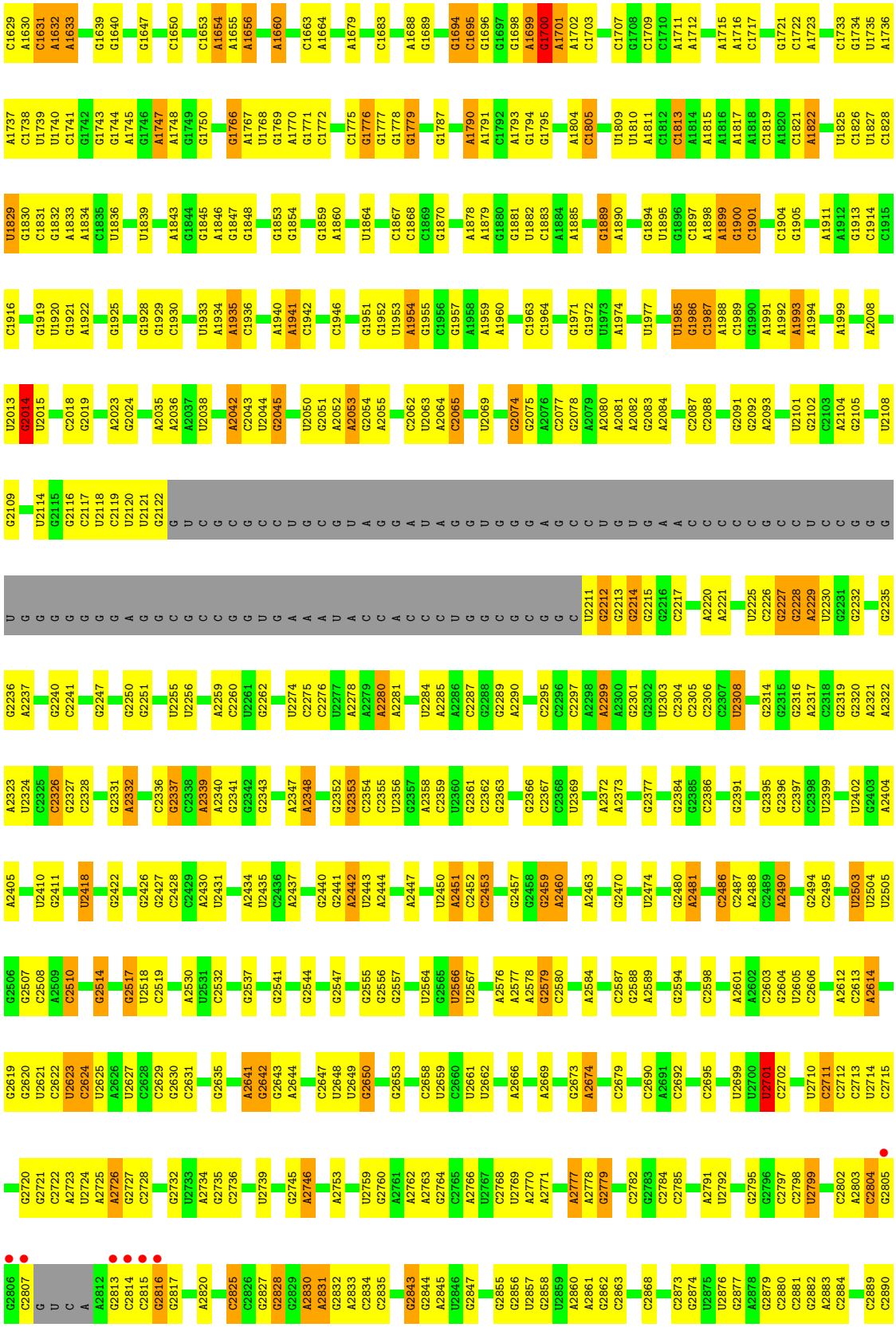
Chain CW:

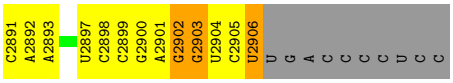
• Molecule 25: 23S Ribosomal RNA

Chain BA:



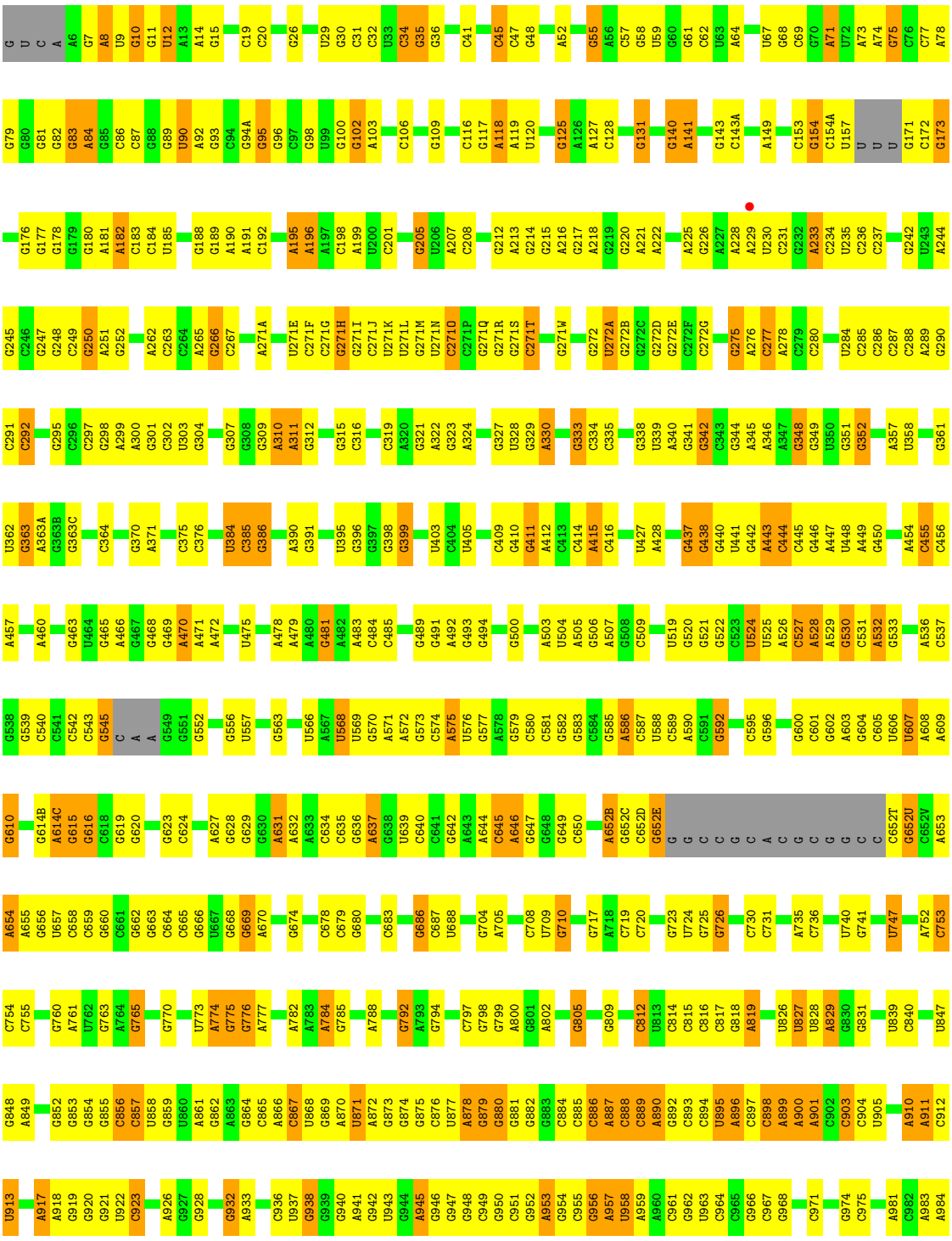


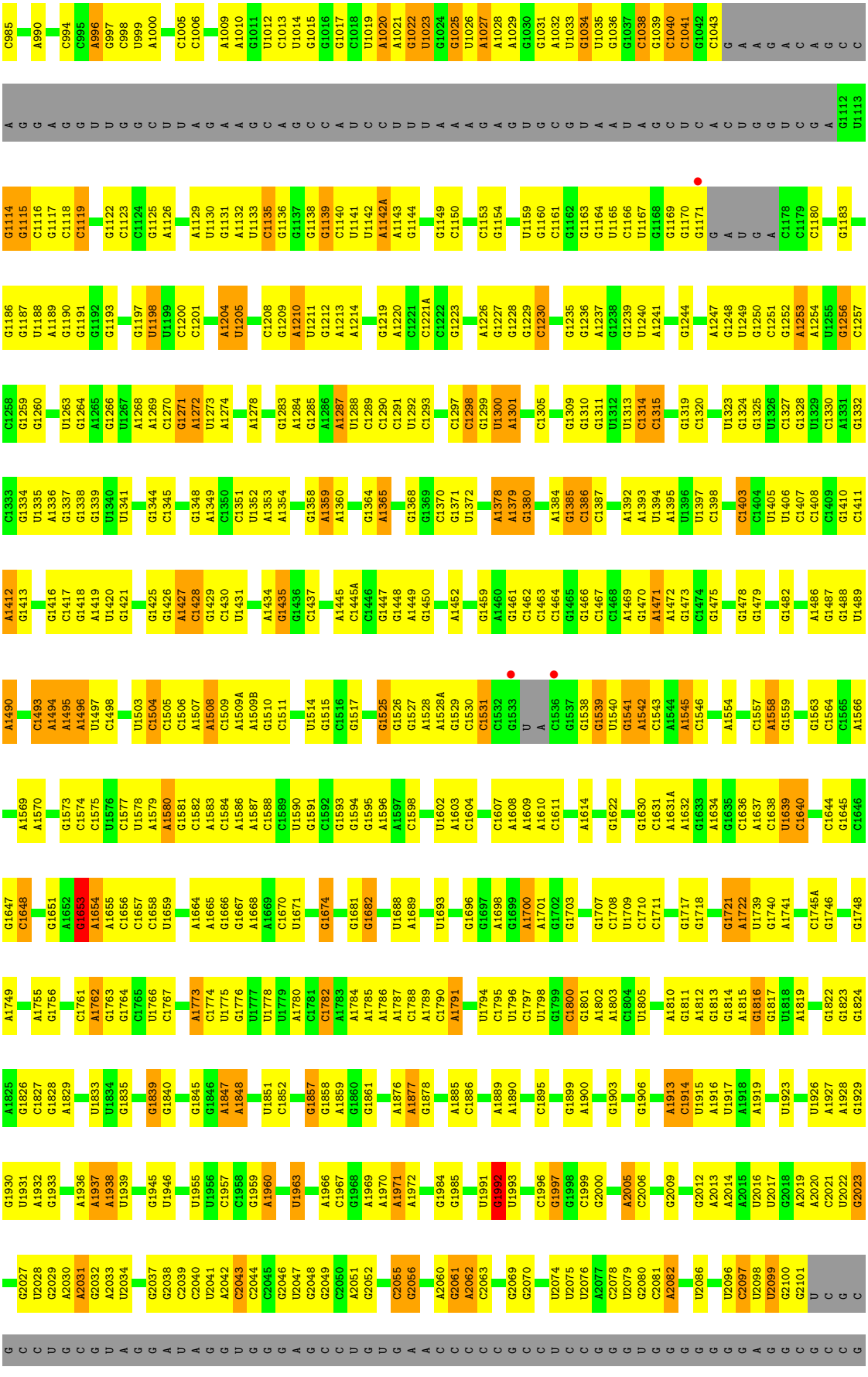


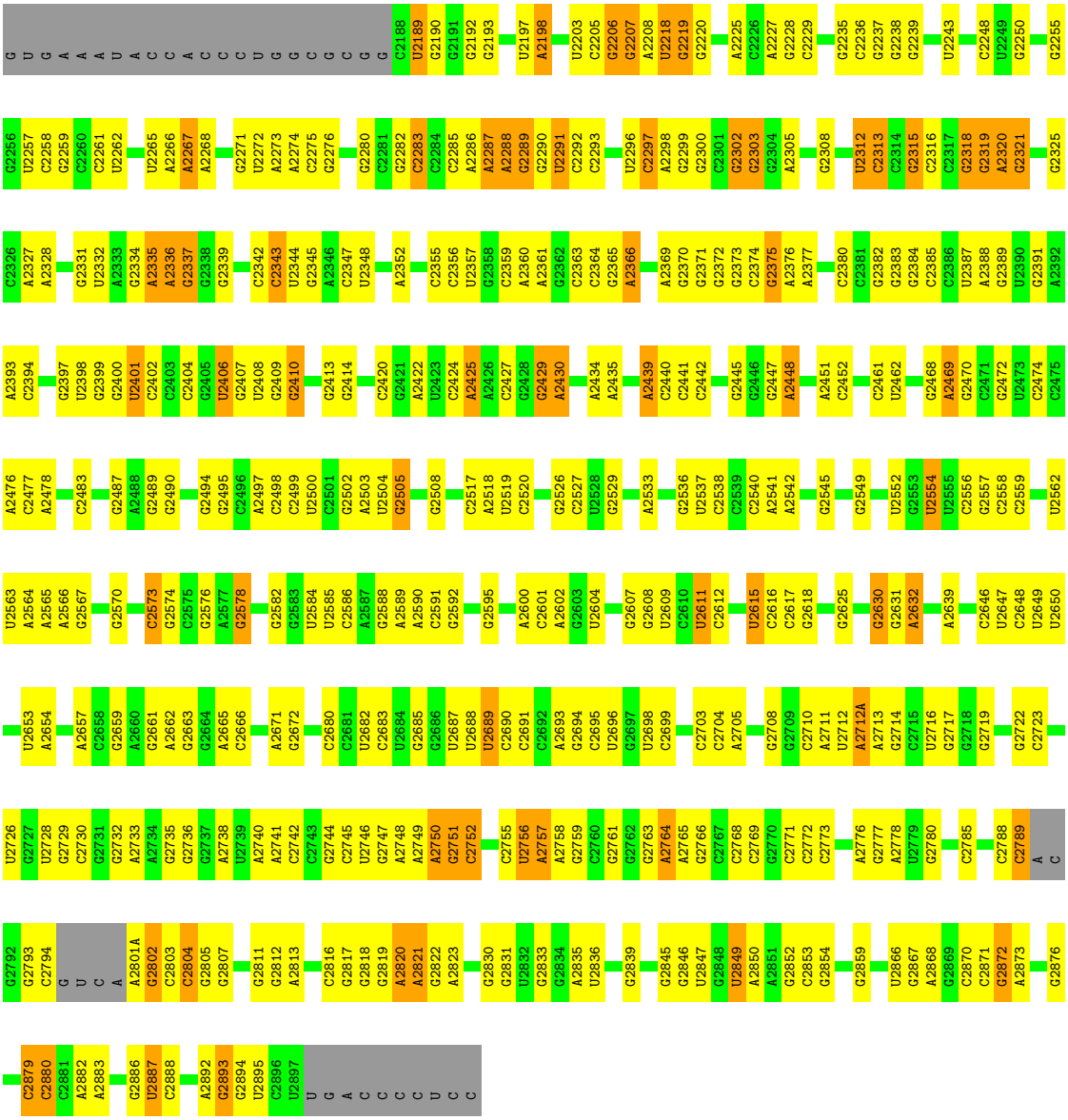


• Molecule 25: 23S Ribosomal RNA

Chain DA:

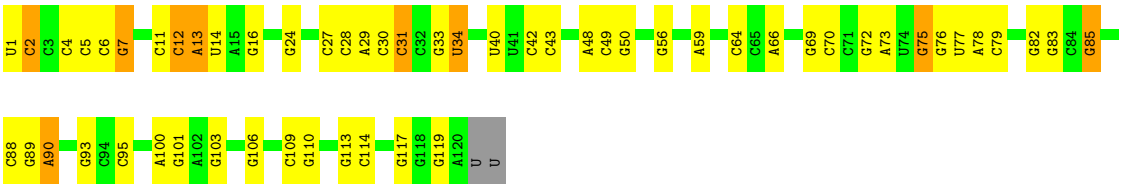






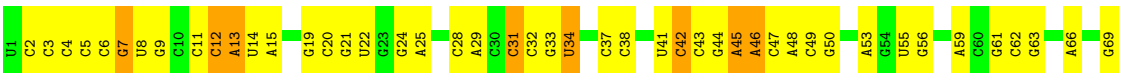
• Molecule 26: 5S Ribosomal RNA

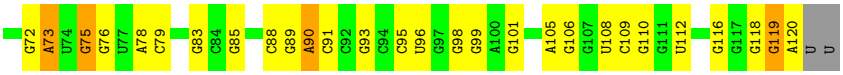
Chain BB:



• Molecule 26: 5S Ribosomal RNA

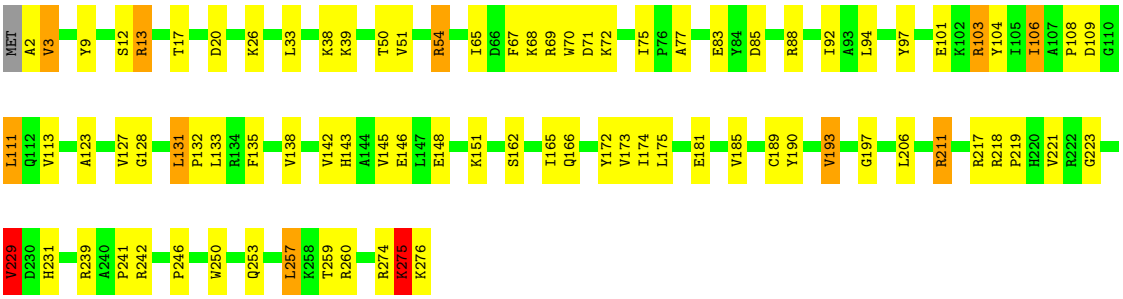
Chain DB:





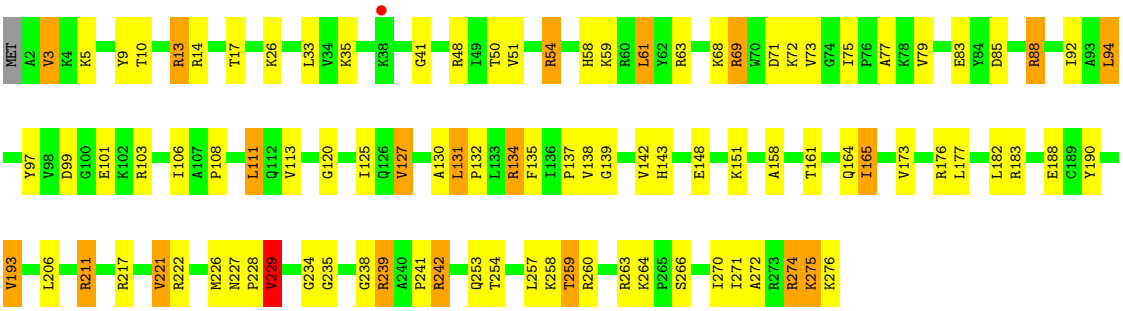
• Molecule 27: 50S Ribosomal Protein L2

Chain BD:



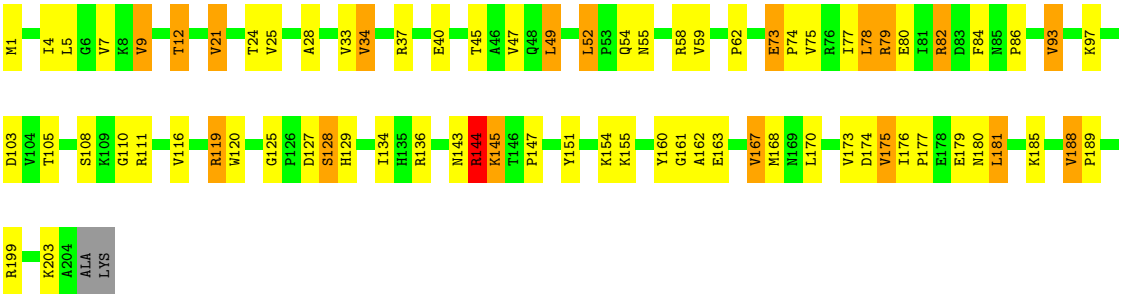
• Molecule 27: 50S Ribosomal Protein L2

Chain DD:



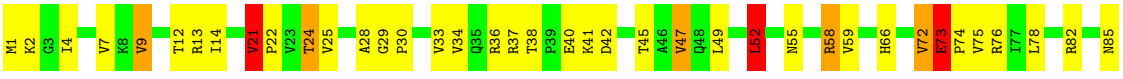
• Molecule 28: 50S Ribosomal Protein L3

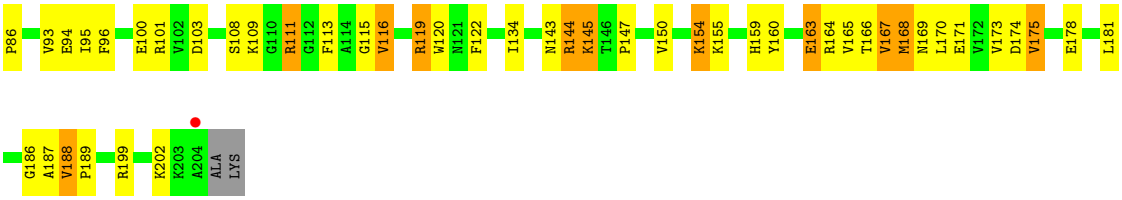
Chain BE:



• Molecule 28: 50S Ribosomal Protein L3

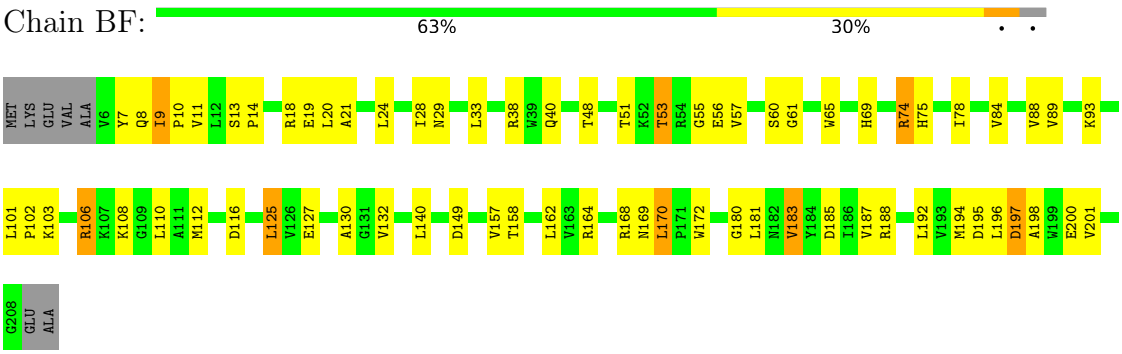
Chain DE:





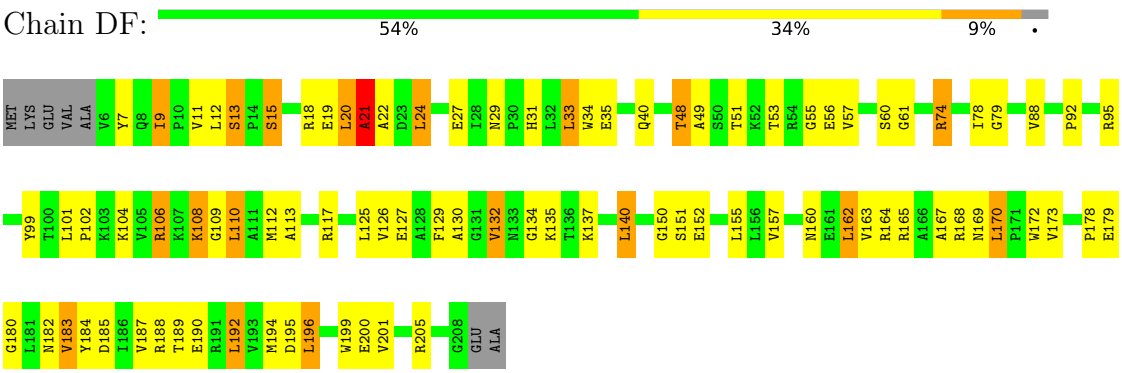
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



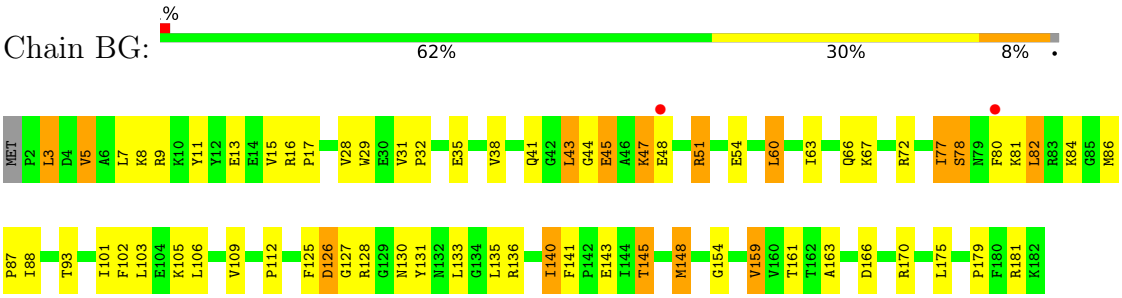
• Molecule 29: 50S Ribosomal Protein L4

Chain DF:



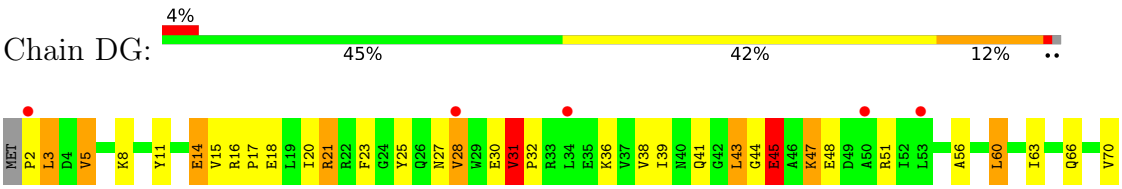
• Molecule 30: 50S Ribosomal Protein L5

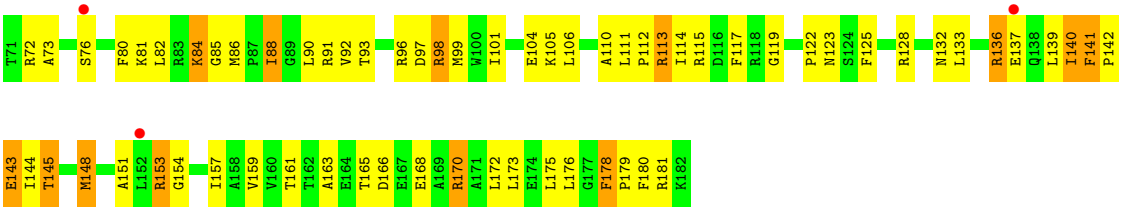
Chain BG:



• Molecule 30: 50S Ribosomal Protein L5

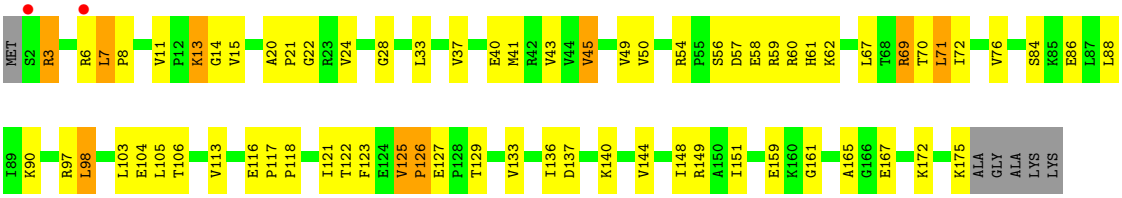
Chain DG:





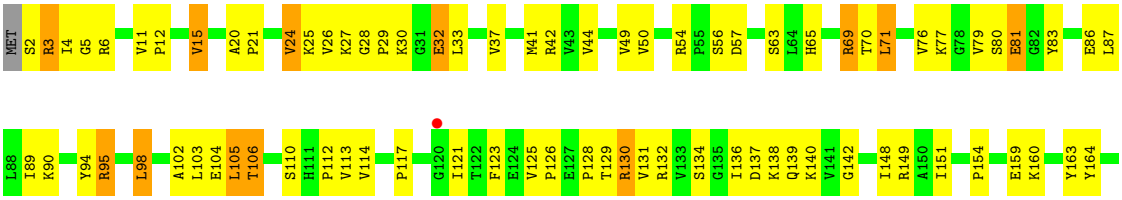
• Molecule 31: 50S Ribosomal Protein L6

Chain BH:



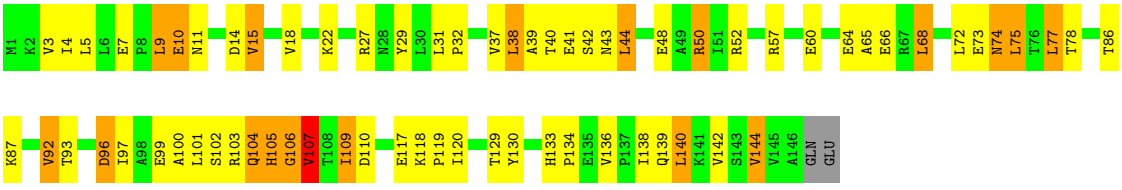
• Molecule 31: 50S Ribosomal Protein L6

Chain DH:



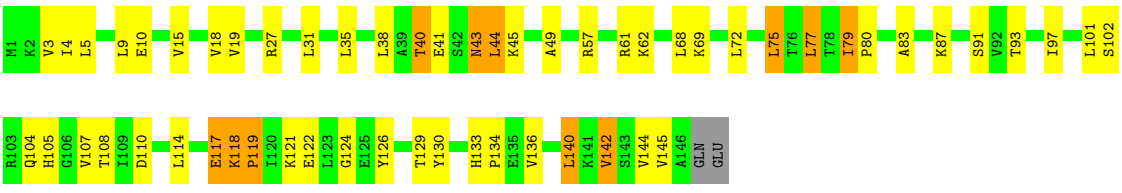
• Molecule 32: 50S Ribosomal Protein L9

Chain BI:



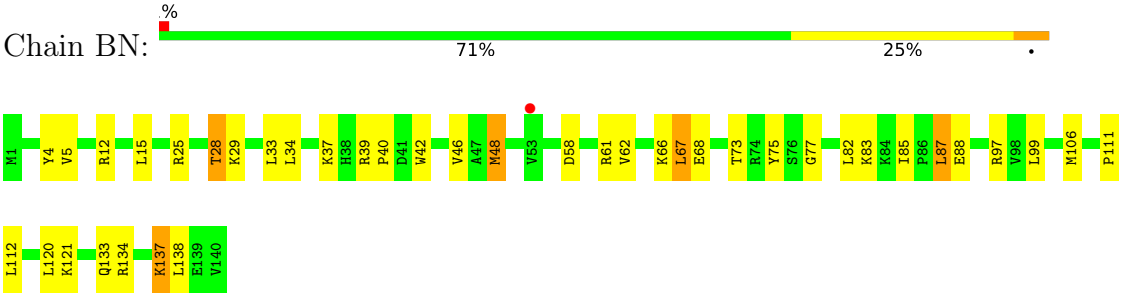
• Molecule 32: 50S Ribosomal Protein L9

Chain DI:



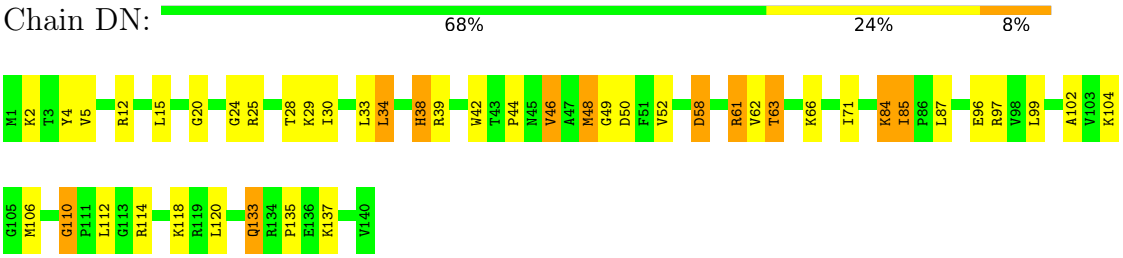
• Molecule 33: 50S Ribosomal Protein L13

Chain BN:



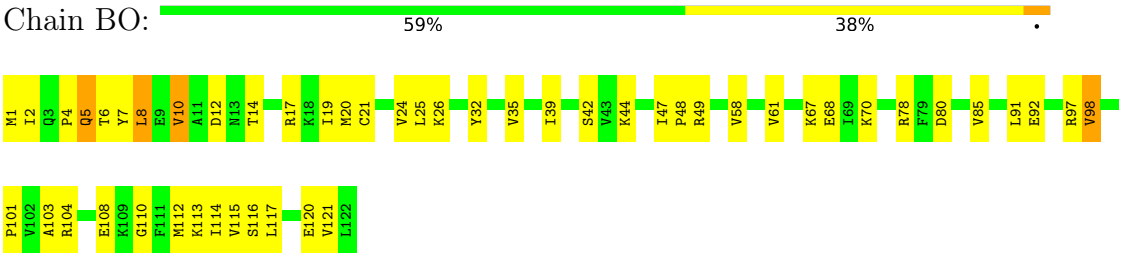
• Molecule 33: 50S Ribosomal Protein L13

Chain DN:



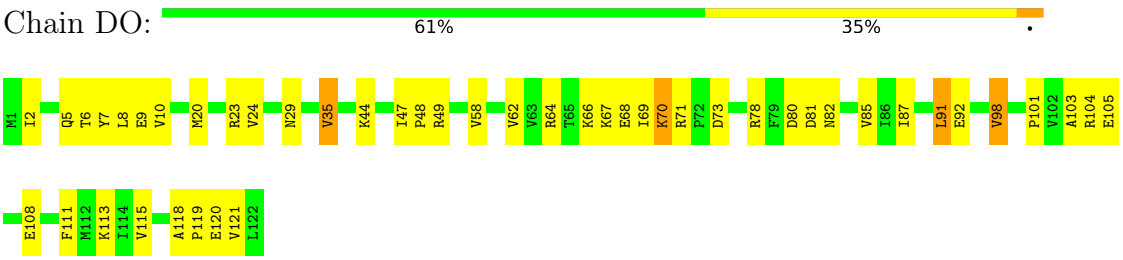
• Molecule 34: 50S Ribosomal Protein L14

Chain BO:



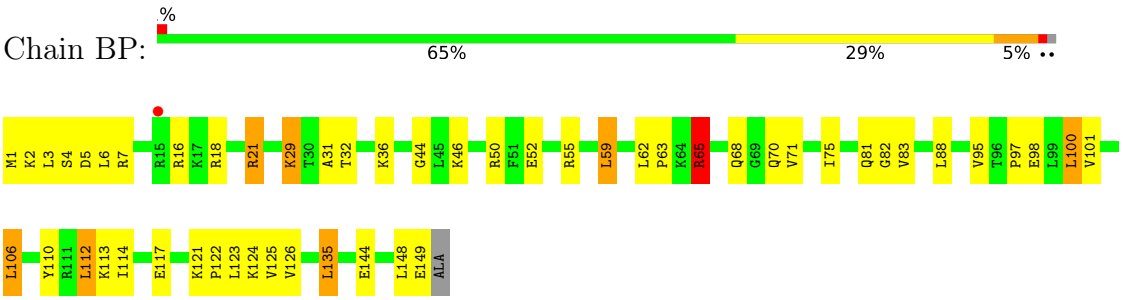
• Molecule 34: 50S Ribosomal Protein L14

Chain DO:



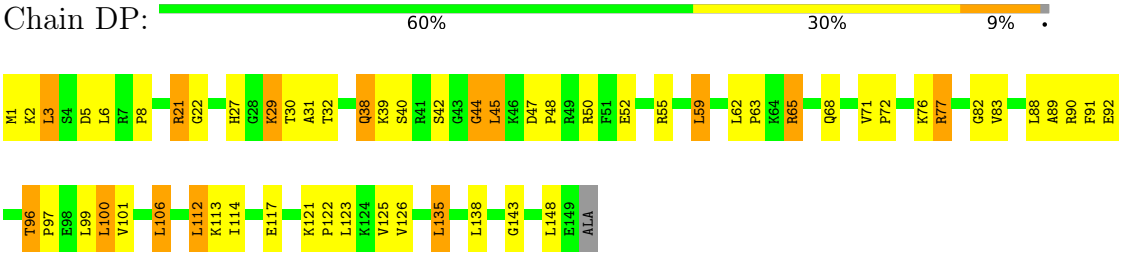
• Molecule 35: 50S Ribosomal Protein L15

Chain BP:



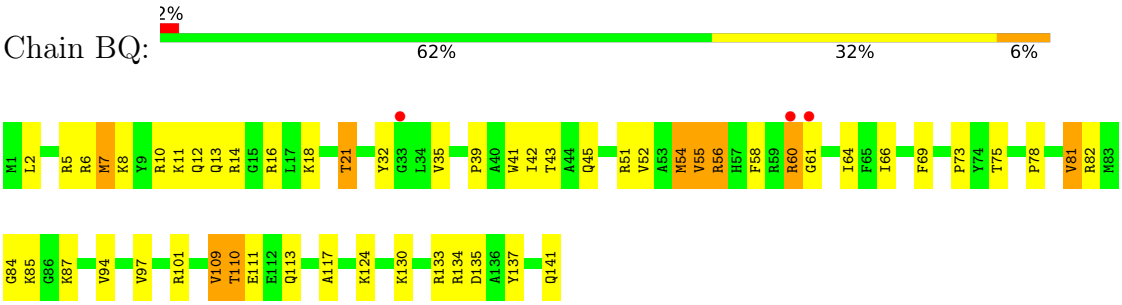
• Molecule 35: 50S Ribosomal Protein L15

Chain DP:



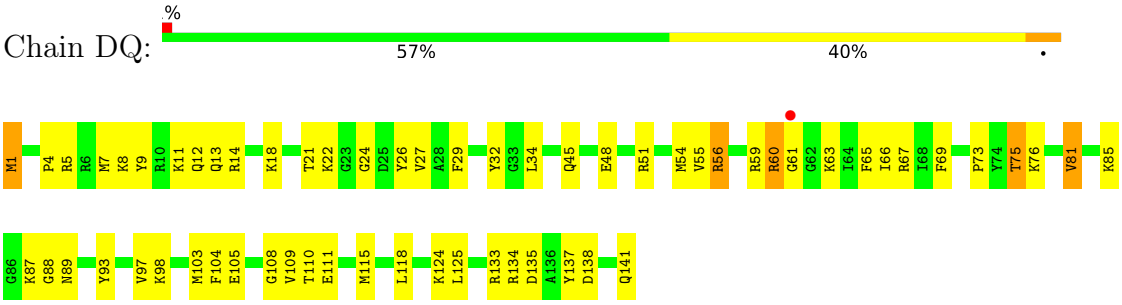
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



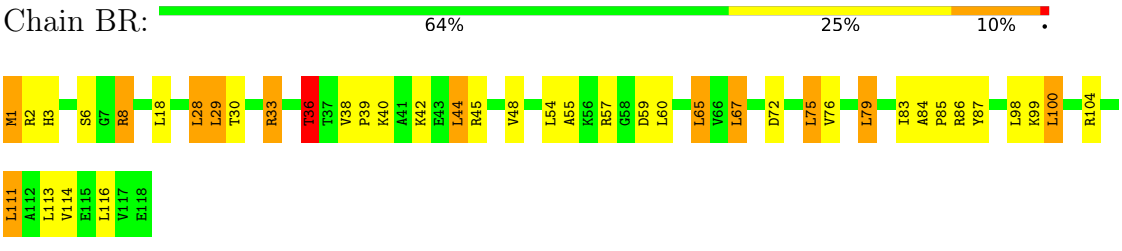
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



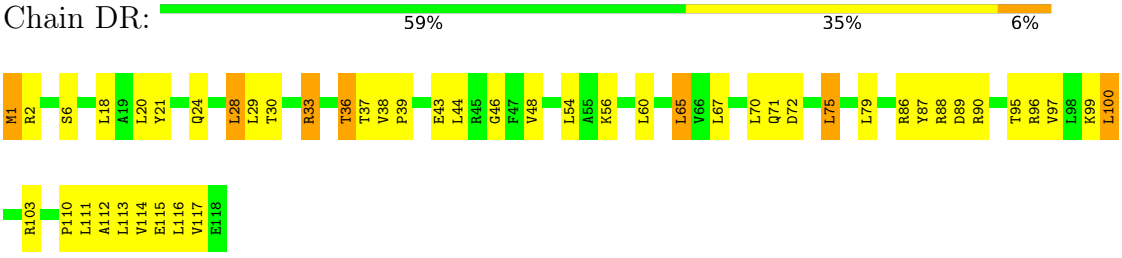
• Molecule 37: 50S Ribosomal Protein L17

Chain BR:



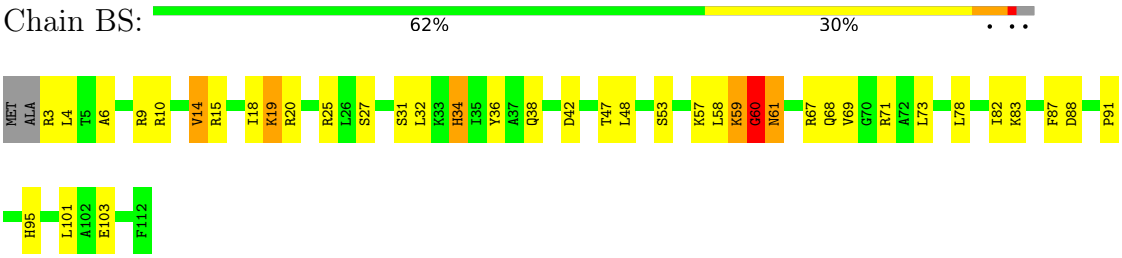
• Molecule 37: 50S Ribosomal Protein L17

Chain DR:



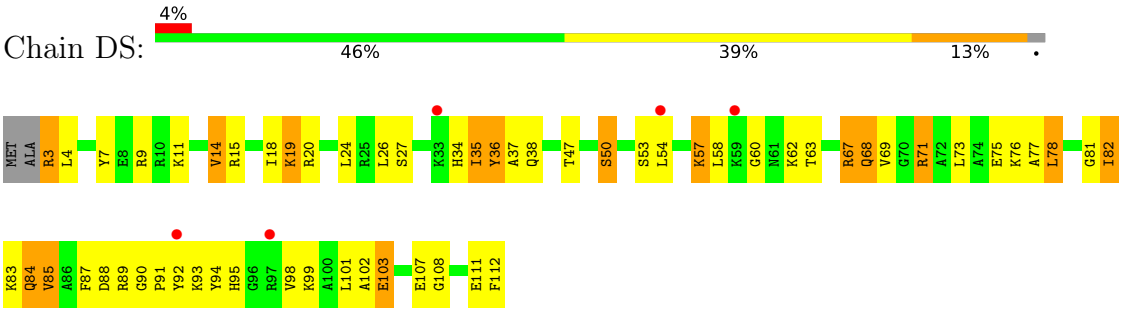
• Molecule 38: 50S Ribosomal Protein L18

Chain BS:



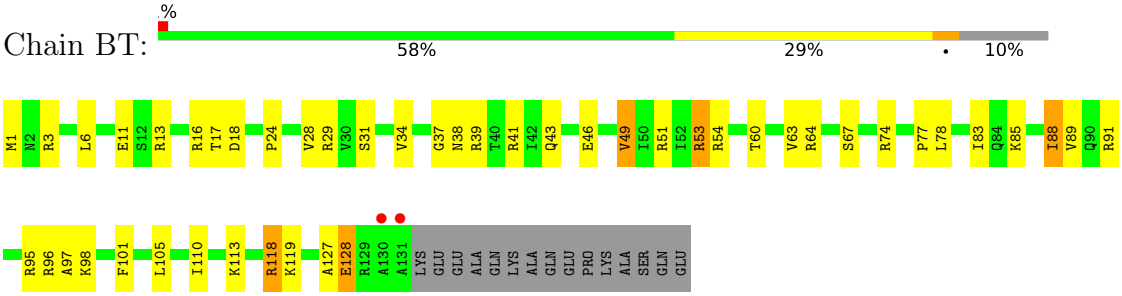
• Molecule 38: 50S Ribosomal Protein L18

Chain DS:



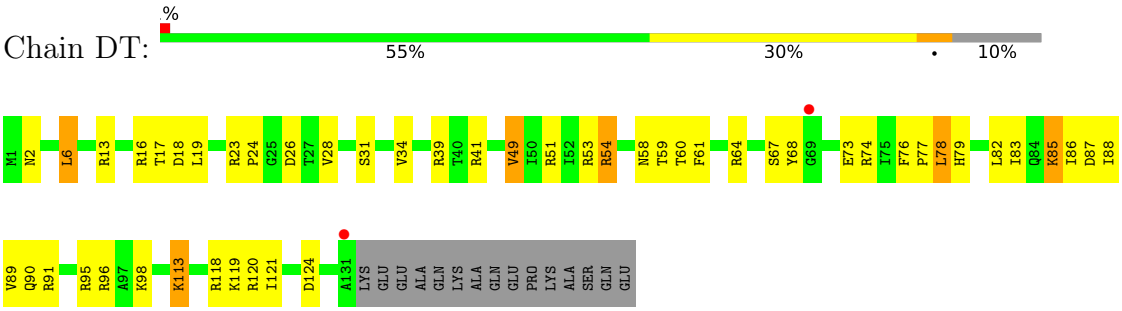
• Molecule 39: 50S Ribosomal Protein L19

Chain BT:



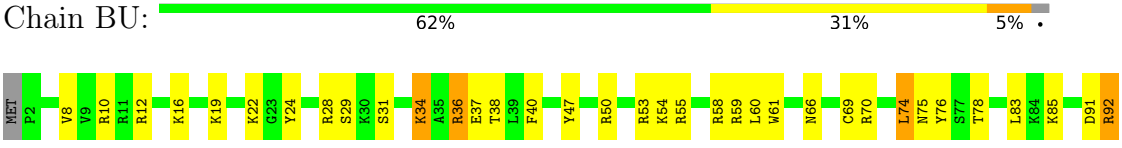
• Molecule 39: 50S Ribosomal Protein L19

Chain DT:



• Molecule 40: 50S Ribosomal Protein L20

Chain BU:



• Molecule 40: 50S Ribosomal Protein L20

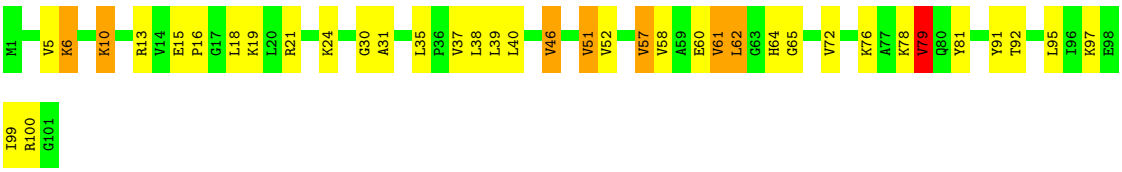
Chain DU:

• Molecule 41: 50S Ribosomal Protein L21

Chain BV:

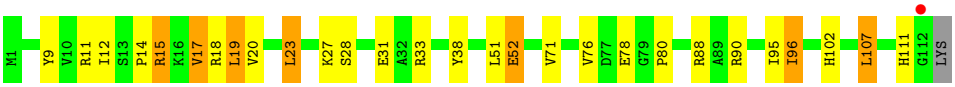
• Molecule 41: 50S Ribosomal Protein L21

Chain DV:



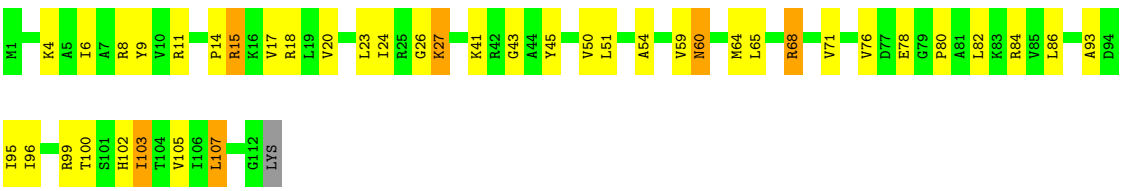
• Molecule 42: 50S Ribosomal Protein L22

Chain BW:



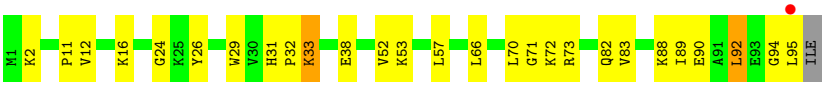
• Molecule 42: 50S Ribosomal Protein L22

Chain DW:



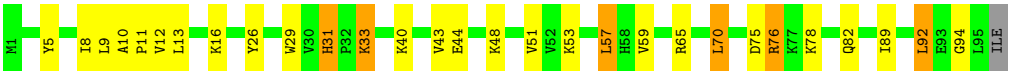
• Molecule 43: 50S Ribosomal Protein L23

Chain BX:



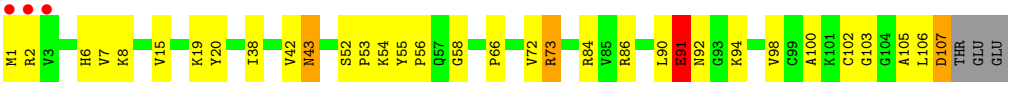
• Molecule 43: 50S Ribosomal Protein L23

Chain DX:



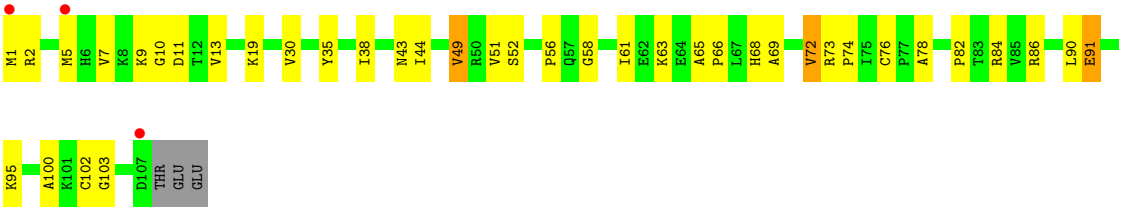
• Molecule 44: 50S Ribosomal Protein L24

Chain BY:



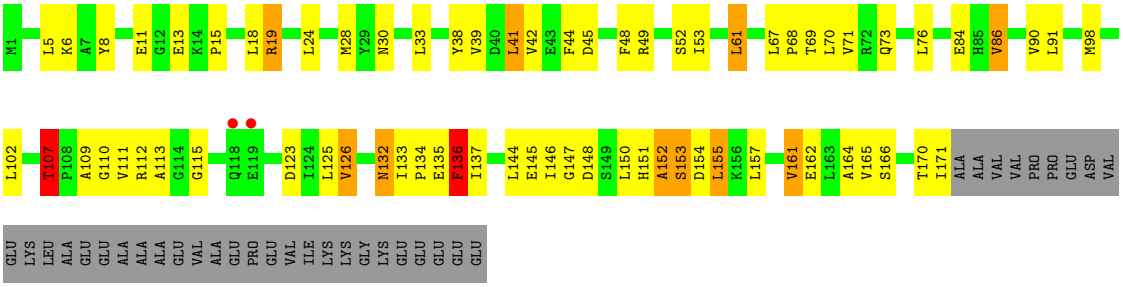
• Molecule 44: 50S Ribosomal Protein L24

Chain DY:



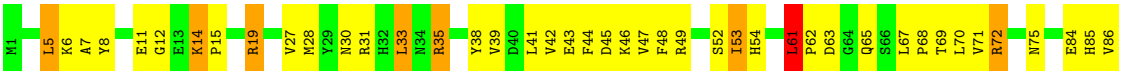
• Molecule 45: 50S Ribosomal Protein L25

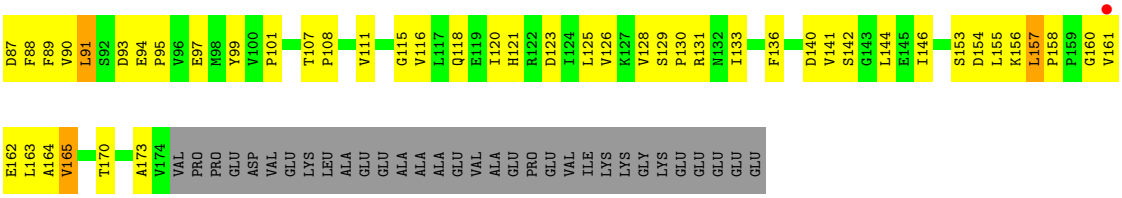
Chain BZ:



• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:



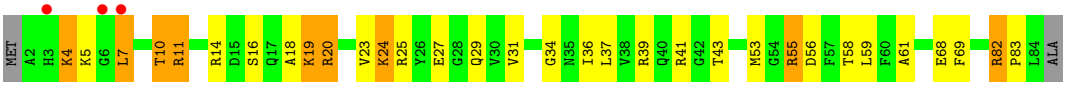


• Molecule 46: 50S Ribosomal Protein L27

Chain B0:

• Molecule 46: 50S Ribosomal Protein L27

Chain D0:

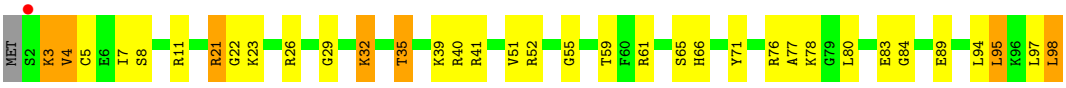


• Molecule 47: 50S Ribosomal Protein L28

Chain B1:

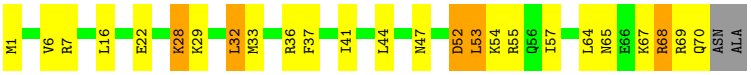
• Molecule 47: 50S Ribosomal Protein L28

Chain D1:



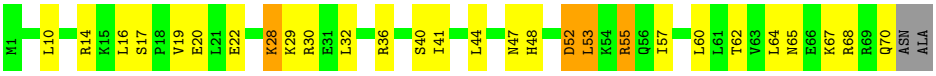
• Molecule 48: 50S Ribosomal Protein L29

Chain B2:



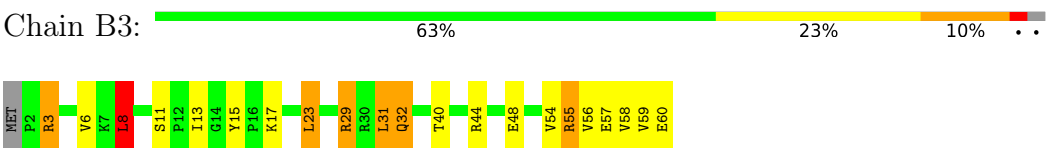
• Molecule 48: 50S Ribosomal Protein L29

Chain D2:



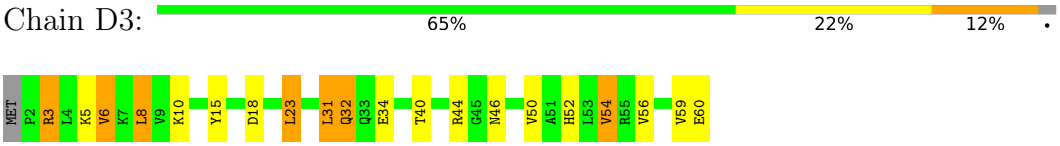
• Molecule 49: 50S Ribosomal Protein L30

Chain B3:



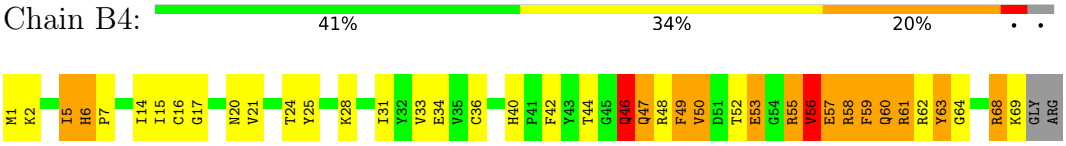
• Molecule 49: 50S Ribosomal Protein L30

Chain D3:



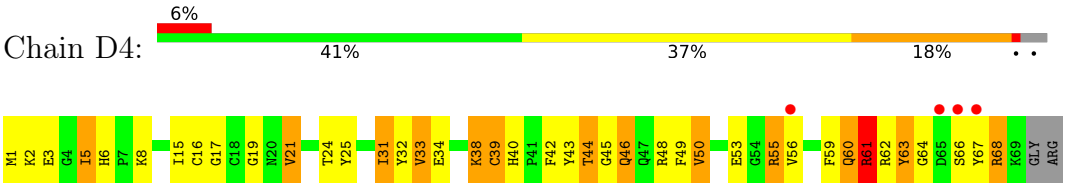
• Molecule 50: 50S Ribosomal Protein L31

Chain B4:



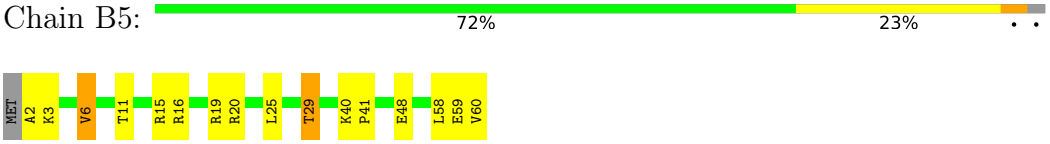
• Molecule 50: 50S Ribosomal Protein L31

Chain D4:



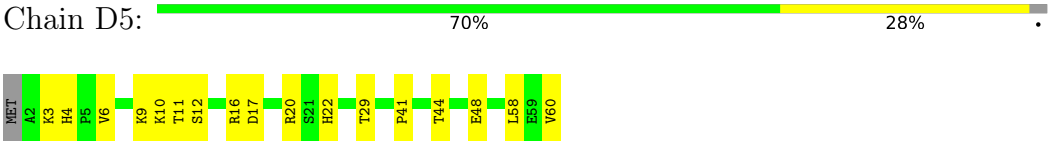
• Molecule 51: 50S Ribosomal Protein L32

Chain B5:



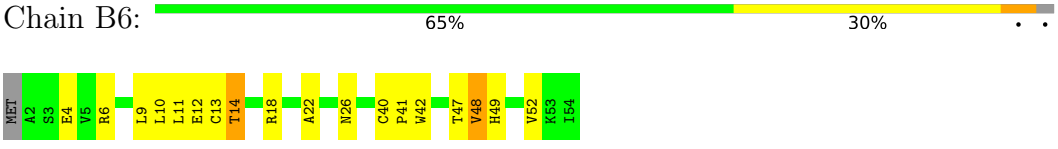
• Molecule 51: 50S Ribosomal Protein L32

Chain D5:



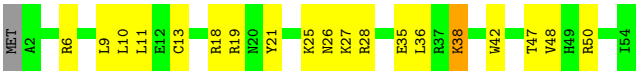
• Molecule 52: 50S Ribosomal Protein L33

Chain B6:



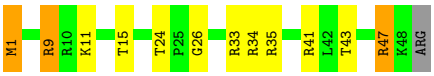
• Molecule 52: 50S Ribosomal Protein L33

Chain D6:



• Molecule 53: 50S Ribosomal Protein L34

Chain B7:



• Molecule 53: 50S Ribosomal Protein L34

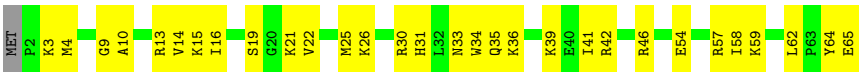
Chain D7:

• Molecule 54: 50S Ribosomal Protein L35

Chain B8:

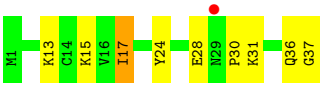
• Molecule 54: 50S Ribosomal Protein L35

Chain D8:



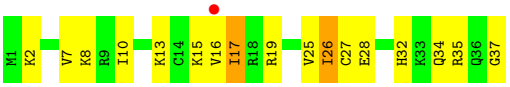
• Molecule 55: 50S Ribosomal Protein L36

Chain B9:



• Molecule 55: 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	210.08Å 449.83Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.00 49.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.74-3.00) 98.8 (49.74-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.259 0.203 , 0.257	Depositor DCC
R_{free} test set	57319 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: SF4, K, 2R3, 2QY, MG, MVA, 004, ZN, 2QZ, FME, 2R1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.42	1/36038 (0.0%)	0.66	6/56244 (0.0%)
1	CA	0.41	0/36170	0.65	12/56452 (0.0%)
2	AB	0.61	0/1881	1.21	23/2542 (0.9%)
2	CB	0.70	0/1860	1.20	17/2518 (0.7%)
3	AC	0.62	0/1576	1.02	1/2130 (0.0%)
3	CC	0.64	0/1566	1.10	6/2119 (0.3%)
4	AD	0.63	0/1689	1.13	5/2267 (0.2%)
4	CD	0.63	0/1704	1.07	8/2284 (0.4%)
5	AE	0.62	0/1145	1.11	9/1543 (0.6%)
5	CE	0.66	0/1149	1.21	9/1548 (0.6%)
6	AF	0.61	0/819	0.97	1/1111 (0.1%)
6	CF	0.68	0/829	1.03	1/1123 (0.1%)
7	AG	0.59	0/1250	1.02	4/1679 (0.2%)
7	CG	0.60	0/1254	1.16	7/1683 (0.4%)
8	AH	0.60	0/1108	1.06	2/1494 (0.1%)
8	CH	0.56	0/1108	1.11	3/1494 (0.2%)
9	AI	0.61	0/1002	1.06	2/1346 (0.1%)
9	CI	0.72	0/997	1.09	3/1343 (0.2%)
10	AJ	0.71	0/722	1.12	3/982 (0.3%)
10	CJ	0.72	0/727	1.10	3/988 (0.3%)
11	AK	0.57	0/844	1.05	7/1145 (0.6%)
11	CK	0.58	0/848	1.01	4/1149 (0.3%)
12	AL	0.63	0/946	1.13	2/1274 (0.2%)
12	CL	0.64	0/946	1.03	1/1274 (0.1%)
13	AM	0.61	0/969	1.08	3/1302 (0.2%)
13	CM	0.64	0/961	1.07	4/1291 (0.3%)
14	AN	0.54	0/501	1.05	2/664 (0.3%)
14	CN	0.62	0/501	1.06	1/664 (0.2%)
15	AO	0.63	0/739	1.07	3/985 (0.3%)
15	CO	0.59	0/739	1.03	0/985
16	AP	0.62	0/697	1.06	3/939 (0.3%)
16	CP	0.66	0/693	0.98	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.61	0/836	0.95	0/1117
17	CQ	0.59	0/836	1.02	2/1117 (0.2%)
18	AR	0.61	0/560	1.03	1/746 (0.1%)
18	CR	0.58	0/560	0.95	0/746
19	AS	0.62	0/667	1.05	2/900 (0.2%)
19	CS	0.70	0/661	1.15	2/893 (0.2%)
20	AT	0.59	0/730	1.21	2/965 (0.2%)
20	CT	0.57	0/729	1.02	1/965 (0.1%)
21	AU	0.53	0/203	0.98	0/266
21	CU	0.64	0/203	1.05	2/266 (0.8%)
22	AV	0.52	0/127	0.65	0/198
22	CV	0.51	0/126	0.65	0/195
23	AX	0.42	0/1813	0.64	1/2825 (0.0%)
23	CX	0.45	0/1813	0.75	1/2825 (0.0%)
24	AW	0.45	0/20	0.87	0/23
24	CW	0.32	0/20	0.55	0/23
25	BA	0.58	0/65892	0.69	5/102850 (0.0%)
25	DA	0.45	0/65466	0.67	2/102184 (0.0%)
26	BB	0.46	0/2878	0.62	0/4490
26	DB	0.48	0/2878	0.69	0/4490
27	BD	0.90	0/2186	1.14	6/2944 (0.2%)
27	DD	0.78	0/2186	1.11	7/2944 (0.2%)
28	BE	0.90	0/1592	1.16	7/2149 (0.3%)
28	DE	0.73	0/1592	1.20	7/2149 (0.3%)
29	BF	0.93	1/1619 (0.1%)	1.09	8/2193 (0.4%)
29	DF	0.65	0/1615	1.18	9/2188 (0.4%)
30	BG	0.61	0/1450	1.03	5/1959 (0.3%)
30	DG	0.65	0/1449	1.20	9/1958 (0.5%)
31	BH	0.81	0/1356	1.15	11/1834 (0.6%)
31	DH	0.66	0/1356	1.10	5/1834 (0.3%)
32	BI	0.65	0/1100	1.04	5/1501 (0.3%)
32	DI	0.66	0/1076	1.11	6/1471 (0.4%)
33	BN	0.88	0/1144	1.10	2/1543 (0.1%)
33	DN	0.68	0/1144	1.15	10/1543 (0.6%)
34	BO	0.85	0/943	1.08	0/1269
34	DO	0.73	0/943	1.08	0/1269
35	BP	0.83	0/1152	1.05	1/1533 (0.1%)
35	DP	0.67	0/1152	1.17	8/1533 (0.5%)
36	BQ	0.89	0/1143	1.12	2/1527 (0.1%)
36	DQ	0.72	0/1143	1.10	2/1527 (0.1%)
37	BR	0.87	1/982 (0.1%)	1.04	2/1312 (0.2%)
37	DR	0.69	0/982	0.94	0/1312
38	BS	0.69	0/887	1.05	3/1180 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DS	0.64	0/880	1.09	2/1172 (0.2%)
39	BT	0.78	0/1105	1.08	3/1477 (0.2%)
39	DT	0.68	0/1097	1.06	1/1468 (0.1%)
40	BU	0.89	0/977	1.07	2/1301 (0.2%)
40	DU	0.66	0/977	0.97	0/1301
41	BV	0.87	0/782	1.01	0/1049
41	DV	0.69	0/782	1.00	0/1049
42	BW	0.99	1/897 (0.1%)	1.06	1/1205 (0.1%)
42	DW	0.79	1/897 (0.1%)	1.09	0/1205
43	BX	0.89	0/764	0.98	0/1025
43	DX	0.66	0/764	1.12	5/1025 (0.5%)
44	BY	0.87	0/819	1.12	3/1095 (0.3%)
44	DY	0.68	0/819	1.12	3/1095 (0.3%)
45	BZ	0.72	0/1379	1.17	12/1873 (0.6%)
45	DZ	0.66	0/1390	1.10	11/1890 (0.6%)
46	B0	0.78	0/662	1.09	2/881 (0.2%)
46	D0	0.64	0/662	1.14	3/881 (0.3%)
47	B1	0.88	1/762 (0.1%)	1.11	4/1014 (0.4%)
47	D1	0.68	0/762	1.02	0/1014
48	B2	0.83	0/590	1.12	0/781
48	D2	0.57	0/590	0.95	0/781
49	B3	0.84	0/474	1.19	6/635 (0.9%)
49	D3	0.63	0/469	1.05	2/630 (0.3%)
50	B4	0.67	0/564	1.31	8/759 (1.1%)
50	D4	0.80	0/544	1.32	4/735 (0.5%)
51	B5	0.92	0/469	1.14	0/635
51	D5	0.75	0/469	1.07	2/635 (0.3%)
52	B6	0.78	0/460	0.89	0/613
52	D6	0.67	0/456	0.97	0/608
53	B7	0.97	0/426	1.02	1/561 (0.2%)
53	D7	0.76	0/426	1.01	0/561
54	B8	0.91	0/519	1.00	0/684
54	D8	0.69	0/525	1.01	0/691
55	B9	0.88	0/310	1.02	0/407
55	D9	0.67	0/310	1.12	0/407
All	All	0.56	6/305966 (0.0%)	0.81	366/457396 (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	3
4	CD	0	1
7	AG	0	1
9	AI	0	1
19	CS	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
45	BZ	0	1
50	B4	0	1
50	D4	0	1
All	All	1	15

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BR	38	VAL	CA-CB	-7.72	1.50	1.54
47	B1	67	ILE	CA-CB	-6.61	1.50	1.54
29	BF	84	VAL	CA-CB	-6.23	1.46	1.54
42	DW	103	ILE	CA-CB	-5.46	1.47	1.54
1	AA	343	U	C4-O4	5.11	1.33	1.23

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CX	76	A	O4'-C1'-N9	17.86	135.29	108.50
8	CH	73	ASP	CA-C-N	11.99	132.99	120.04
8	CH	73	ASP	C-N-CA	11.99	132.99	120.04
50	B4	60	GLN	N-CA-C	-10.28	100.41	113.16
7	CG	79	ARG	N-CA-C	10.02	123.53	108.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
9	AI	52	ALA	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	32196	0	16250	915	0
1	CA	32312	0	16307	1009	0
2	AB	1846	0	1867	109	0
2	CB	1825	0	1828	122	0
3	AC	1552	0	1546	52	0
3	CC	1542	0	1517	83	0
4	AD	1659	0	1676	90	0
4	CD	1674	0	1714	89	0
5	AE	1129	0	1185	44	0
5	CE	1133	0	1191	58	0
6	AF	806	0	793	36	0
6	CF	816	0	808	26	0
7	AG	1231	0	1238	33	0
7	CG	1235	0	1249	53	0
8	AH	1088	0	1126	45	0
8	CH	1088	0	1126	57	0
9	AI	983	0	986	47	0
9	CI	978	0	966	57	0
10	AJ	709	0	650	42	0
10	CJ	714	0	672	58	0
11	AK	829	0	825	17	0
11	CK	833	0	836	27	0
12	AL	930	0	980	35	0
12	CL	930	0	980	40	0
13	AM	958	0	1002	35	0
13	CM	950	0	988	54	0
14	AN	492	0	529	26	0
14	CN	492	0	529	32	0
15	AO	728	0	760	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	728	0	760	26	0
16	AP	681	0	697	36	0
16	CP	677	0	686	31	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	27	0
18	AR	555	0	618	25	0
18	CR	555	0	618	22	0
19	AS	652	0	662	43	0
19	CS	646	0	644	52	0
20	AT	728	0	798	37	0
20	CT	727	0	796	29	0
21	AU	199	0	208	7	0
21	CU	199	0	208	8	0
22	AV	114	0	54	1	0
22	CV	113	0	54	1	0
23	AX	1623	0	823	23	0
23	CX	1623	0	823	22	0
24	AW	93	0	84	10	0
24	CW	93	0	84	10	0
25	BA	58834	0	29666	844	0
25	DA	58458	0	29481	1173	0
26	BB	2573	0	1306	36	0
26	DB	2573	0	1306	66	0
27	BD	2136	0	2218	62	0
27	DD	2136	0	2218	75	0
28	BE	1559	0	1618	57	0
28	DE	1559	0	1618	65	0
29	BF	1584	0	1625	39	0
29	DF	1580	0	1619	67	0
30	BG	1425	0	1443	42	0
30	DG	1424	0	1434	92	0
31	BH	1330	0	1407	37	0
31	DH	1330	0	1407	51	0
32	BI	1085	0	1114	45	0
32	DI	1061	0	1080	28	0
33	BN	1117	0	1183	20	0
33	DN	1117	0	1184	25	0
34	BO	933	0	996	31	0
34	DO	933	0	996	31	0
35	BP	1135	0	1212	43	0
35	DP	1135	0	1212	50	0
36	BQ	1122	0	1179	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DQ	1122	0	1179	42	0
37	BR	968	0	1033	26	0
37	DR	968	0	1032	29	0
38	BS	877	0	938	30	0
38	DS	870	0	923	45	0
39	BT	1091	0	1151	36	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	28	0
40	DU	959	0	1019	28	0
41	BV	771	0	830	16	0
41	DV	771	0	830	23	0
42	BW	886	0	940	15	0
42	DW	886	0	940	26	0
43	BX	750	0	814	20	0
43	DX	750	0	814	23	0
44	BY	806	0	881	25	0
44	DY	806	0	881	28	0
45	BZ	1349	0	1355	45	0
45	DZ	1360	0	1363	57	0
46	B0	653	0	674	19	0
46	D0	653	0	674	32	0
47	B1	755	0	826	19	0
47	D1	755	0	826	20	0
48	B2	588	0	643	15	0
48	D2	588	0	643	18	0
49	B3	469	0	518	12	0
49	D3	464	0	514	11	0
50	B4	551	0	532	42	0
50	D4	531	0	502	41	0
51	B5	455	0	465	13	0
51	D5	455	0	465	11	0
52	B6	453	0	473	10	0
52	D6	449	0	469	13	0
53	B7	418	0	467	10	0
53	D7	418	0	467	9	0
54	B8	511	0	571	33	0
54	D8	517	0	582	24	0
55	B9	307	0	335	7	0
55	D9	307	0	335	14	0
56	AA	222	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	2	0	0	0	0
56	AN	1	0	0	0	0
56	AS	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0
56	BA	739	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	9	0	0	0	0
56	BF	6	0	0	0	0
56	BG	4	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	3	0	0	0	0
56	BW	5	0	0	0	0
56	BX	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	657	0	0	0	0
56	DB	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DD	5	0	0	0	0
56	DE	6	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	10	0	10	1	0
59	CX	10	0	10	3	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	147	0	0	23	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	0	0
61	AO	2	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B5	2	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1086	0	0	94	0
61	BB	26	0	0	2	0
61	BD	6	0	0	0	0
61	BE	13	0	0	3	0
61	BF	5	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	2	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	5	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	4	0	0	1	0
61	CA	186	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	3	0	0	1	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	906	0	0	117	0
61	DB	7	0	0	0	0
61	DD	10	0	0	0	0
61	DE	11	0	0	1	0
61	DF	4	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	2	0
61	DQ	3	0	0	1	0
61	DR	1	0	0	0	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	1	0
61	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	286321	0	191124	6816	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 15.

The worst 5 of 6816 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)
1:AA:1129:C:N4	1:AA:1143:G:H1	1.46	1.12
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.09
1:AA:348:G:H2'	1:AA:349:A:H5'	1.30	1.06
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.39	1.04
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.36	1.03

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%)	201 (88%)	23 (10%)	5 (2%)	5 26
2	CB	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3 19
3	AC	204/239 (85%)	182 (89%)	20 (10%)	2 (1%)	12 45
3	CC	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	12 45
4	AD	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	12 45
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	8 35
5	AE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	9 36
5	CE	146/162 (90%)	134 (92%)	12 (8%)	0	100 100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	53
7	CG	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	18	53
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	18	53
9	AI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	4	24
9	CI	125/128 (98%)	115 (92%)	8 (6%)	2 (2%)	7	34
10	AJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	18
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	27
11	AK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	48
11	CK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	48
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	16	50
13	CM	120/126 (95%)	113 (94%)	6 (5%)	1 (1%)	16	50
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
16	CP	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9	38
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	35
18	CR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	11	43
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	18
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	AW	3/10 (30%)	0	2 (67%)	1 (33%)	0 0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0 0
27	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30 65
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	18 53
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24 60
28	DE	202/206 (98%)	195 (96%)	4 (2%)	3 (2%)	8 35
29	BF	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24 60
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12 45
30	BG	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	7 32
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5 26
31	BH	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	21 56
31	DH	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	21 56
32	BI	144/148 (97%)	124 (86%)	14 (10%)	6 (4%)	2 13
32	DI	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5 27
33	BN	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
33	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18 53
34	BO	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	16 50
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	16 50
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18 53
35	DP	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	6 28
36	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18 53
36	DQ	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18 53
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14 48
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14 48
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14 48
39	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100 100
39	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100 100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
41	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12 45
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
43	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100 100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
44	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100 100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
45	BZ	169/206 (82%)	150 (89%)	18 (11%)	1 (1%)	21 56
45	DZ	172/206 (84%)	162 (94%)	10 (6%)	0	100 100
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10 40
46	D0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10 40
47	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 43
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 43
48	B2	68/72 (94%)	68 (100%)	0	0	100 100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
49	D3	57/60 (95%)	57 (100%)	0	0	100 100
50	B4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1 4
50	D4	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0 2
51	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
51	D5	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
52	D6	51/54 (94%)	47 (92%)	4 (8%)	0	100 100
53	B7	46/49 (94%)	46 (100%)	0	0	100 100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5 26
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
All	All	11415/12148 (94%)	10659 (93%)	648 (6%)	108 (1%)	14 48

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	125	PRO
3	AC	107	GLN
4	AD	166	LYS
9	AI	54	ASP
10	AJ	31	GLY

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%)	147 (77%)	45 (23%)	1	4
2	CB	187/220 (85%)	148 (79%)	39 (21%)	1	7
3	AC	143/188 (76%)	122 (85%)	21 (15%)	3	15
3	CC	140/188 (74%)	118 (84%)	22 (16%)	2	13
4	AD	170/181 (94%)	146 (86%)	24 (14%)	3	16
4	CD	173/181 (96%)	145 (84%)	28 (16%)	2	12
5	AE	113/123 (92%)	100 (88%)	13 (12%)	5	24
5	CE	114/123 (93%)	98 (86%)	16 (14%)	3	16
6	AF	83/90 (92%)	75 (90%)	8 (10%)	8	31
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	32
7	AG	119/127 (94%)	92 (77%)	27 (23%)	1	5
7	CG	120/127 (94%)	97 (81%)	23 (19%)	1	8
8	AH	114/119 (96%)	95 (83%)	19 (17%)	2	12
8	CH	114/119 (96%)	97 (85%)	17 (15%)	3	15
9	AI	90/99 (91%)	75 (83%)	15 (17%)	2	12
9	CI	89/99 (90%)	77 (86%)	12 (14%)	4	18
10	AJ	66/92 (72%)	57 (86%)	9 (14%)	3	17
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7	29
11	AK	82/99 (83%)	73 (89%)	9 (11%)	6	25
11	CK	83/99 (84%)	72 (87%)	11 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	AL	97/109 (89%)	85 (88%)	12 (12%)	4 20
12	CL	97/109 (89%)	83 (86%)	14 (14%)	3 15
13	AM	93/101 (92%)	81 (87%)	12 (13%)	4 19
13	CM	92/101 (91%)	77 (84%)	15 (16%)	2 12
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1 7
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1 9
15	AO	78/80 (98%)	69 (88%)	9 (12%)	5 24
15	CO	78/80 (98%)	67 (86%)	11 (14%)	3 16
16	AP	69/74 (93%)	61 (88%)	8 (12%)	5 23
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7 28
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13 42
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8 31
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10 36
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3 17
19	AS	69/80 (86%)	63 (91%)	6 (9%)	9 35
19	CS	67/80 (84%)	58 (87%)	9 (13%)	4 18
20	AT	70/82 (85%)	59 (84%)	11 (16%)	2 13
20	CT	70/82 (85%)	61 (87%)	9 (13%)	4 19
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2 12
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2 12
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0 1
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0 1
27	BD	215/218 (99%)	194 (90%)	21 (10%)	7 30
27	DD	215/218 (99%)	187 (87%)	28 (13%)	4 19
28	BE	164/166 (99%)	135 (82%)	29 (18%)	2 10
28	DE	164/166 (99%)	135 (82%)	29 (18%)	2 10
29	BF	160/166 (96%)	134 (84%)	26 (16%)	2 12
29	DF	159/166 (96%)	133 (84%)	26 (16%)	2 12
30	BG	143/156 (92%)	120 (84%)	23 (16%)	2 12
30	DG	142/156 (91%)	119 (84%)	23 (16%)	2 12
31	BH	144/148 (97%)	125 (87%)	19 (13%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	DH	144/148 (97%)	126 (88%)	18 (12%)	4 20
32	BI	110/124 (89%)	84 (76%)	26 (24%)	1 4
32	DI	104/124 (84%)	84 (81%)	20 (19%)	1 8
33	BN	118/119 (99%)	97 (82%)	21 (18%)	2 10
33	DN	118/119 (99%)	98 (83%)	20 (17%)	2 11
34	BO	100/100 (100%)	90 (90%)	10 (10%)	7 29
34	DO	100/100 (100%)	85 (85%)	15 (15%)	3 14
35	BP	115/116 (99%)	99 (86%)	16 (14%)	3 17
35	DP	115/116 (99%)	98 (85%)	17 (15%)	3 15
36	BQ	111/111 (100%)	98 (88%)	13 (12%)	5 23
36	DQ	111/111 (100%)	99 (89%)	12 (11%)	6 26
37	BR	101/101 (100%)	82 (81%)	19 (19%)	1 9
37	DR	101/101 (100%)	82 (81%)	19 (19%)	1 9
38	BS	87/88 (99%)	75 (86%)	12 (14%)	3 17
38	DS	85/88 (97%)	66 (78%)	19 (22%)	1 5
39	BT	115/127 (91%)	101 (88%)	14 (12%)	5 21
39	DT	113/127 (89%)	100 (88%)	13 (12%)	5 24
40	BU	93/94 (99%)	80 (86%)	13 (14%)	3 16
40	DU	93/94 (99%)	78 (84%)	15 (16%)	2 12
41	BV	80/82 (98%)	65 (81%)	15 (19%)	1 9
41	DV	80/82 (98%)	64 (80%)	16 (20%)	1 7
42	BW	90/92 (98%)	79 (88%)	11 (12%)	5 21
42	DW	90/92 (98%)	79 (88%)	11 (12%)	5 21
43	BX	77/78 (99%)	71 (92%)	6 (8%)	11 39
43	DX	77/78 (99%)	71 (92%)	6 (8%)	11 39
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8 32
44	DY	85/91 (93%)	79 (93%)	6 (7%)	13 43
45	BZ	145/179 (81%)	124 (86%)	21 (14%)	3 15
45	DZ	145/179 (81%)	127 (88%)	18 (12%)	4 20
46	B0	65/67 (97%)	61 (94%)	4 (6%)	16 49
46	D0	65/67 (97%)	59 (91%)	6 (9%)	8 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	B1	80/83 (96%)	70 (88%)	10 (12%)	4 20
47	D1	80/83 (96%)	67 (84%)	13 (16%)	2 12
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3 17
48	D2	65/67 (97%)	56 (86%)	9 (14%)	3 17
49	B3	51/52 (98%)	40 (78%)	11 (22%)	1 6
49	D3	50/52 (96%)	41 (82%)	9 (18%)	2 10
50	B4	59/63 (94%)	48 (81%)	11 (19%)	1 9
50	D4	53/63 (84%)	43 (81%)	10 (19%)	1 9
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5 22
51	D5	50/52 (96%)	47 (94%)	3 (6%)	17 50
52	B6	51/52 (98%)	47 (92%)	4 (8%)	11 39
52	D6	50/52 (96%)	46 (92%)	4 (8%)	11 38
53	B7	41/42 (98%)	37 (90%)	4 (10%)	7 30
53	D7	41/42 (98%)	37 (90%)	4 (10%)	7 30
54	B8	53/55 (96%)	49 (92%)	4 (8%)	12 41
54	D8	54/55 (98%)	51 (94%)	3 (6%)	19 52
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37 70
55	D9	34/34 (100%)	31 (91%)	3 (9%)	9 35
All	All	9325/10072 (93%)	7991 (86%)	1334 (14%)	3 16

5 of 1334 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	24	LEU
36	DQ	110	THR
27	DD	165	ILE
19	CS	65	ASN
30	DG	145	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
28	DE	85	ASN
52	D6	20	ASN
29	DF	169	ASN

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Mol	Chain	Res	Type
38	DS	68	GLN
30	BG	26	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	422 (28%)	24 (1%)
1	CA	1501/1522 (98%)	423 (28%)	30 (1%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	18 (24%)	0
23	CX	75/77 (97%)	19 (25%)	0
25	BA	2722/2915 (93%)	533 (19%)	41 (1%)
25	DA	2704/2915 (92%)	529 (19%)	35 (1%)
26	BB	119/122 (97%)	21 (17%)	0
26	DB	119/122 (97%)	23 (19%)	1 (0%)
All	All	8818/9320 (94%)	1990 (22%)	131 (1%)

5 of 1990 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	16	A
1	AA	22	G

5 of 131 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1427	A
25	DA	1608	A
26	DB	45	A
25	BA	1466	U
25	BA	1321	A

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

14 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	$\#\|Z\| > 2$
24	2R3	CW	8	24	12,14,15	0.71	0	16,18,20	2.15	6 (37%)
24	2QY	CW	10	24	12,13,14	2.04	2 (16%)	14,16,18	3.56	3 (21%)
24	004	AW	3	24	9,10,11	1.20	1 (11%)	9,12,14	1.16	0
24	MVA	CW	5	24	6,7,8	0.81	0	6,8,10	1.51	2 (33%)
24	MVA	CW	9	24	6,7,8	0.89	0	6,8,10	1.10	0
24	2QZ	AW	1	24	7,8,9	0.41	0	7,10,12	2.50	1 (14%)
24	2R1	CW	6	24	10,10,11	1.82	3 (30%)	8,13,15	3.68	3 (37%)
24	2QZ	CW	1	24	7,8,9	0.83	0	7,10,12	3.69	2 (28%)
24	004	CW	3	24	9,10,11	1.35	1 (11%)	9,12,14	0.68	0
24	2QY	AW	10	24	12,13,14	1.94	2 (16%)	14,16,18	3.62	6 (42%)
24	2R3	AW	8	24	12,14,15	0.81	0	16,18,20	2.05	7 (43%)
24	MVA	AW	5	24	6,7,8	0.57	0	6,8,10	1.28	0
24	2R1	AW	6	24	10,10,11	2.43	4 (40%)	8,13,15	4.19	3 (37%)
24	MVA	AW	9	24	6,7,8	0.38	0	6,8,10	0.94	1 (16%)

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
24	2R3	CW	8	24	-	6/11/12/14	0/1/1/1
24	2QY	CW	10	24	-	1/5/8/10	0/1/1/1
24	004	AW	3	24	-	1/4/6/8	0/1/1/1
24	MVA	CW	5	24	-	5/6/8/10	-
24	MVA	CW	9	24	-	5/6/8/10	-
24	2QZ	AW	1	24	-	3/8/10/12	-
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2QZ	CW	1	24	-	1/8/10/12	-
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2QY	AW	10	24	-	3/5/8/10	0/1/1/1
24	2R3	AW	8	24	-	6/11/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MVA	AW	5	24	-	2/6/8/10	-
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	MVA	AW	9	24	-	5/6/8/10	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	10	2QY	C-CA	6.08	1.53	1.43
24	AW	10	2QY	C-CA	5.76	1.53	1.43
24	AW	6	2R1	OD1-CG1	4.61	1.56	1.42
24	AW	6	2R1	CA-N	4.13	1.46	1.36
24	CW	6	2R1	CA-N	3.84	1.45	1.36

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AW	6	2R1	OD2-CG2-CB	-10.70	92.15	111.99
24	CW	10	2QY	CN-N-CA	-9.76	109.17	123.98
24	AW	10	2QY	CN-N-CA	-9.66	109.33	123.98
24	CW	1	2QZ	OG1-CB-CG2	9.20	137.20	109.68
24	CW	6	2R1	OD2-CG2-CB	-8.95	95.40	111.99

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	5	MVA	CB-CA-N-CN
24	AW	8	2R3	N-CA-CB-OB
24	AW	8	2R3	N-CA-CB-CG
24	AW	8	2R3	C-CA-CB-OB

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	8	2R3	2	0
24	CW	10	2QY	4	0
24	AW	3	004	1	0
24	CW	5	MVA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	9	MVA	3	0
24	AW	1	2QZ	2	0
24	CW	6	2R1	1	0
24	CW	1	2QZ	3	0
24	CW	3	004	1	0
24	AW	10	2QY	3	0
24	AW	8	2R3	4	0
24	AW	5	MVA	1	0
24	AW	6	2R1	3	0
24	AW	9	MVA	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
59	FME	AX	101	23	8,9,10	0.94	0	8,9,11	1.49	2 (25%)
59	FME	CX	101	23	8,9,10	0.82	0	8,9,11	1.37	1 (12%)
57	SF4	CD	501	4	0,12,12	-	-	-		
57	SF4	AD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	AX	101	23	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	CX	101	23	-	1/7/9/11	-
57	SF4	CD	501	4	-	-	0/6/5/5
57	SF4	AD	501	4	-	-	0/6/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	AX	101	FME	CA-N-CN	-2.47	119.03	122.82
59	CX	101	FME	CA-N-CN	-2.33	119.25	122.82
59	AX	101	FME	CB-CA-N	2.31	114.72	110.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	CX	101	FME	O1-CN-N-CA
59	AX	101	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AX	101	FME	1	0
59	CX	101	FME	3	0
57	CD	501	SF4	1	0
57	AD	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1498/1522 (98%)	0.01	25 (1%) 69 45	39, 80, 103, 118	0
1	CA	1503/1522 (98%)	0.01	22 (1%) 72 49	41, 80, 103, 119	0
2	AB	231/256 (90%)	0.47	6 (2%) 57 34	69, 86, 97, 105	0
2	CB	231/256 (90%)	0.54	11 (4%) 35 19	70, 88, 98, 107	0
3	AC	206/239 (86%)	0.44	5 (2%) 59 36	73, 87, 95, 104	0
3	CC	206/239 (86%)	0.62	6 (2%) 53 31	72, 89, 97, 104	0
4	AD	208/209 (99%)	0.55	6 (2%) 53 31	61, 80, 90, 97	0
4	CD	208/209 (99%)	0.43	2 (0%) 79 59	61, 79, 89, 97	0
5	AE	148/162 (91%)	-0.10	0 100 100	51, 73, 82, 93	0
5	CE	148/162 (91%)	0.18	0 100 100	53, 75, 84, 96	0
6	AF	100/101 (99%)	0.11	1 (1%) 79 59	63, 77, 87, 94	0
6	CF	100/101 (99%)	0.15	0 100 100	62, 78, 87, 95	0
7	AG	155/156 (99%)	0.29	5 (3%) 50 29	74, 86, 99, 106	0
7	CG	155/156 (99%)	0.43	5 (3%) 50 29	75, 86, 99, 105	0
8	AH	137/138 (99%)	0.17	0 100 100	60, 74, 82, 89	0
8	CH	137/138 (99%)	0.32	3 (2%) 62 39	62, 75, 83, 89	0
9	AI	127/128 (99%)	0.81	9 (7%) 22 11	73, 91, 99, 101	0
9	CI	127/128 (99%)	1.33	27 (21%) 2 1	72, 93, 100, 102	0
10	AJ	97/105 (92%)	1.05	14 (14%) 6 3	73, 91, 100, 105	0
10	CJ	96/105 (91%)	1.19	14 (14%) 6 3	77, 93, 100, 104	0
11	AK	114/129 (88%)	-0.00	1 (0%) 81 61	53, 74, 87, 91	0
11	CK	114/129 (88%)	0.02	0 100 100	55, 76, 87, 92	0
12	AL	122/132 (92%)	0.24	4 (3%) 49 28	53, 68, 80, 87	0
12	CL	122/132 (92%)	0.14	2 (1%) 70 47	53, 69, 80, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.40	7 (5%) 29 15	67, 85, 95, 105	0
13	CM	122/126 (96%)	0.75	7 (5%) 29 15	77, 92, 100, 109	0
14	AN	60/61 (98%)	0.85	6 (10%) 12 7	75, 87, 94, 103	0
14	CN	60/61 (98%)	1.32	14 (23%) 2 1	77, 89, 94, 100	0
15	AO	88/89 (98%)	0.17	1 (1%) 78 57	55, 72, 85, 90	0
15	CO	88/89 (98%)	0.09	1 (1%) 78 57	55, 72, 85, 91	0
16	AP	82/88 (93%)	0.66	5 (6%) 27 14	67, 78, 89, 94	0
16	CP	82/88 (93%)	0.58	3 (3%) 45 25	66, 76, 88, 94	0
17	AQ	99/105 (94%)	0.22	1 (1%) 79 59	59, 72, 83, 90	0
17	CQ	99/105 (94%)	0.18	0 100 100	58, 72, 83, 89	0
18	AR	68/88 (77%)	0.18	0 100 100	65, 73, 87, 91	0
18	CR	68/88 (77%)	0.08	0 100 100	64, 75, 87, 91	0
19	AS	83/93 (89%)	0.79	7 (8%) 17 9	77, 92, 99, 106	0
19	CS	83/93 (89%)	1.14	15 (18%) 3 2	79, 92, 101, 106	0
20	AT	96/106 (90%)	0.63	7 (7%) 21 11	62, 76, 86, 90	0
20	CT	96/106 (90%)	0.32	3 (3%) 51 30	62, 74, 86, 92	0
21	AU	23/27 (85%)	1.34	4 (17%) 4 3	73, 88, 93, 94	0
21	CU	23/27 (85%)	1.81	8 (34%) 1 1	73, 89, 92, 94	0
22	AV	7/24 (29%)	0.35	0 100 100	65, 77, 102, 104	0
22	CV	6/24 (25%)	0.46	1 (16%) 4 3	67, 78, 103, 103	0
23	AX	76/77 (98%)	-0.38	0 100 100	52, 80, 97, 105	0
23	CX	76/77 (98%)	-0.13	0 100 100	52, 82, 100, 106	0
24	AW	3/10 (30%)	0.50	0 100 100	67, 67, 82, 98	0
24	CW	3/10 (30%)	-0.32	0 100 100	67, 67, 78, 82	0
25	BA	2731/2915 (93%)	-0.69	13 (0%) 87 72	23, 44, 85, 111	0
25	DA	2714/2915 (93%)	-0.69	4 (0%) 92 86	26, 47, 85, 118	0
26	BB	120/122 (98%)	-0.27	0 100 100	42, 68, 80, 95	0
26	DB	120/122 (98%)	0.09	0 100 100	48, 74, 84, 97	0
27	BD	275/276 (99%)	-0.44	0 100 100	22, 42, 58, 77	0
27	DD	275/276 (99%)	-0.45	1 (0%) 88 76	23, 44, 60, 79	0
28	BE	204/206 (99%)	-0.42	0 100 100	23, 45, 67, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DE	204/206 (99%)	-0.39	1 (0%) 87 72	24, 47, 70, 88	0
29	BF	203/210 (96%)	-0.23	0 100 100	20, 51, 77, 94	0
29	DF	203/210 (96%)	-0.26	0 100 100	22, 54, 78, 93	0
30	BG	181/182 (99%)	0.18	2 (1%) 78 57	59, 77, 90, 103	0
30	DG	181/182 (99%)	0.59	8 (4%) 39 21	63, 80, 92, 102	0
31	BH	174/180 (96%)	0.12	2 (1%) 78 57	50, 66, 78, 84	0
31	DH	174/180 (96%)	0.31	1 (0%) 85 69	54, 71, 82, 87	0
32	BI	146/148 (98%)	-0.08	0 100 100	45, 75, 87, 92	0
32	DI	146/148 (98%)	0.17	0 100 100	48, 76, 86, 91	0
33	BN	140/140 (100%)	-0.16	1 (0%) 84 66	32, 49, 68, 80	0
33	DN	140/140 (100%)	-0.23	0 100 100	34, 53, 72, 81	0
34	BO	122/122 (100%)	-0.57	0 100 100	25, 39, 60, 78	0
34	DO	122/122 (100%)	-0.39	0 100 100	34, 52, 68, 79	0
35	BP	149/150 (99%)	-0.19	1 (0%) 84 66	26, 54, 76, 84	0
35	DP	149/150 (99%)	-0.08	0 100 100	30, 57, 79, 86	0
36	BQ	141/141 (100%)	-0.05	3 (2%) 63 40	33, 51, 65, 79	0
36	DQ	141/141 (100%)	-0.15	1 (0%) 84 66	35, 54, 70, 80	0
37	BR	118/118 (100%)	-0.53	0 100 100	22, 35, 51, 64	0
37	DR	118/118 (100%)	-0.26	0 100 100	36, 50, 64, 81	0
38	BS	110/112 (98%)	-0.30	0 100 100	38, 55, 69, 81	0
38	DS	110/112 (98%)	0.57	5 (4%) 38 20	66, 78, 90, 100	0
39	BT	131/146 (89%)	-0.30	2 (1%) 72 49	33, 45, 75, 91	0
39	DT	131/146 (89%)	-0.21	2 (1%) 72 49	44, 56, 80, 86	0
40	BU	116/118 (98%)	-0.71	0 100 100	19, 30, 50, 63	0
40	DU	116/118 (98%)	-0.10	0 100 100	39, 61, 79, 88	0
41	BV	101/101 (100%)	-0.29	0 100 100	29, 52, 70, 77	0
41	DV	101/101 (100%)	-0.31	0 100 100	32, 58, 74, 79	0
42	BW	112/113 (99%)	-0.47	1 (0%) 81 61	27, 37, 61, 94	0
42	DW	112/113 (99%)	-0.42	0 100 100	31, 40, 63, 94	0
43	BX	95/96 (98%)	-0.16	1 (1%) 78 57	32, 46, 69, 82	0
43	DX	95/96 (98%)	-0.04	0 100 100	38, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BY	107/110 (97%)	0.11	3 (2%) 55 32	44, 59, 77, 82	0
44	DY	107/110 (97%)	0.30	3 (2%) 55 32	46, 63, 80, 85	0
45	BZ	171/206 (83%)	0.11	2 (1%) 76 55	52, 71, 85, 93	0
45	DZ	174/206 (84%)	0.33	1 (0%) 85 69	56, 74, 87, 95	0
46	B0	83/85 (97%)	-0.13	6 (7%) 21 11	22, 40, 75, 104	0
46	D0	83/85 (97%)	0.28	3 (3%) 46 26	45, 66, 87, 98	0
47	B1	97/98 (98%)	-0.41	0 100 100	25, 42, 71, 77	0
47	D1	97/98 (98%)	-0.17	1 (1%) 79 59	35, 56, 79, 85	0
48	B2	70/72 (97%)	-0.23	0 100 100	31, 48, 64, 77	0
48	D2	70/72 (97%)	0.09	0 100 100	56, 73, 84, 86	0
49	B3	59/60 (98%)	-0.44	0 100 100	26, 38, 63, 86	0
49	D3	59/60 (98%)	-0.14	0 100 100	49, 62, 80, 93	0
50	B4	69/71 (97%)	0.27	0 100 100	64, 87, 101, 104	0
50	D4	69/71 (97%)	0.72	4 (5%) 29 15	85, 95, 104, 107	0
51	B5	59/60 (98%)	-0.75	0 100 100	14, 35, 55, 71	0
51	D5	59/60 (98%)	-0.34	0 100 100	29, 51, 70, 77	0
52	B6	53/54 (98%)	-0.38	0 100 100	40, 54, 68, 74	0
52	D6	53/54 (98%)	-0.30	0 100 100	42, 58, 68, 74	0
53	B7	48/49 (97%)	-0.39	0 100 100	26, 32, 67, 78	0
53	D7	48/49 (97%)	-0.27	1 (2%) 63 40	27, 34, 66, 79	0
54	B8	64/65 (98%)	-0.33	0 100 100	33, 43, 51, 56	0
54	D8	64/65 (98%)	-0.14	0 100 100	34, 46, 56, 60	0
55	B9	37/37 (100%)	0.14	1 (2%) 56 33	43, 52, 68, 77	0
55	D9	37/37 (100%)	0.26	1 (2%) 56 33	48, 57, 72, 78	0
All	All	20462/21468 (95%)	-0.13	333 (1%) 70 47	14, 65, 95, 119	0

The worst 5 of 333 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	6.6
13	AM	123	ALA	6.0
13	CM	123	ALA	5.9
9	CI	11	LYS	5.2
44	BY	1	MET	5.0

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, 95^{th} 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
24	2R1	AW	6	10/11	0.76	0.14	66,72,84,91	0
24	MVA	AW	5	8/9	0.77	0.15	69,82,86,91	0
24	004	AW	3	10/11	0.81	0.12	67,87,95,97	0
24	2QY	CW	10	13/14	0.85	0.11	60,72,80,86	0
24	2R1	CW	6	10/11	0.86	0.12	68,82,90,91	0
24	2R3	AW	8	14/15	0.86	0.13	70,78,86,87	0
24	MVA	CW	5	8/9	0.87	0.12	76,88,91,99	0
24	MVA	CW	9	8/9	0.88	0.11	70,73,84,91	0
24	2QY	AW	10	13/14	0.90	0.10	49,70,87,100	0
24	MVA	AW	9	8/9	0.92	0.11	63,74,87,88	0
24	2QZ	AW	1	9/10	0.92	0.10	50,71,82,83	0
24	2R3	CW	8	14/15	0.93	0.08	62,69,77,78	0
24	2QZ	CW	1	9/10	0.94	0.10	63,71,80,101	0
24	004	CW	3	10/11	0.94	0.08	69,78,82,83	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
56	MG	CA	3147	1/1	0.28	0.30	77,77,77,77	0
56	MG	CA	3139	1/1	0.48	0.22	76,76,76,76	0
56	MG	CA	3114	1/1	0.55	0.18	67,67,67,67	0
56	MG	AA	3180	1/1	0.58	0.29	75,75,75,75	0
56	MG	BA	3661	1/1	0.61	0.19	69,69,69,69	0
56	MG	CA	3156	1/1	0.62	0.21	80,80,80,80	0
56	MG	AA	3093	1/1	0.63	0.25	90,90,90,90	0
56	MG	CA	3142	1/1	0.65	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3164	1/1	0.65	0.16	43,43,43,43	0
56	MG	DA	3356	1/1	0.65	0.14	57,57,57,57	0
56	MG	CA	3030	1/1	0.66	0.44	74,74,74,74	0
56	MG	CA	3053	1/1	0.66	0.50	87,87,87,87	0
56	MG	AA	3164	1/1	0.66	0.28	61,61,61,61	0
56	MG	AA	3076	1/1	0.67	0.37	74,74,74,74	0
56	MG	AA	3129	1/1	0.68	0.25	77,77,77,77	0
56	MG	BA	3103	1/1	0.68	0.28	58,58,58,58	0
56	MG	AA	3072	1/1	0.68	0.20	69,69,69,69	0
56	MG	DG	3001	1/1	0.68	0.16	68,68,68,68	0
56	MG	BB	3005	1/1	0.69	0.27	62,62,62,62	0
56	MG	BA	3625	1/1	0.69	0.17	80,80,80,80	0
56	MG	CA	3161	1/1	0.69	0.15	71,71,71,71	0
56	MG	AX	108	1/1	0.70	0.26	66,66,66,66	0
56	MG	BA	3203	1/1	0.70	0.17	45,45,45,45	0
56	MG	DA	3540	1/1	0.71	0.16	76,76,76,76	0
56	MG	AA	3200	1/1	0.71	0.24	79,79,79,79	0
56	MG	AA	3021	1/1	0.72	0.18	76,76,76,76	0
56	MG	BA	3704	1/1	0.72	0.20	58,58,58,58	0
56	MG	AA	3094	1/1	0.72	0.13	78,78,78,78	0
56	MG	DA	3568	1/1	0.73	0.18	58,58,58,58	0
56	MG	DA	3619	1/1	0.73	0.17	67,67,67,67	0
56	MG	AA	3133	1/1	0.73	0.41	71,71,71,71	0
56	MG	CA	3025	1/1	0.74	0.18	102,102,102,102	0
56	MG	AA	3087	1/1	0.74	0.21	87,87,87,87	0
56	MG	DA	3567	1/1	0.74	0.15	68,68,68,68	0
56	MG	AS	3001	1/1	0.74	0.16	79,79,79,79	0
56	MG	AX	104	1/1	0.74	0.11	62,62,62,62	0
56	MG	BA	3620	1/1	0.74	0.22	57,57,57,57	0
56	MG	CA	3129	1/1	0.75	0.21	54,54,54,54	0
56	MG	AA	3002	1/1	0.75	0.14	74,74,74,74	0
56	MG	DA	3464	1/1	0.75	0.11	51,51,51,51	0
56	MG	DA	3630	1/1	0.75	0.12	67,67,67,67	0
56	MG	DB	3003	1/1	0.75	0.21	70,70,70,70	0
56	MG	AA	3022	1/1	0.75	0.19	56,56,56,56	0
56	MG	DA	3001	1/1	0.76	0.37	76,76,76,76	0
56	MG	DA	3115	1/1	0.76	0.11	64,64,64,64	0
56	MG	CA	3073	1/1	0.76	0.22	74,74,74,74	0
56	MG	DA	3436	1/1	0.76	0.11	61,61,61,61	0
56	MG	DA	3456	1/1	0.76	0.20	58,58,58,58	0
56	MG	AA	3209	1/1	0.76	0.16	66,66,66,66	0
56	MG	DA	3500	1/1	0.76	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BF	306	1/1	0.76	0.13	52,52,52,52	0
56	MG	AA	3063	1/1	0.76	0.18	57,57,57,57	0
56	MG	CA	3027	1/1	0.76	0.14	64,64,64,64	0
56	MG	DA	3602	1/1	0.76	0.17	63,63,63,63	0
56	MG	AA	3131	1/1	0.76	0.25	65,65,65,65	0
56	MG	BA	3582	1/1	0.76	0.16	52,52,52,52	0
56	MG	DA	3639	1/1	0.76	0.22	55,55,55,55	0
56	MG	CA	3061	1/1	0.76	0.36	68,68,68,68	0
56	MG	CA	3070	1/1	0.76	0.21	59,59,59,59	0
56	MG	CA	3119	1/1	0.77	0.29	73,73,73,73	0
56	MG	DA	3603	1/1	0.77	0.17	66,66,66,66	0
56	MG	BA	3711	1/1	0.77	0.28	64,64,64,64	0
56	MG	CA	3009	1/1	0.77	0.14	55,55,55,55	0
56	MG	BA	3708	1/1	0.77	0.16	38,38,38,38	0
56	MG	CA	3056	1/1	0.77	0.19	63,63,63,63	0
56	MG	CA	3117	1/1	0.77	0.11	58,58,58,58	0
56	MG	BA	3740	1/1	0.78	0.26	57,57,57,57	0
56	MG	CA	3172	1/1	0.78	0.19	65,65,65,65	0
56	MG	BA	3133	1/1	0.78	0.34	53,53,53,53	0
56	MG	DA	3462	1/1	0.78	0.19	71,71,71,71	0
56	MG	DA	3066	1/1	0.78	0.25	59,59,59,59	0
56	MG	CA	3144	1/1	0.78	0.26	84,84,84,84	0
56	MG	DA	3123	1/1	0.78	0.10	61,61,61,61	0
56	MG	DA	3220	1/1	0.78	0.06	61,61,61,61	0
56	MG	AA	3189	1/1	0.79	0.13	74,74,74,74	0
56	MG	CA	3152	1/1	0.79	0.21	45,45,45,45	0
56	MG	DA	3131	1/1	0.79	0.09	60,60,60,60	0
56	MG	DA	3141	1/1	0.79	0.22	63,63,63,63	0
56	MG	BA	3358	1/1	0.79	0.12	78,78,78,78	0
56	MG	DA	3296	1/1	0.79	0.19	65,65,65,65	0
56	MG	CA	3007	1/1	0.79	0.11	63,63,63,63	0
56	MG	AA	3115	1/1	0.79	0.27	67,67,67,67	0
56	MG	AA	3067	1/1	0.79	0.29	76,76,76,76	0
56	MG	DB	3001	1/1	0.79	0.17	80,80,80,80	0
56	MG	AA	3112	1/1	0.79	0.14	53,53,53,53	0
56	MG	CA	3091	1/1	0.79	0.11	95,95,95,95	0
56	MG	CA	3028	1/1	0.80	0.44	62,62,62,62	0
56	MG	DA	3241	1/1	0.80	0.08	74,74,74,74	0
56	MG	AA	3136	1/1	0.80	0.14	68,68,68,68	0
56	MG	AA	3117	1/1	0.80	0.18	64,64,64,64	0
56	MG	DA	3073	1/1	0.80	0.23	50,50,50,50	0
56	MG	DA	3441	1/1	0.80	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3627	1/1	0.80	0.14	52,52,52,52	0
56	MG	AA	3030	1/1	0.80	0.39	66,66,66,66	0
56	MG	CA	3060	1/1	0.80	0.27	59,59,59,59	0
56	MG	BA	3247	1/1	0.80	0.26	58,58,58,58	0
56	MG	BA	3292	1/1	0.80	0.27	59,59,59,59	0
56	MG	DA	3506	1/1	0.80	0.11	61,61,61,61	0
56	MG	BA	3636	1/1	0.81	0.13	54,54,54,54	0
56	MG	CA	3159	1/1	0.81	0.25	76,76,76,76	0
56	MG	DA	3113	1/1	0.81	0.45	61,61,61,61	0
56	MG	DA	3346	1/1	0.81	0.10	64,64,64,64	0
56	MG	BA	3510	1/1	0.81	0.24	66,66,66,66	0
56	MG	AA	3184	1/1	0.81	0.16	81,81,81,81	0
56	MG	AA	3217	1/1	0.81	0.30	64,64,64,64	0
56	MG	AD	502	1/1	0.81	0.30	56,56,56,56	0
56	MG	CA	3048	1/1	0.82	0.32	70,70,70,70	0
56	MG	DA	3414	1/1	0.82	0.18	59,59,59,59	0
56	MG	DA	3418	1/1	0.82	0.14	57,57,57,57	0
56	MG	BA	3338	1/1	0.82	0.18	62,62,62,62	0
56	MG	BA	3710	1/1	0.82	0.15	57,57,57,57	0
56	MG	AA	3127	1/1	0.82	0.20	50,50,50,50	0
56	MG	BA	3060	1/1	0.82	0.31	64,64,64,64	0
56	MG	AA	3114	1/1	0.82	0.18	73,73,73,73	0
56	MG	DA	3496	1/1	0.82	0.20	76,76,76,76	0
56	MG	BB	3014	1/1	0.82	0.17	68,68,68,68	0
56	MG	BB	3017	1/1	0.82	0.29	80,80,80,80	0
56	MG	DA	3537	1/1	0.82	0.15	74,74,74,74	0
56	MG	CA	3110	1/1	0.82	0.15	93,93,93,93	0
56	MG	DA	3554	1/1	0.82	0.06	62,62,62,62	0
56	MG	DA	3566	1/1	0.82	0.18	55,55,55,55	0
56	MG	AA	3171	1/1	0.82	0.15	77,77,77,77	0
56	MG	BA	3177	1/1	0.82	0.43	35,35,35,35	0
56	MG	AA	3023	1/1	0.82	0.13	56,56,56,56	0
56	MG	AA	3132	1/1	0.82	0.16	59,59,59,59	0
56	MG	DA	3606	1/1	0.82	0.14	58,58,58,58	0
56	MG	DA	3617	1/1	0.82	0.12	51,51,51,51	0
56	MG	BA	3693	1/1	0.82	0.22	57,57,57,57	0
56	MG	DA	3162	1/1	0.82	0.18	69,69,69,69	0
56	MG	DA	3169	1/1	0.82	0.24	58,58,58,58	0
56	MG	CA	3141	1/1	0.82	0.39	85,85,85,85	0
56	MG	DA	3642	1/1	0.82	0.21	67,67,67,67	0
56	MG	AA	3032	1/1	0.82	0.28	65,65,65,65	0
56	MG	BA	3705	1/1	0.82	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3033	1/1	0.82	0.14	64,64,64,64	0
56	MG	AA	3039	1/1	0.83	0.10	62,62,62,62	0
56	MG	AA	3162	1/1	0.83	0.17	79,79,79,79	0
56	MG	AA	3126	1/1	0.83	0.21	54,54,54,54	0
56	MG	DA	3086	1/1	0.83	0.20	43,43,43,43	0
56	MG	DA	3108	1/1	0.83	0.11	50,50,50,50	0
56	MG	AA	3016	1/1	0.83	0.10	70,70,70,70	0
56	MG	CA	3029	1/1	0.83	0.16	54,54,54,54	0
56	MG	DA	3122	1/1	0.83	0.12	60,60,60,60	0
56	MG	AA	3178	1/1	0.83	0.16	63,63,63,63	0
56	MG	CA	3136	1/1	0.83	0.25	70,70,70,70	0
56	MG	CA	3032	1/1	0.83	0.20	44,44,44,44	0
56	MG	AA	3098	1/1	0.83	0.37	76,76,76,76	0
56	MG	CA	3039	1/1	0.83	0.32	82,82,82,82	0
56	MG	DA	3171	1/1	0.83	0.26	58,58,58,58	0
56	MG	AA	3029	1/1	0.83	0.32	60,60,60,60	0
56	MG	BA	3601	1/1	0.83	0.16	61,61,61,61	0
56	MG	AA	3089	1/1	0.83	0.24	80,80,80,80	0
56	MG	AA	3196	1/1	0.83	0.33	78,78,78,78	0
56	MG	AA	3092	1/1	0.83	0.25	59,59,59,59	0
56	MG	DA	3393	1/1	0.83	0.17	35,35,35,35	0
56	MG	CA	3065	1/1	0.83	0.17	81,81,81,81	0
56	MG	BW	3001	1/1	0.83	0.13	55,55,55,55	0
56	MG	BA	3180	1/1	0.83	0.25	48,48,48,48	0
56	MG	CX	103	1/1	0.83	0.08	57,57,57,57	0
59	FME	CX	101	10/11	0.83	0.25	59,80,100,106	0
56	MG	CA	3081	1/1	0.84	0.14	72,72,72,72	0
56	MG	BA	3648	1/1	0.84	0.13	54,54,54,54	0
56	MG	AA	3106	1/1	0.84	0.29	68,68,68,68	0
56	MG	DA	3514	1/1	0.84	0.17	60,60,60,60	0
56	MG	DA	3531	1/1	0.84	0.08	44,44,44,44	0
56	MG	BA	3686	1/1	0.84	0.25	65,65,65,65	0
56	MG	BD	305	1/1	0.84	0.17	41,41,41,41	0
56	MG	DA	3549	1/1	0.84	0.19	73,73,73,73	0
56	MG	CA	3041	1/1	0.84	0.31	71,71,71,71	0
56	MG	AA	3017	1/1	0.84	0.25	57,57,57,57	0
56	MG	DA	3246	1/1	0.84	0.10	55,55,55,55	0
56	MG	CA	3135	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3586	1/1	0.84	0.12	57,57,57,57	0
56	MG	DA	3314	1/1	0.84	0.14	56,56,56,56	0
56	MG	AA	3134	1/1	0.84	0.29	70,70,70,70	0
56	MG	AA	3045	1/1	0.84	0.26	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3613	1/1	0.84	0.20	64,64,64,64	0
56	MG	DA	3096	1/1	0.84	0.14	68,68,68,68	0
56	MG	DA	3405	1/1	0.84	0.24	53,53,53,53	0
56	MG	DA	3098	1/1	0.84	0.35	45,45,45,45	0
56	MG	BA	3616	1/1	0.84	0.18	73,73,73,73	0
56	MG	DA	3424	1/1	0.84	0.13	58,58,58,58	0
56	MG	AA	3147	1/1	0.84	0.14	51,51,51,51	0
56	MG	BA	3294	1/1	0.84	0.20	59,59,59,59	0
56	MG	BA	3716	1/1	0.84	0.20	77,77,77,77	0
56	MG	DB	3011	1/1	0.84	0.17	49,49,49,49	0
56	MG	AA	3148	1/1	0.84	0.14	72,72,72,72	0
56	MG	DA	3124	1/1	0.84	0.17	66,66,66,66	0
56	MG	CA	3122	1/1	0.85	0.18	70,70,70,70	0
56	MG	DA	3102	1/1	0.85	0.11	49,49,49,49	0
56	MG	CA	3125	1/1	0.85	0.17	64,64,64,64	0
56	MG	DA	3109	1/1	0.85	0.14	55,55,55,55	0
56	MG	CA	3127	1/1	0.85	0.12	72,72,72,72	0
56	MG	DA	3468	1/1	0.85	0.13	47,47,47,47	0
56	MG	DA	3491	1/1	0.85	0.23	55,55,55,55	0
56	MG	AA	3064	1/1	0.85	0.07	65,65,65,65	0
56	MG	BA	3465	1/1	0.85	0.12	51,51,51,51	0
56	MG	BA	3467	1/1	0.85	0.09	44,44,44,44	0
56	MG	BA	3473	1/1	0.85	0.13	55,55,55,55	0
56	MG	AA	3079	1/1	0.85	0.27	65,65,65,65	0
56	MG	BA	3538	1/1	0.85	0.13	29,29,29,29	0
56	MG	DA	3153	1/1	0.85	0.21	51,51,51,51	0
56	MG	DA	3155	1/1	0.85	0.15	50,50,50,50	0
56	MG	BA	3567	1/1	0.85	0.07	54,54,54,54	0
56	MG	DA	3557	1/1	0.85	0.13	74,74,74,74	0
56	MG	DA	3563	1/1	0.85	0.14	49,49,49,49	0
56	MG	AA	3053	1/1	0.85	0.20	56,56,56,56	0
56	MG	BA	3186	1/1	0.85	0.18	50,50,50,50	0
56	MG	DA	3212	1/1	0.85	0.17	48,48,48,48	0
56	MG	AA	3088	1/1	0.85	0.25	53,53,53,53	0
56	MG	DA	3591	1/1	0.85	0.13	67,67,67,67	0
56	MG	BA	3223	1/1	0.85	0.22	49,49,49,49	0
56	MG	AA	3025	1/1	0.85	0.11	78,78,78,78	0
56	MG	DA	3251	1/1	0.85	0.22	50,50,50,50	0
56	MG	DA	3607	1/1	0.85	0.21	68,68,68,68	0
56	MG	DA	3263	1/1	0.85	0.14	48,48,48,48	0
56	MG	BA	3248	1/1	0.85	0.33	68,68,68,68	0
56	MG	DA	3618	1/1	0.85	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3306	1/1	0.85	0.11	51,51,51,51	0
56	MG	DA	3620	1/1	0.85	0.15	66,66,66,66	0
56	MG	BA	3022	1/1	0.85	0.23	66,66,66,66	0
56	MG	DA	3333	1/1	0.85	0.09	61,61,61,61	0
56	MG	BA	3293	1/1	0.85	0.29	69,69,69,69	0
56	MG	CA	3103	1/1	0.85	0.14	101,101,101,101	0
56	MG	DA	3005	1/1	0.85	0.09	50,50,50,50	0
56	MG	BA	3667	1/1	0.85	0.18	72,72,72,72	0
56	MG	DB	3010	1/1	0.85	0.17	66,66,66,66	0
56	MG	AA	3090	1/1	0.85	0.23	64,64,64,64	0
56	MG	AA	3074	1/1	0.85	0.20	40,40,40,40	0
56	MG	DQ	3004	1/1	0.85	0.12	52,52,52,52	0
59	FME	AX	101	10/11	0.85	0.22	55,74,92,107	0
56	MG	BA	3694	1/1	0.85	0.15	48,48,48,48	0
56	MG	DA	3060	1/1	0.86	0.07	51,51,51,51	0
56	MG	BB	3001	1/1	0.86	0.17	56,56,56,56	0
56	MG	BA	3028	1/1	0.86	0.25	59,59,59,59	0
56	MG	DA	3074	1/1	0.86	0.24	60,60,60,60	0
56	MG	DA	3084	1/1	0.86	0.10	55,55,55,55	0
56	MG	BA	3597	1/1	0.86	0.14	46,46,46,46	0
56	MG	DA	3093	1/1	0.86	0.14	51,51,51,51	0
56	MG	AA	3061	1/1	0.86	0.10	57,57,57,57	0
56	MG	CA	3109	1/1	0.86	0.16	79,79,79,79	0
56	MG	BB	3018	1/1	0.86	0.15	54,54,54,54	0
56	MG	DA	3504	1/1	0.86	0.10	46,46,46,46	0
56	MG	BA	3257	1/1	0.86	0.21	56,56,56,56	0
56	MG	CA	3116	1/1	0.86	0.16	76,76,76,76	0
56	MG	BA	3289	1/1	0.86	0.17	53,53,53,53	0
56	MG	BA	3066	1/1	0.86	0.20	49,49,49,49	0
56	MG	B7	101	1/1	0.86	0.16	45,45,45,45	0
56	MG	BA	3068	1/1	0.86	0.26	43,43,43,43	0
56	MG	BA	3641	1/1	0.86	0.09	33,33,33,33	0
56	MG	AF	3001	1/1	0.86	0.16	62,62,62,62	0
56	MG	BA	3651	1/1	0.86	0.23	52,52,52,52	0
56	MG	BA	3301	1/1	0.86	0.18	44,44,44,44	0
56	MG	BA	3123	1/1	0.86	0.11	47,47,47,47	0
56	MG	AA	3020	1/1	0.86	0.09	80,80,80,80	0
56	MG	BA	3433	1/1	0.86	0.24	46,46,46,46	0
56	MG	DA	3589	1/1	0.86	0.14	65,65,65,65	0
56	MG	AA	3097	1/1	0.86	0.31	53,53,53,53	0
56	MG	DA	3596	1/1	0.86	0.22	68,68,68,68	0
56	MG	BA	3701	1/1	0.86	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3702	1/1	0.86	0.11	56,56,56,56	0
56	MG	CA	3153	1/1	0.86	0.15	85,85,85,85	0
56	MG	DA	3243	1/1	0.86	0.22	49,49,49,49	0
56	MG	DA	3608	1/1	0.86	0.23	63,63,63,63	0
56	MG	AX	105	1/1	0.86	0.20	72,72,72,72	0
56	MG	CA	3158	1/1	0.86	0.12	64,64,64,64	0
56	MG	AA	3082	1/1	0.86	0.26	52,52,52,52	0
56	MG	DA	3281	1/1	0.86	0.09	33,33,33,33	0
56	MG	DA	3289	1/1	0.86	0.21	64,64,64,64	0
56	MG	BA	3014	1/1	0.86	0.29	48,48,48,48	0
56	MG	CA	3162	1/1	0.86	0.16	60,60,60,60	0
56	MG	BA	3530	1/1	0.86	0.14	72,72,72,72	0
56	MG	CA	3168	1/1	0.86	0.28	79,79,79,79	0
56	MG	DA	3645	1/1	0.86	0.19	57,57,57,57	0
56	MG	AA	3028	1/1	0.86	0.24	72,72,72,72	0
56	MG	CE	3001	1/1	0.86	0.19	66,66,66,66	0
56	MG	DA	3361	1/1	0.86	0.18	58,58,58,58	0
56	MG	DA	3392	1/1	0.86	0.10	60,60,60,60	0
56	MG	BA	3565	1/1	0.86	0.14	75,75,75,75	0
56	MG	CA	3067	1/1	0.86	0.16	66,66,66,66	0
56	MG	D3	101	1/1	0.86	0.12	54,54,54,54	0
56	MG	BA	3224	1/1	0.86	0.15	48,48,48,48	0
56	MG	DA	3035	1/1	0.86	0.16	58,58,58,58	0
60	K	BA	3304	1/1	0.86	0.19	93,93,93,93	0
56	MG	BA	3143	1/1	0.87	0.39	41,41,41,41	0
56	MG	BA	3156	1/1	0.87	0.25	61,61,61,61	0
56	MG	BA	3173	1/1	0.87	0.17	41,41,41,41	0
56	MG	BA	3357	1/1	0.87	0.15	45,45,45,45	0
56	MG	BA	3027	1/1	0.87	0.13	53,53,53,53	0
56	MG	BA	3674	1/1	0.87	0.17	67,67,67,67	0
56	MG	BA	3369	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3015	1/1	0.87	0.12	74,74,74,74	0
56	MG	BA	3184	1/1	0.87	0.23	51,51,51,51	0
56	MG	CA	3145	1/1	0.87	0.08	67,67,67,67	0
56	MG	DA	3534	1/1	0.87	0.12	62,62,62,62	0
56	MG	CA	3146	1/1	0.87	0.15	61,61,61,61	0
56	MG	CA	3038	1/1	0.87	0.09	54,54,54,54	0
56	MG	CA	3150	1/1	0.87	0.12	63,63,63,63	0
56	MG	AA	3078	1/1	0.87	0.31	55,55,55,55	0
56	MG	BA	3469	1/1	0.87	0.12	60,60,60,60	0
56	MG	DA	3189	1/1	0.87	0.19	55,55,55,55	0
56	MG	AA	3068	1/1	0.87	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3157	1/1	0.87	0.11	56,56,56,56	0
56	MG	DA	3224	1/1	0.87	0.23	53,53,53,53	0
56	MG	DA	3585	1/1	0.87	0.25	62,62,62,62	0
56	MG	CA	3050	1/1	0.87	0.22	54,54,54,54	0
56	MG	BA	3212	1/1	0.87	0.20	47,47,47,47	0
56	MG	CA	3054	1/1	0.87	0.23	74,74,74,74	0
56	MG	AA	3141	1/1	0.87	0.18	51,51,51,51	0
56	MG	BA	3071	1/1	0.87	0.19	55,55,55,55	0
56	MG	BA	3563	1/1	0.87	0.38	66,66,66,66	0
56	MG	DA	3287	1/1	0.87	0.08	53,53,53,53	0
56	MG	BA	3088	1/1	0.87	0.08	55,55,55,55	0
56	MG	BA	3739	1/1	0.87	0.10	50,50,50,50	0
56	MG	AA	3080	1/1	0.87	0.22	58,58,58,58	0
56	MG	BA	3119	1/1	0.87	0.12	56,56,56,56	0
56	MG	DA	3323	1/1	0.87	0.09	60,60,60,60	0
56	MG	CA	3074	1/1	0.87	0.15	56,56,56,56	0
56	MG	BA	3596	1/1	0.87	0.11	79,79,79,79	0
56	MG	DA	3621	1/1	0.87	0.16	46,46,46,46	0
56	MG	BA	3262	1/1	0.87	0.32	44,44,44,44	0
56	MG	DA	3628	1/1	0.87	0.10	38,38,38,38	0
56	MG	DA	3062	1/1	0.87	0.23	58,58,58,58	0
56	MG	DA	3367	1/1	0.87	0.19	55,55,55,55	0
56	MG	DA	3391	1/1	0.87	0.10	54,54,54,54	0
56	MG	BA	3267	1/1	0.87	0.19	56,56,56,56	0
56	MG	BA	3272	1/1	0.87	0.21	49,49,49,49	0
56	MG	AA	3219	1/1	0.87	0.16	54,54,54,54	0
56	MG	DB	3006	1/1	0.87	0.10	54,54,54,54	0
56	MG	AA	3081	1/1	0.87	0.25	46,46,46,46	0
56	MG	BA	3634	1/1	0.87	0.14	77,77,77,77	0
56	MG	BX	102	1/1	0.87	0.22	60,60,60,60	0
56	MG	DA	3095	1/1	0.87	0.22	53,53,53,53	0
56	MG	DY	502	1/1	0.87	0.13	66,66,66,66	0
56	MG	BA	3137	1/1	0.87	0.15	59,59,59,59	0
56	MG	DA	3448	1/1	0.87	0.21	67,67,67,67	0
56	MG	CA	3004	1/1	0.87	0.15	88,88,88,88	0
56	MG	DA	3460	1/1	0.87	0.13	47,47,47,47	0
56	MG	DA	3344	1/1	0.88	0.07	48,48,48,48	0
56	MG	AA	3047	1/1	0.88	0.22	59,59,59,59	0
56	MG	BA	3644	1/1	0.88	0.13	38,38,38,38	0
56	MG	CA	3160	1/1	0.88	0.14	49,49,49,49	0
56	MG	AA	3207	1/1	0.88	0.16	51,51,51,51	0
56	MG	BA	3328	1/1	0.88	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3335	1/1	0.88	0.19	51,51,51,51	0
56	MG	CA	3034	1/1	0.88	0.26	66,66,66,66	0
56	MG	CA	3171	1/1	0.88	0.16	61,61,61,61	0
56	MG	BA	3172	1/1	0.88	0.13	54,54,54,54	0
56	MG	BA	3669	1/1	0.88	0.12	61,61,61,61	0
56	MG	CN	502	1/1	0.88	0.18	70,70,70,70	0
56	MG	AA	3100	1/1	0.88	0.18	43,43,43,43	0
56	MG	BA	3675	1/1	0.88	0.28	68,68,68,68	0
56	MG	AA	3215	1/1	0.88	0.33	77,77,77,77	0
56	MG	DA	3008	1/1	0.88	0.12	56,56,56,56	0
56	MG	BA	3039	1/1	0.88	0.15	44,44,44,44	0
56	MG	DA	3039	1/1	0.88	0.25	46,46,46,46	0
56	MG	DA	3040	1/1	0.88	0.15	45,45,45,45	0
56	MG	DA	3055	1/1	0.88	0.20	55,55,55,55	0
56	MG	DA	3057	1/1	0.88	0.17	57,57,57,57	0
56	MG	BA	3373	1/1	0.88	0.07	48,48,48,48	0
56	MG	BA	3429	1/1	0.88	0.20	55,55,55,55	0
56	MG	AA	3102	1/1	0.88	0.20	68,68,68,68	0
56	MG	BA	3064	1/1	0.88	0.10	49,49,49,49	0
56	MG	CA	3064	1/1	0.88	0.11	74,74,74,74	0
56	MG	AA	3218	1/1	0.88	0.14	73,73,73,73	0
56	MG	DA	3532	1/1	0.88	0.14	60,60,60,60	0
56	MG	BA	3204	1/1	0.88	0.12	48,48,48,48	0
56	MG	DA	3536	1/1	0.88	0.09	57,57,57,57	0
56	MG	BA	3709	1/1	0.88	0.14	77,77,77,77	0
56	MG	CA	3071	1/1	0.88	0.25	64,64,64,64	0
56	MG	BA	3209	1/1	0.88	0.22	39,39,39,39	0
56	MG	BA	3499	1/1	0.88	0.22	50,50,50,50	0
56	MG	AA	3070	1/1	0.88	0.14	68,68,68,68	0
56	MG	CA	3086	1/1	0.88	0.19	70,70,70,70	0
56	MG	BA	3717	1/1	0.88	0.13	51,51,51,51	0
56	MG	DA	3112	1/1	0.88	0.21	49,49,49,49	0
56	MG	BA	3514	1/1	0.88	0.13	49,49,49,49	0
56	MG	BA	3213	1/1	0.88	0.14	63,63,63,63	0
56	MG	BA	3070	1/1	0.88	0.10	46,46,46,46	0
56	MG	CA	3111	1/1	0.88	0.16	69,69,69,69	0
56	MG	CA	3112	1/1	0.88	0.20	69,69,69,69	0
56	MG	AA	3176	1/1	0.88	0.16	60,60,60,60	0
56	MG	DA	3134	1/1	0.88	0.13	37,37,37,37	0
56	MG	BA	3238	1/1	0.88	0.15	48,48,48,48	0
56	MG	BA	3240	1/1	0.88	0.24	54,54,54,54	0
56	MG	BA	3571	1/1	0.88	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3121	1/1	0.88	0.27	59,59,59,59	0
56	MG	BD	304	1/1	0.88	0.17	41,41,41,41	0
56	MG	DA	3170	1/1	0.88	0.09	45,45,45,45	0
56	MG	CA	3124	1/1	0.88	0.12	64,64,64,64	0
56	MG	AA	3071	1/1	0.88	0.23	60,60,60,60	0
56	MG	AA	3027	1/1	0.88	0.11	67,67,67,67	0
56	MG	BG	3003	1/1	0.88	0.14	53,53,53,53	0
56	MG	BN	3002	1/1	0.88	0.11	52,52,52,52	0
56	MG	DA	3230	1/1	0.88	0.19	61,61,61,61	0
56	MG	DA	3240	1/1	0.88	0.23	58,58,58,58	0
56	MG	BQ	3002	1/1	0.88	0.09	51,51,51,51	0
56	MG	BA	3107	1/1	0.88	0.23	60,60,60,60	0
56	MG	AX	103	1/1	0.88	0.06	57,57,57,57	0
56	MG	BA	3122	1/1	0.88	0.10	68,68,68,68	0
56	MG	DA	3255	1/1	0.88	0.17	46,46,46,46	0
56	MG	CA	3003	1/1	0.88	0.13	69,69,69,69	0
56	MG	AA	3065	1/1	0.88	0.25	50,50,50,50	0
56	MG	AA	3086	1/1	0.88	0.12	65,65,65,65	0
56	MG	CA	3008	1/1	0.88	0.35	59,59,59,59	0
56	MG	DQ	3003	1/1	0.88	0.18	58,58,58,58	0
56	MG	BA	3135	1/1	0.88	0.22	57,57,57,57	0
56	MG	CA	3021	1/1	0.88	0.16	54,54,54,54	0
56	MG	CA	3022	1/1	0.88	0.10	67,67,67,67	0
56	MG	AA	3033	1/1	0.88	0.23	68,68,68,68	0
56	MG	BA	3638	1/1	0.88	0.11	73,73,73,73	0
56	MG	DA	3336	1/1	0.88	0.12	36,36,36,36	0
56	MG	BA	3317	1/1	0.89	0.16	40,40,40,40	0
56	MG	CA	3042	1/1	0.89	0.27	69,69,69,69	0
56	MG	DA	3119	1/1	0.89	0.10	44,44,44,44	0
56	MG	DA	3121	1/1	0.89	0.10	46,46,46,46	0
56	MG	CA	3047	1/1	0.89	0.14	56,56,56,56	0
56	MG	DA	3465	1/1	0.89	0.08	41,41,41,41	0
56	MG	AA	3003	1/1	0.89	0.13	70,70,70,70	0
56	MG	BA	3604	1/1	0.89	0.20	64,64,64,64	0
56	MG	AA	3203	1/1	0.89	0.12	76,76,76,76	0
56	MG	BB	3003	1/1	0.89	0.14	40,40,40,40	0
56	MG	BA	3208	1/1	0.89	0.18	50,50,50,50	0
56	MG	BA	3621	1/1	0.89	0.11	57,57,57,57	0
56	MG	AA	3128	1/1	0.89	0.22	64,64,64,64	0
56	MG	DA	3524	1/1	0.89	0.09	51,51,51,51	0
56	MG	DA	3529	1/1	0.89	0.22	72,72,72,72	0
56	MG	DA	3157	1/1	0.89	0.29	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3633	1/1	0.89	0.20	54,54,54,54	0
56	MG	BA	3021	1/1	0.89	0.15	62,62,62,62	0
56	MG	AA	3004	1/1	0.89	0.17	50,50,50,50	0
56	MG	BD	309	1/1	0.89	0.18	43,43,43,43	0
56	MG	BD	311	1/1	0.89	0.28	53,53,53,53	0
56	MG	CA	3072	1/1	0.89	0.19	57,57,57,57	0
56	MG	BF	303	1/1	0.89	0.18	42,42,42,42	0
56	MG	DA	3222	1/1	0.89	0.08	45,45,45,45	0
56	MG	BA	3637	1/1	0.89	0.60	52,52,52,52	0
56	MG	AA	3085	1/1	0.89	0.23	57,57,57,57	0
56	MG	DA	3235	1/1	0.89	0.17	46,46,46,46	0
56	MG	AA	3013	1/1	0.89	0.07	75,75,75,75	0
56	MG	BA	3230	1/1	0.89	0.30	70,70,70,70	0
56	MG	BA	3447	1/1	0.89	0.09	76,76,76,76	0
56	MG	DA	3587	1/1	0.89	0.16	57,57,57,57	0
56	MG	CA	3107	1/1	0.89	0.23	71,71,71,71	0
56	MG	DA	3022	1/1	0.89	0.13	41,41,41,41	0
56	MG	DA	3595	1/1	0.89	0.11	53,53,53,53	0
56	MG	DA	3029	1/1	0.89	0.17	62,62,62,62	0
56	MG	DA	3598	1/1	0.89	0.07	45,45,45,45	0
56	MG	DA	3256	1/1	0.89	0.13	41,41,41,41	0
56	MG	BA	3460	1/1	0.89	0.17	66,66,66,66	0
56	MG	AA	3056	1/1	0.89	0.24	61,61,61,61	0
56	MG	DA	3282	1/1	0.89	0.14	58,58,58,58	0
56	MG	AA	3037	1/1	0.89	0.16	53,53,53,53	0
56	MG	DA	3043	1/1	0.89	0.27	56,56,56,56	0
56	MG	BA	3149	1/1	0.89	0.13	58,58,58,58	0
56	MG	AA	3120	1/1	0.89	0.22	53,53,53,53	0
56	MG	BA	3158	1/1	0.89	0.32	43,43,43,43	0
56	MG	BA	3681	1/1	0.89	0.24	54,54,54,54	0
56	MG	DA	3326	1/1	0.89	0.16	61,61,61,61	0
56	MG	CA	3015	1/1	0.89	0.14	53,53,53,53	0
56	MG	DA	3069	1/1	0.89	0.17	49,49,49,49	0
56	MG	BA	3164	1/1	0.89	0.17	57,57,57,57	0
56	MG	DA	3637	1/1	0.89	0.17	59,59,59,59	0
56	MG	AA	3140	1/1	0.89	0.10	65,65,65,65	0
56	MG	DA	3351	1/1	0.89	0.12	58,58,58,58	0
56	MG	DA	3078	1/1	0.89	0.15	49,49,49,49	0
56	MG	DA	3646	1/1	0.89	0.08	42,42,42,42	0
56	MG	BA	3520	1/1	0.89	0.12	69,69,69,69	0
56	MG	AM	3002	1/1	0.89	0.25	60,60,60,60	0
56	MG	AA	3019	1/1	0.89	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3178	1/1	0.89	0.17	51,51,51,51	0
56	MG	AA	3194	1/1	0.89	0.16	50,50,50,50	0
56	MG	DB	3012	1/1	0.89	0.22	50,50,50,50	0
56	MG	DF	304	1/1	0.89	0.24	39,39,39,39	0
56	MG	AA	3143	1/1	0.89	0.15	67,67,67,67	0
56	MG	DA	3099	1/1	0.89	0.20	39,39,39,39	0
56	MG	BA	3299	1/1	0.89	0.24	56,56,56,56	0
56	MG	BA	3300	1/1	0.89	0.18	48,48,48,48	0
56	MG	DA	3425	1/1	0.89	0.17	51,51,51,51	0
56	MG	D8	5001	1/1	0.89	0.21	53,53,53,53	0
56	MG	BA	3583	1/1	0.89	0.20	57,57,57,57	0
56	MG	BA	3094	1/1	0.89	0.19	62,62,62,62	0
56	MG	DA	3445	1/1	0.89	0.33	60,60,60,60	0
60	K	DA	3234	1/1	0.89	0.21	102,102,102,102	0
56	MG	BQ	3004	1/1	0.90	0.10	41,41,41,41	0
56	MG	DA	3079	1/1	0.90	0.09	44,44,44,44	0
56	MG	BR	203	1/1	0.90	0.14	48,48,48,48	0
56	MG	BV	3002	1/1	0.90	0.28	42,42,42,42	0
56	MG	DA	3087	1/1	0.90	0.15	43,43,43,43	0
56	MG	DA	3089	1/1	0.90	0.07	51,51,51,51	0
56	MG	DA	3431	1/1	0.90	0.15	56,56,56,56	0
56	MG	DA	3435	1/1	0.90	0.11	56,56,56,56	0
56	MG	CA	3113	1/1	0.90	0.23	84,84,84,84	0
56	MG	DA	3437	1/1	0.90	0.18	46,46,46,46	0
56	MG	BA	3477	1/1	0.90	0.17	52,52,52,52	0
56	MG	DA	3444	1/1	0.90	0.17	43,43,43,43	0
56	MG	BA	3663	1/1	0.90	0.23	73,73,73,73	0
56	MG	DA	3447	1/1	0.90	0.12	56,56,56,56	0
56	MG	B2	101	1/1	0.90	0.09	34,34,34,34	0
56	MG	DA	3452	1/1	0.90	0.23	64,64,64,64	0
56	MG	BA	3666	1/1	0.90	0.31	54,54,54,54	0
56	MG	DA	3458	1/1	0.90	0.11	47,47,47,47	0
56	MG	BA	3485	1/1	0.90	0.11	67,67,67,67	0
56	MG	DA	3106	1/1	0.90	0.29	45,45,45,45	0
56	MG	AX	106	1/1	0.90	0.10	64,64,64,64	0
56	MG	BA	3672	1/1	0.90	0.15	63,63,63,63	0
56	MG	DA	3110	1/1	0.90	0.13	46,46,46,46	0
56	MG	DA	3475	1/1	0.90	0.08	35,35,35,35	0
56	MG	DA	3477	1/1	0.90	0.28	35,35,35,35	0
56	MG	AA	3005	1/1	0.90	0.34	66,66,66,66	0
56	MG	DA	3495	1/1	0.90	0.08	53,53,53,53	0
56	MG	CA	3126	1/1	0.90	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3498	1/1	0.90	0.15	75,75,75,75	0
56	MG	BA	3512	1/1	0.90	0.12	42,42,42,42	0
56	MG	DA	3116	1/1	0.90	0.12	43,43,43,43	0
56	MG	BA	3006	1/1	0.90	0.10	46,46,46,46	0
56	MG	BA	3284	1/1	0.90	0.45	76,76,76,76	0
56	MG	DA	3523	1/1	0.90	0.08	47,47,47,47	0
56	MG	BA	3007	1/1	0.90	0.13	55,55,55,55	0
56	MG	DA	3528	1/1	0.90	0.10	33,33,33,33	0
56	MG	AA	3099	1/1	0.90	0.21	49,49,49,49	0
56	MG	BA	3696	1/1	0.90	0.13	36,36,36,36	0
56	MG	BA	3549	1/1	0.90	0.24	49,49,49,49	0
56	MG	BA	3561	1/1	0.90	0.15	39,39,39,39	0
56	MG	DA	3135	1/1	0.90	0.13	58,58,58,58	0
56	MG	AA	3182	1/1	0.90	0.09	48,48,48,48	0
56	MG	BA	3111	1/1	0.90	0.17	43,43,43,43	0
56	MG	BA	3187	1/1	0.90	0.10	53,53,53,53	0
56	MG	CA	3149	1/1	0.90	0.09	81,81,81,81	0
56	MG	BA	3196	1/1	0.90	0.17	45,45,45,45	0
56	MG	DA	3166	1/1	0.90	0.06	37,37,37,37	0
56	MG	CA	3037	1/1	0.90	0.13	45,45,45,45	0
56	MG	BA	3118	1/1	0.90	0.22	53,53,53,53	0
56	MG	AA	3009	1/1	0.90	0.27	71,71,71,71	0
56	MG	DA	3180	1/1	0.90	0.24	47,47,47,47	0
56	MG	BA	3714	1/1	0.90	0.12	72,72,72,72	0
56	MG	DA	3196	1/1	0.90	0.17	54,54,54,54	0
56	MG	DA	3200	1/1	0.90	0.22	48,48,48,48	0
56	MG	DA	3201	1/1	0.90	0.09	43,43,43,43	0
56	MG	DA	3594	1/1	0.90	0.13	63,63,63,63	0
56	MG	BA	3591	1/1	0.90	0.12	38,38,38,38	0
56	MG	CA	3043	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3324	1/1	0.90	0.19	54,54,54,54	0
56	MG	BA	3722	1/1	0.90	0.09	49,49,49,49	0
56	MG	AA	3001	1/1	0.90	0.18	74,74,74,74	0
56	MG	AA	3150	1/1	0.90	0.27	67,67,67,67	0
56	MG	DA	3236	1/1	0.90	0.08	38,38,38,38	0
56	MG	BA	3131	1/1	0.90	0.08	31,31,31,31	0
56	MG	BA	3610	1/1	0.90	0.61	49,49,49,49	0
56	MG	BA	3038	1/1	0.90	0.19	51,51,51,51	0
56	MG	BB	3006	1/1	0.90	0.20	34,34,34,34	0
56	MG	CA	3063	1/1	0.90	0.08	57,57,57,57	0
56	MG	BA	3214	1/1	0.90	0.17	37,37,37,37	0
56	MG	AA	3095	1/1	0.90	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3003	1/1	0.90	0.07	43,43,43,43	0
56	MG	DA	3278	1/1	0.90	0.08	39,39,39,39	0
56	MG	BA	3043	1/1	0.90	0.20	33,33,33,33	0
56	MG	CA	3069	1/1	0.90	0.22	63,63,63,63	0
56	MG	DA	3015	1/1	0.90	0.18	54,54,54,54	0
56	MG	BA	3044	1/1	0.90	0.19	32,32,32,32	0
56	MG	AA	3018	1/1	0.90	0.19	51,51,51,51	0
56	MG	AA	3168	1/1	0.90	0.16	80,80,80,80	0
56	MG	DA	3655	1/1	0.90	0.18	62,62,62,62	0
56	MG	DA	3036	1/1	0.90	0.11	35,35,35,35	0
56	MG	DA	3318	1/1	0.90	0.13	47,47,47,47	0
56	MG	AA	3139	1/1	0.90	0.17	58,58,58,58	0
56	MG	BA	3163	1/1	0.90	0.13	50,50,50,50	0
56	MG	CA	3075	1/1	0.90	0.26	76,76,76,76	0
56	MG	BA	3255	1/1	0.90	0.18	53,53,53,53	0
56	MG	DE	303	1/1	0.90	0.14	36,36,36,36	0
56	MG	AA	3113	1/1	0.90	0.16	56,56,56,56	0
56	MG	BG	3004	1/1	0.90	0.14	53,53,53,53	0
56	MG	DA	3061	1/1	0.90	0.20	47,47,47,47	0
56	MG	DA	3353	1/1	0.90	0.16	54,54,54,54	0
56	MG	DV	202	1/1	0.90	0.19	45,45,45,45	0
56	MG	BA	3470	1/1	0.90	0.11	44,44,44,44	0
56	MG	CA	3106	1/1	0.90	0.22	72,72,72,72	0
56	MG	DA	3363	1/1	0.90	0.16	56,56,56,56	0
56	MG	BN	3005	1/1	0.90	0.33	63,63,63,63	0
56	MG	DA	3373	1/1	0.90	0.14	52,52,52,52	0
56	MG	CA	3108	1/1	0.90	0.11	45,45,45,45	0
56	MG	BA	3261	1/1	0.90	0.25	45,45,45,45	0
56	MG	BA	3263	1/1	0.91	0.33	35,35,35,35	0
56	MG	BA	3144	1/1	0.91	0.10	52,52,52,52	0
56	MG	AA	3026	1/1	0.91	0.15	52,52,52,52	0
56	MG	BU	202	1/1	0.91	0.47	41,41,41,41	0
56	MG	BA	3279	1/1	0.91	0.23	60,60,60,60	0
56	MG	BA	3600	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3299	1/1	0.91	0.08	35,35,35,35	0
56	MG	BA	3150	1/1	0.91	0.18	42,42,42,42	0
56	MG	BZ	3001	1/1	0.91	0.11	47,47,47,47	0
56	MG	B1	3001	1/1	0.91	0.45	63,63,63,63	0
56	MG	AA	3084	1/1	0.91	0.21	71,71,71,71	0
56	MG	BA	3047	1/1	0.91	0.21	30,30,30,30	0
56	MG	DA	3331	1/1	0.91	0.11	27,27,27,27	0
56	MG	CA	3163	1/1	0.91	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B7	104	1/1	0.91	0.17	55,55,55,55	0
56	MG	B8	5001	1/1	0.91	0.10	62,62,62,62	0
56	MG	CA	3169	1/1	0.91	0.16	52,52,52,52	0
56	MG	BA	3612	1/1	0.91	0.13	41,41,41,41	0
56	MG	BA	3614	1/1	0.91	0.10	48,48,48,48	0
56	MG	AA	3075	1/1	0.91	0.11	50,50,50,50	0
56	MG	AA	3096	1/1	0.91	0.21	52,52,52,52	0
56	MG	BA	3296	1/1	0.91	0.23	69,69,69,69	0
56	MG	BA	3624	1/1	0.91	0.10	73,73,73,73	0
56	MG	CA	3018	1/1	0.91	0.07	55,55,55,55	0
56	MG	CA	3019	1/1	0.91	0.09	62,62,62,62	0
56	MG	BA	3166	1/1	0.91	0.10	41,41,41,41	0
56	MG	DA	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	BA	3627	1/1	0.91	0.22	50,50,50,50	0
56	MG	DA	3018	1/1	0.91	0.17	41,41,41,41	0
56	MG	CA	3024	1/1	0.91	0.26	57,57,57,57	0
56	MG	DA	3023	1/1	0.91	0.34	64,64,64,64	0
56	MG	BA	3631	1/1	0.91	0.11	41,41,41,41	0
56	MG	DA	3031	1/1	0.91	0.15	60,60,60,60	0
56	MG	DA	3432	1/1	0.91	0.17	37,37,37,37	0
56	MG	BA	3632	1/1	0.91	0.11	55,55,55,55	0
56	MG	AA	3038	1/1	0.91	0.38	64,64,64,64	0
56	MG	AA	3187	1/1	0.91	0.08	72,72,72,72	0
56	MG	BA	3309	1/1	0.91	0.17	43,43,43,43	0
56	MG	CA	3031	1/1	0.91	0.32	55,55,55,55	0
56	MG	BA	3310	1/1	0.91	0.14	59,59,59,59	0
56	MG	AX	102	1/1	0.91	0.14	66,66,66,66	0
56	MG	BA	3318	1/1	0.91	0.11	30,30,30,30	0
56	MG	DA	3449	1/1	0.91	0.25	46,46,46,46	0
56	MG	CA	3036	1/1	0.91	0.11	56,56,56,56	0
56	MG	DA	3455	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3643	1/1	0.91	0.10	59,59,59,59	0
56	MG	DA	3064	1/1	0.91	0.09	55,55,55,55	0
56	MG	AA	3188	1/1	0.91	0.18	52,52,52,52	0
56	MG	DA	3068	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3647	1/1	0.91	0.08	40,40,40,40	0
56	MG	BA	3072	1/1	0.91	0.25	45,45,45,45	0
56	MG	BA	3331	1/1	0.91	0.11	61,61,61,61	0
56	MG	BA	3654	1/1	0.91	0.16	49,49,49,49	0
56	MG	CA	3044	1/1	0.91	0.14	52,52,52,52	0
56	MG	DA	3483	1/1	0.91	0.13	55,55,55,55	0
56	MG	DA	3485	1/1	0.91	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3081	1/1	0.91	0.20	56,56,56,56	0
56	MG	BA	3656	1/1	0.91	0.12	70,70,70,70	0
56	MG	BA	3181	1/1	0.91	0.09	37,37,37,37	0
56	MG	CA	3049	1/1	0.91	0.18	51,51,51,51	0
56	MG	BA	3082	1/1	0.91	0.20	54,54,54,54	0
56	MG	DA	3090	1/1	0.91	0.20	59,59,59,59	0
56	MG	DA	3092	1/1	0.91	0.21	48,48,48,48	0
56	MG	DA	3513	1/1	0.91	0.12	58,58,58,58	0
56	MG	BA	3342	1/1	0.91	0.18	46,46,46,46	0
56	MG	DA	3521	1/1	0.91	0.11	46,46,46,46	0
56	MG	BA	3185	1/1	0.91	0.16	40,40,40,40	0
56	MG	BA	3083	1/1	0.91	0.14	33,33,33,33	0
56	MG	DA	3525	1/1	0.91	0.11	56,56,56,56	0
56	MG	DA	3097	1/1	0.91	0.14	58,58,58,58	0
56	MG	CA	3058	1/1	0.91	0.08	36,36,36,36	0
56	MG	BA	3087	1/1	0.91	0.20	48,48,48,48	0
56	MG	DA	3100	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3673	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3371	1/1	0.91	0.13	38,38,38,38	0
56	MG	BA	3191	1/1	0.91	0.09	56,56,56,56	0
56	MG	BA	3676	1/1	0.91	0.08	63,63,63,63	0
56	MG	DA	3542	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3543	1/1	0.91	0.11	52,52,52,52	0
56	MG	DA	3547	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3376	1/1	0.91	0.21	35,35,35,35	0
56	MG	DA	3111	1/1	0.91	0.20	67,67,67,67	0
56	MG	BA	3394	1/1	0.91	0.20	45,45,45,45	0
56	MG	DA	3559	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3395	1/1	0.91	0.22	56,56,56,56	0
56	MG	BA	3405	1/1	0.91	0.10	57,57,57,57	0
56	MG	BA	3195	1/1	0.91	0.16	37,37,37,37	0
56	MG	BA	3697	1/1	0.91	0.13	63,63,63,63	0
56	MG	DA	3569	1/1	0.91	0.07	54,54,54,54	0
56	MG	DA	3571	1/1	0.91	0.17	57,57,57,57	0
56	MG	AA	3118	1/1	0.91	0.27	39,39,39,39	0
56	MG	AA	3191	1/1	0.91	0.10	56,56,56,56	0
56	MG	BA	3455	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3099	1/1	0.91	0.32	55,55,55,55	0
56	MG	DA	3128	1/1	0.91	0.16	54,54,54,54	0
56	MG	AA	3077	1/1	0.91	0.30	67,67,67,67	0
56	MG	CA	3099	1/1	0.91	0.21	64,64,64,64	0
56	MG	BA	3466	1/1	0.91	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3104	1/1	0.91	0.16	60,60,60,60	0
56	MG	DA	3600	1/1	0.91	0.14	73,73,73,73	0
56	MG	DA	3152	1/1	0.91	0.15	43,43,43,43	0
56	MG	BA	3105	1/1	0.91	0.28	54,54,54,54	0
56	MG	AA	3124	1/1	0.91	0.15	61,61,61,61	0
56	MG	AA	3197	1/1	0.91	0.16	64,64,64,64	0
56	MG	DA	3161	1/1	0.91	0.16	51,51,51,51	0
56	MG	DA	3611	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3117	1/1	0.91	0.14	37,37,37,37	0
56	MG	AA	3048	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3718	1/1	0.91	0.13	52,52,52,52	0
56	MG	BA	3478	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3732	1/1	0.91	0.18	56,56,56,56	0
56	MG	DA	3172	1/1	0.91	0.20	46,46,46,46	0
56	MG	DA	3175	1/1	0.91	0.20	52,52,52,52	0
56	MG	AA	3036	1/1	0.91	0.14	69,69,69,69	0
56	MG	AA	3204	1/1	0.91	0.13	70,70,70,70	0
56	MG	DA	3636	1/1	0.91	0.18	64,64,64,64	0
56	MG	DA	3190	1/1	0.91	0.08	54,54,54,54	0
56	MG	DA	3194	1/1	0.91	0.34	65,65,65,65	0
56	MG	BA	3502	1/1	0.91	0.17	59,59,59,59	0
56	MG	DA	3198	1/1	0.91	0.18	34,34,34,34	0
56	MG	BA	3505	1/1	0.91	0.10	45,45,45,45	0
56	MG	BB	3004	1/1	0.91	0.22	57,57,57,57	0
56	MG	BA	3231	1/1	0.91	0.18	50,50,50,50	0
56	MG	DB	3002	1/1	0.91	0.23	72,72,72,72	0
56	MG	AA	3055	1/1	0.91	0.23	56,56,56,56	0
56	MG	DB	3004	1/1	0.91	0.14	56,56,56,56	0
56	MG	BA	3126	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3242	1/1	0.91	0.23	45,45,45,45	0
56	MG	BA	3246	1/1	0.91	0.21	38,38,38,38	0
56	MG	BA	3535	1/1	0.91	0.16	42,42,42,42	0
56	MG	BA	3026	1/1	0.91	0.06	36,36,36,36	0
56	MG	AA	3073	1/1	0.91	0.11	63,63,63,63	0
56	MG	BA	3552	1/1	0.91	0.18	30,30,30,30	0
56	MG	DN	5001	1/1	0.91	0.07	71,71,71,71	0
56	MG	DQ	3002	1/1	0.91	0.16	51,51,51,51	0
56	MG	BA	3251	1/1	0.91	0.06	45,45,45,45	0
56	MG	BA	3252	1/1	0.91	0.28	65,65,65,65	0
56	MG	DA	3249	1/1	0.91	0.10	25,25,25,25	0
56	MG	AA	3107	1/1	0.91	0.21	44,44,44,44	0
56	MG	DA	3254	1/1	0.91	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3216	1/1	0.91	0.20	60,60,60,60	0
56	MG	BA	3139	1/1	0.91	0.22	50,50,50,50	0
56	MG	AA	3108	1/1	0.91	0.15	72,72,72,72	0
56	MG	DA	3268	1/1	0.91	0.12	42,42,42,42	0
56	MG	DA	3273	1/1	0.91	0.13	32,32,32,32	0
56	MG	BA	3273	1/1	0.92	0.29	35,35,35,35	0
56	MG	BU	208	1/1	0.92	0.13	42,42,42,42	0
56	MG	AA	3154	1/1	0.92	0.12	60,60,60,60	0
56	MG	BA	3280	1/1	0.92	0.26	44,44,44,44	0
56	MG	BA	3649	1/1	0.92	0.20	43,43,43,43	0
56	MG	BA	3061	1/1	0.92	0.21	44,44,44,44	0
56	MG	BA	3476	1/1	0.92	0.08	47,47,47,47	0
56	MG	BA	3004	1/1	0.92	0.18	45,45,45,45	0
56	MG	B3	3403	1/1	0.92	0.13	37,37,37,37	0
56	MG	BA	3657	1/1	0.92	0.11	29,29,29,29	0
56	MG	BA	3658	1/1	0.92	0.16	62,62,62,62	0
56	MG	BA	3291	1/1	0.92	0.16	44,44,44,44	0
56	MG	DA	3454	1/1	0.92	0.07	52,52,52,52	0
56	MG	CA	3131	1/1	0.92	0.07	48,48,48,48	0
56	MG	BA	3190	1/1	0.92	0.08	42,42,42,42	0
56	MG	DA	3457	1/1	0.92	0.08	44,44,44,44	0
56	MG	BA	3487	1/1	0.92	0.18	47,47,47,47	0
56	MG	AA	3135	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3461	1/1	0.92	0.09	40,40,40,40	0
56	MG	AA	3083	1/1	0.92	0.15	56,56,56,56	0
56	MG	BA	3671	1/1	0.92	0.12	44,44,44,44	0
56	MG	DA	3126	1/1	0.92	0.14	61,61,61,61	0
56	MG	CA	3014	1/1	0.92	0.22	56,56,56,56	0
56	MG	BA	3295	1/1	0.92	0.07	30,30,30,30	0
56	MG	CA	3016	1/1	0.92	0.13	72,72,72,72	0
56	MG	DA	3478	1/1	0.92	0.06	58,58,58,58	0
56	MG	BA	3012	1/1	0.92	0.07	34,34,34,34	0
56	MG	DA	3484	1/1	0.92	0.10	47,47,47,47	0
56	MG	BA	3202	1/1	0.92	0.24	29,29,29,29	0
56	MG	DA	3487	1/1	0.92	0.06	44,44,44,44	0
56	MG	DA	3146	1/1	0.92	0.20	34,34,34,34	0
56	MG	DA	3149	1/1	0.92	0.08	47,47,47,47	0
56	MG	AA	3116	1/1	0.92	0.32	62,62,62,62	0
56	MG	AA	3111	1/1	0.92	0.08	70,70,70,70	0
56	MG	DA	3154	1/1	0.92	0.30	45,45,45,45	0
56	MG	DA	3502	1/1	0.92	0.16	48,48,48,48	0
56	MG	BA	3524	1/1	0.92	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3155	1/1	0.92	0.07	71,71,71,71	0
56	MG	BA	3075	1/1	0.92	0.19	36,36,36,36	0
56	MG	BA	3081	1/1	0.92	0.21	44,44,44,44	0
56	MG	DA	3515	1/1	0.92	0.12	57,57,57,57	0
56	MG	DA	3163	1/1	0.92	0.14	52,52,52,52	0
56	MG	BA	3311	1/1	0.92	0.27	52,52,52,52	0
56	MG	BA	3540	1/1	0.92	0.18	29,29,29,29	0
56	MG	BA	3316	1/1	0.92	0.14	51,51,51,51	0
56	MG	DA	3527	1/1	0.92	0.15	58,58,58,58	0
56	MG	AA	3173	1/1	0.92	0.06	37,37,37,37	0
56	MG	AA	3174	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3530	1/1	0.92	0.12	57,57,57,57	0
56	MG	BA	3145	1/1	0.92	0.14	40,40,40,40	0
56	MG	AA	3198	1/1	0.92	0.08	73,73,73,73	0
56	MG	AA	3046	1/1	0.92	0.19	60,60,60,60	0
56	MG	BA	3155	1/1	0.92	0.07	56,56,56,56	0
56	MG	AA	3069	1/1	0.92	0.11	77,77,77,77	0
56	MG	DA	3195	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3340	1/1	0.92	0.17	57,57,57,57	0
56	MG	BA	3235	1/1	0.92	0.25	44,44,44,44	0
56	MG	BA	3593	1/1	0.92	0.08	51,51,51,51	0
56	MG	CT	3001	1/1	0.92	0.19	57,57,57,57	0
56	MG	DA	3551	1/1	0.92	0.07	43,43,43,43	0
56	MG	DA	3203	1/1	0.92	0.06	48,48,48,48	0
56	MG	DA	3205	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3558	1/1	0.92	0.15	77,77,77,77	0
56	MG	BA	3343	1/1	0.92	0.07	37,37,37,37	0
56	MG	BA	3356	1/1	0.92	0.09	33,33,33,33	0
56	MG	BA	3719	1/1	0.92	0.08	63,63,63,63	0
56	MG	DA	3223	1/1	0.92	0.09	41,41,41,41	0
56	MG	BA	3721	1/1	0.92	0.21	56,56,56,56	0
56	MG	DA	3225	1/1	0.92	0.17	64,64,64,64	0
56	MG	DA	3570	1/1	0.92	0.18	67,67,67,67	0
56	MG	BA	3599	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3231	1/1	0.92	0.09	45,45,45,45	0
56	MG	BA	3098	1/1	0.92	0.24	42,42,42,42	0
56	MG	BA	3737	1/1	0.92	0.11	39,39,39,39	0
56	MG	AA	3121	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3359	1/1	0.92	0.12	63,63,63,63	0
56	MG	CA	3057	1/1	0.92	0.14	40,40,40,40	0
56	MG	DA	3024	1/1	0.92	0.28	59,59,59,59	0
56	MG	BA	3607	1/1	0.92	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3250	1/1	0.92	0.11	42,42,42,42	0
56	MG	BB	3002	1/1	0.92	0.16	49,49,49,49	0
56	MG	DA	3252	1/1	0.92	0.20	36,36,36,36	0
56	MG	BA	3368	1/1	0.92	0.12	22,22,22,22	0
56	MG	CA	3062	1/1	0.92	0.33	67,67,67,67	0
56	MG	BA	3042	1/1	0.92	0.21	50,50,50,50	0
56	MG	DA	3259	1/1	0.92	0.09	45,45,45,45	0
56	MG	AA	3123	1/1	0.92	0.25	38,38,38,38	0
56	MG	DA	3612	1/1	0.92	0.17	46,46,46,46	0
56	MG	DA	3041	1/1	0.92	0.20	54,54,54,54	0
56	MG	DA	3615	1/1	0.92	0.09	57,57,57,57	0
56	MG	DA	3270	1/1	0.92	0.14	55,55,55,55	0
56	MG	BA	3167	1/1	0.92	0.40	50,50,50,50	0
56	MG	DA	3048	1/1	0.92	0.21	29,29,29,29	0
56	MG	DA	3049	1/1	0.92	0.13	56,56,56,56	0
56	MG	DA	3054	1/1	0.92	0.13	34,34,34,34	0
56	MG	DA	3622	1/1	0.92	0.10	40,40,40,40	0
56	MG	DA	3285	1/1	0.92	0.12	41,41,41,41	0
56	MG	AA	3052	1/1	0.92	0.18	58,58,58,58	0
56	MG	BB	3016	1/1	0.92	0.14	24,24,24,24	0
56	MG	DA	3631	1/1	0.92	0.15	49,49,49,49	0
56	MG	BA	3390	1/1	0.92	0.12	40,40,40,40	0
56	MG	BA	3109	1/1	0.92	0.34	62,62,62,62	0
56	MG	BA	3174	1/1	0.92	0.06	52,52,52,52	0
56	MG	BA	3253	1/1	0.92	0.29	63,63,63,63	0
56	MG	DA	3065	1/1	0.92	0.14	40,40,40,40	0
56	MG	BA	3629	1/1	0.92	0.07	51,51,51,51	0
56	MG	BA	3425	1/1	0.92	0.15	42,42,42,42	0
56	MG	CA	3079	1/1	0.92	0.07	37,37,37,37	0
56	MG	DA	3070	1/1	0.92	0.24	51,51,51,51	0
56	MG	DA	3071	1/1	0.92	0.28	46,46,46,46	0
56	MG	BD	312	1/1	0.92	0.33	72,72,72,72	0
56	MG	CA	3084	1/1	0.92	0.18	80,80,80,80	0
56	MG	DA	3075	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3077	1/1	0.92	0.12	48,48,48,48	0
56	MG	BA	3046	1/1	0.92	0.13	52,52,52,52	0
56	MG	CA	3090	1/1	0.92	0.10	63,63,63,63	0
56	MG	DE	305	1/1	0.92	0.17	68,68,68,68	0
56	MG	BA	3112	1/1	0.92	0.20	46,46,46,46	0
56	MG	BG	3002	1/1	0.92	0.17	51,51,51,51	0
56	MG	BA	3179	1/1	0.92	0.30	53,53,53,53	0
56	MG	DP	201	1/1	0.92	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DP	202	1/1	0.92	0.19	54,54,54,54	0
56	MG	DA	3380	1/1	0.92	0.07	40,40,40,40	0
56	MG	BA	3453	1/1	0.92	0.20	54,54,54,54	0
56	MG	BA	3114	1/1	0.92	0.25	46,46,46,46	0
56	MG	DU	3001	1/1	0.92	0.19	61,61,61,61	0
56	MG	BA	3116	1/1	0.92	0.23	30,30,30,30	0
56	MG	DW	202	1/1	0.92	0.09	53,53,53,53	0
56	MG	BP	202	1/1	0.92	0.27	47,47,47,47	0
56	MG	BA	3640	1/1	0.92	0.13	31,31,31,31	0
56	MG	DA	3416	1/1	0.92	0.19	34,34,34,34	0
56	MG	BA	3182	1/1	0.92	0.17	43,43,43,43	0
56	MG	DA	3419	1/1	0.92	0.09	53,53,53,53	0
56	MG	BR	201	1/1	0.92	0.14	44,44,44,44	0
56	MG	AA	3211	1/1	0.92	0.09	58,58,58,58	0
56	MG	BA	3148	1/1	0.93	0.38	49,49,49,49	0
56	MG	BA	3544	1/1	0.93	0.12	35,35,35,35	0
56	MG	DA	3184	1/1	0.93	0.15	54,54,54,54	0
56	MG	DA	3030	1/1	0.93	0.14	49,49,49,49	0
56	MG	AA	3181	1/1	0.93	0.17	46,46,46,46	0
56	MG	DA	3032	1/1	0.93	0.06	36,36,36,36	0
56	MG	DA	3033	1/1	0.93	0.15	41,41,41,41	0
56	MG	BA	3193	1/1	0.93	0.16	53,53,53,53	0
56	MG	BA	3018	1/1	0.93	0.10	54,54,54,54	0
56	MG	BA	3152	1/1	0.93	0.11	52,52,52,52	0
56	MG	DA	3486	1/1	0.93	0.07	52,52,52,52	0
56	MG	BA	3198	1/1	0.93	0.20	29,29,29,29	0
56	MG	CA	3088	1/1	0.93	0.09	49,49,49,49	0
56	MG	BW	3004	1/1	0.93	0.27	46,46,46,46	0
56	MG	DA	3209	1/1	0.93	0.10	44,44,44,44	0
56	MG	BA	3199	1/1	0.93	0.15	31,31,31,31	0
56	MG	DA	3214	1/1	0.93	0.12	48,48,48,48	0
56	MG	BA	3375	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3221	1/1	0.93	0.18	56,56,56,56	0
56	MG	DA	3053	1/1	0.93	0.14	47,47,47,47	0
56	MG	DA	3507	1/1	0.93	0.16	53,53,53,53	0
56	MG	DA	3509	1/1	0.93	0.06	57,57,57,57	0
56	MG	B0	101	1/1	0.93	0.13	57,57,57,57	0
56	MG	B0	106	1/1	0.93	0.05	43,43,43,43	0
56	MG	BA	3680	1/1	0.93	0.16	62,62,62,62	0
56	MG	DA	3517	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3520	1/1	0.93	0.07	38,38,38,38	0
56	MG	DA	3058	1/1	0.93	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3277	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3682	1/1	0.93	0.27	50,50,50,50	0
56	MG	BA	3201	1/1	0.93	0.21	36,36,36,36	0
56	MG	B7	103	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3687	1/1	0.93	0.13	59,59,59,59	0
56	MG	BA	3590	1/1	0.93	0.12	23,23,23,23	0
56	MG	B9	502	1/1	0.93	0.15	49,49,49,49	0
56	MG	BA	3392	1/1	0.93	0.11	53,53,53,53	0
56	MG	BA	3154	1/1	0.93	0.14	55,55,55,55	0
56	MG	BA	3283	1/1	0.93	0.22	61,61,61,61	0
56	MG	BA	3019	1/1	0.93	0.17	42,42,42,42	0
56	MG	AA	3166	1/1	0.93	0.14	55,55,55,55	0
56	MG	CA	3010	1/1	0.93	0.11	34,34,34,34	0
56	MG	DA	3541	1/1	0.93	0.09	55,55,55,55	0
56	MG	CA	3123	1/1	0.93	0.14	75,75,75,75	0
56	MG	AN	101	1/1	0.93	0.07	64,64,64,64	0
56	MG	DA	3544	1/1	0.93	0.32	42,42,42,42	0
56	MG	AA	3007	1/1	0.93	0.08	68,68,68,68	0
56	MG	BA	3435	1/1	0.93	0.11	59,59,59,59	0
56	MG	BA	3605	1/1	0.93	0.08	35,35,35,35	0
56	MG	AA	3185	1/1	0.93	0.19	47,47,47,47	0
56	MG	DA	3555	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3276	1/1	0.93	0.07	26,26,26,26	0
56	MG	CA	3130	1/1	0.93	0.11	59,59,59,59	0
56	MG	AA	3169	1/1	0.93	0.08	62,62,62,62	0
56	MG	AA	3101	1/1	0.93	0.20	61,61,61,61	0
56	MG	DA	3284	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3091	1/1	0.93	0.41	50,50,50,50	0
56	MG	BA	3217	1/1	0.93	0.10	59,59,59,59	0
56	MG	DA	3288	1/1	0.93	0.10	68,68,68,68	0
56	MG	BA	3297	1/1	0.93	0.12	43,43,43,43	0
56	MG	DA	3094	1/1	0.93	0.16	26,26,26,26	0
56	MG	DA	3575	1/1	0.93	0.16	51,51,51,51	0
56	MG	BA	3618	1/1	0.93	0.18	37,37,37,37	0
56	MG	DA	3302	1/1	0.93	0.12	42,42,42,42	0
56	MG	BA	3120	1/1	0.93	0.19	56,56,56,56	0
56	MG	DA	3310	1/1	0.93	0.17	30,30,30,30	0
56	MG	AA	3043	1/1	0.93	0.28	63,63,63,63	0
56	MG	BA	3622	1/1	0.93	0.18	32,32,32,32	0
56	MG	BA	3468	1/1	0.93	0.19	45,45,45,45	0
56	MG	DA	3325	1/1	0.93	0.16	31,31,31,31	0
56	MG	BA	3734	1/1	0.93	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3328	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3601	1/1	0.93	0.10	50,50,50,50	0
56	MG	BA	3735	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3104	1/1	0.93	0.12	46,46,46,46	0
56	MG	DA	3604	1/1	0.93	0.06	50,50,50,50	0
56	MG	DA	3105	1/1	0.93	0.11	56,56,56,56	0
56	MG	DA	3338	1/1	0.93	0.14	58,58,58,58	0
56	MG	BA	3229	1/1	0.93	0.10	50,50,50,50	0
56	MG	CA	3151	1/1	0.93	0.10	80,80,80,80	0
56	MG	CA	3035	1/1	0.93	0.18	49,49,49,49	0
56	MG	BA	3305	1/1	0.93	0.10	48,48,48,48	0
56	MG	AA	3125	1/1	0.93	0.13	56,56,56,56	0
56	MG	AA	3175	1/1	0.93	0.12	70,70,70,70	0
56	MG	BA	3093	1/1	0.93	0.35	52,52,52,52	0
56	MG	BA	3313	1/1	0.93	0.12	56,56,56,56	0
56	MG	DA	3370	1/1	0.93	0.20	40,40,40,40	0
56	MG	BA	3479	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3378	1/1	0.93	0.07	38,38,38,38	0
56	MG	DA	3117	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3381	1/1	0.93	0.14	68,68,68,68	0
56	MG	DA	3387	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3390	1/1	0.93	0.12	58,58,58,58	0
56	MG	BA	3481	1/1	0.93	0.14	41,41,41,41	0
56	MG	AA	3159	1/1	0.93	0.17	57,57,57,57	0
56	MG	DA	3638	1/1	0.93	0.08	53,53,53,53	0
56	MG	BB	3009	1/1	0.93	0.12	49,49,49,49	0
56	MG	DA	3640	1/1	0.93	0.10	53,53,53,53	0
56	MG	DA	3395	1/1	0.93	0.07	40,40,40,40	0
56	MG	DA	3399	1/1	0.93	0.23	39,39,39,39	0
56	MG	DA	3400	1/1	0.93	0.16	42,42,42,42	0
56	MG	DA	3651	1/1	0.93	0.08	48,48,48,48	0
56	MG	AA	3130	1/1	0.93	0.19	55,55,55,55	0
56	MG	DA	3406	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3409	1/1	0.93	0.07	54,54,54,54	0
56	MG	AA	3222	1/1	0.93	0.20	64,64,64,64	0
56	MG	BA	3100	1/1	0.93	0.15	42,42,42,42	0
56	MG	BA	3503	1/1	0.93	0.12	56,56,56,56	0
56	MG	DB	3007	1/1	0.93	0.24	45,45,45,45	0
56	MG	BA	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	DA	3132	1/1	0.93	0.20	47,47,47,47	0
56	MG	BA	3183	1/1	0.93	0.11	40,40,40,40	0
56	MG	DD	303	1/1	0.93	0.54	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DE	302	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3141	1/1	0.93	0.27	43,43,43,43	0
56	MG	CE	3002	1/1	0.93	0.08	69,69,69,69	0
56	MG	BA	3250	1/1	0.93	0.29	61,61,61,61	0
56	MG	BA	3336	1/1	0.93	0.14	46,46,46,46	0
56	MG	BE	307	1/1	0.93	0.20	51,51,51,51	0
56	MG	BA	3518	1/1	0.93	0.09	52,52,52,52	0
56	MG	DA	3442	1/1	0.93	0.17	58,58,58,58	0
56	MG	DA	3002	1/1	0.93	0.19	47,47,47,47	0
56	MG	BA	3008	1/1	0.93	0.15	30,30,30,30	0
56	MG	DA	3156	1/1	0.93	0.32	38,38,38,38	0
56	MG	BA	3104	1/1	0.93	0.23	34,34,34,34	0
56	MG	AA	3146	1/1	0.93	0.08	55,55,55,55	0
56	MG	DV	203	1/1	0.93	0.18	41,41,41,41	0
56	MG	BA	3660	1/1	0.93	0.15	58,58,58,58	0
56	MG	DA	3014	1/1	0.93	0.08	38,38,38,38	0
56	MG	DA	3164	1/1	0.93	0.06	40,40,40,40	0
56	MG	BA	3254	1/1	0.93	0.10	40,40,40,40	0
58	ZN	B4	501	1/1	0.93	0.10	152,152,152,152	0
56	MG	BA	3189	1/1	0.93	0.05	39,39,39,39	0
56	MG	DA	3019	1/1	0.93	0.13	32,32,32,32	0
56	MG	BA	3664	1/1	0.93	0.17	63,63,63,63	0
56	MG	BA	3665	1/1	0.93	0.23	39,39,39,39	0
56	MG	BA	3268	1/1	0.94	0.19	29,29,29,29	0
56	MG	BW	3003	1/1	0.94	0.14	39,39,39,39	0
56	MG	DA	3434	1/1	0.94	0.10	51,51,51,51	0
56	MG	CA	3132	1/1	0.94	0.13	66,66,66,66	0
56	MG	CA	3134	1/1	0.94	0.11	92,92,92,92	0
56	MG	BA	3436	1/1	0.94	0.12	35,35,35,35	0
56	MG	DA	3438	1/1	0.94	0.19	50,50,50,50	0
56	MG	BW	3005	1/1	0.94	0.14	38,38,38,38	0
56	MG	BA	3444	1/1	0.94	0.14	29,29,29,29	0
56	MG	BA	3001	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3129	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3002	1/1	0.94	0.15	38,38,38,38	0
56	MG	B0	104	1/1	0.94	0.11	55,55,55,55	0
56	MG	BA	3274	1/1	0.94	0.21	54,54,54,54	0
56	MG	BA	3458	1/1	0.94	0.14	46,46,46,46	0
56	MG	DA	3137	1/1	0.94	0.27	62,62,62,62	0
56	MG	DA	3138	1/1	0.94	0.27	53,53,53,53	0
56	MG	DA	3140	1/1	0.94	0.26	55,55,55,55	0
56	MG	B1	3002	1/1	0.94	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3148	1/1	0.94	0.12	65,65,65,65	0
56	MG	AA	3153	1/1	0.94	0.14	46,46,46,46	0
56	MG	AA	3011	1/1	0.94	0.34	44,44,44,44	0
56	MG	AA	3210	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3138	1/1	0.94	0.23	54,54,54,54	0
56	MG	BA	3074	1/1	0.94	0.06	38,38,38,38	0
56	MG	BA	3286	1/1	0.94	0.18	42,42,42,42	0
56	MG	DA	3473	1/1	0.94	0.14	50,50,50,50	0
56	MG	BA	3288	1/1	0.94	0.10	45,45,45,45	0
56	MG	AA	3155	1/1	0.94	0.13	54,54,54,54	0
56	MG	AA	3213	1/1	0.94	0.09	74,74,74,74	0
56	MG	DA	3482	1/1	0.94	0.06	45,45,45,45	0
56	MG	CA	3005	1/1	0.94	0.23	37,37,37,37	0
56	MG	AA	3122	1/1	0.94	0.34	40,40,40,40	0
56	MG	BA	3017	1/1	0.94	0.20	38,38,38,38	0
56	MG	DA	3167	1/1	0.94	0.19	46,46,46,46	0
56	MG	BA	3084	1/1	0.94	0.33	47,47,47,47	0
56	MG	BA	3205	1/1	0.94	0.19	38,38,38,38	0
56	MG	DA	3493	1/1	0.94	0.12	38,38,38,38	0
56	MG	BA	3482	1/1	0.94	0.11	59,59,59,59	0
56	MG	CA	3165	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3173	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3499	1/1	0.94	0.18	44,44,44,44	0
56	MG	CA	3167	1/1	0.94	0.06	68,68,68,68	0
56	MG	DA	3176	1/1	0.94	0.11	52,52,52,52	0
56	MG	DA	3503	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3179	1/1	0.94	0.23	36,36,36,36	0
56	MG	BA	3207	1/1	0.94	0.20	44,44,44,44	0
56	MG	AA	3109	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3187	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3188	1/1	0.94	0.23	52,52,52,52	0
56	MG	BA	3498	1/1	0.94	0.07	81,81,81,81	0
56	MG	BA	3298	1/1	0.94	0.25	45,45,45,45	0
56	MG	DA	3516	1/1	0.94	0.21	54,54,54,54	0
56	MG	AA	3051	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3518	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3211	1/1	0.94	0.08	43,43,43,43	0
56	MG	AA	3041	1/1	0.94	0.08	41,41,41,41	0
56	MG	AA	3035	1/1	0.94	0.07	59,59,59,59	0
56	MG	CX	102	1/1	0.94	0.07	60,60,60,60	0
56	MG	BA	3677	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3507	1/1	0.94	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3509	1/1	0.94	0.13	29,29,29,29	0
56	MG	DA	3206	1/1	0.94	0.24	36,36,36,36	0
56	MG	BA	3307	1/1	0.94	0.08	35,35,35,35	0
56	MG	BA	3685	1/1	0.94	0.20	58,58,58,58	0
56	MG	BA	3097	1/1	0.94	0.17	30,30,30,30	0
56	MG	DA	3216	1/1	0.94	0.10	47,47,47,47	0
56	MG	DA	3535	1/1	0.94	0.08	58,58,58,58	0
56	MG	BA	3513	1/1	0.94	0.20	51,51,51,51	0
56	MG	DA	3013	1/1	0.94	0.16	38,38,38,38	0
56	MG	BA	3215	1/1	0.94	0.08	32,32,32,32	0
56	MG	AA	3190	1/1	0.94	0.26	61,61,61,61	0
56	MG	DA	3017	1/1	0.94	0.07	51,51,51,51	0
56	MG	BA	3219	1/1	0.94	0.24	36,36,36,36	0
56	MG	DA	3227	1/1	0.94	0.08	40,40,40,40	0
56	MG	BA	3315	1/1	0.94	0.22	43,43,43,43	0
56	MG	BA	3221	1/1	0.94	0.27	55,55,55,55	0
56	MG	BA	3533	1/1	0.94	0.14	30,30,30,30	0
56	MG	CA	3040	1/1	0.94	0.21	47,47,47,47	0
56	MG	DA	3238	1/1	0.94	0.07	37,37,37,37	0
56	MG	DA	3027	1/1	0.94	0.21	49,49,49,49	0
56	MG	BA	3157	1/1	0.94	0.07	52,52,52,52	0
56	MG	AA	3054	1/1	0.94	0.13	46,46,46,46	0
56	MG	DA	3244	1/1	0.94	0.15	23,23,23,23	0
56	MG	DA	3565	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3539	1/1	0.94	0.11	23,23,23,23	0
56	MG	DA	3248	1/1	0.94	0.15	30,30,30,30	0
56	MG	BA	3225	1/1	0.94	0.23	42,42,42,42	0
56	MG	CA	3045	1/1	0.94	0.22	60,60,60,60	0
56	MG	DA	3034	1/1	0.94	0.18	40,40,40,40	0
56	MG	BA	3325	1/1	0.94	0.10	39,39,39,39	0
56	MG	BA	3546	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3578	1/1	0.94	0.21	68,68,68,68	0
56	MG	DA	3582	1/1	0.94	0.17	44,44,44,44	0
56	MG	DA	3038	1/1	0.94	0.06	37,37,37,37	0
56	MG	BA	3548	1/1	0.94	0.19	40,40,40,40	0
56	MG	BA	3227	1/1	0.94	0.14	67,67,67,67	0
56	MG	CA	3052	1/1	0.94	0.14	47,47,47,47	0
56	MG	BA	3550	1/1	0.94	0.11	32,32,32,32	0
56	MG	DA	3269	1/1	0.94	0.12	47,47,47,47	0
56	MG	DA	3044	1/1	0.94	0.23	45,45,45,45	0
56	MG	DA	3271	1/1	0.94	0.08	45,45,45,45	0
56	MG	DA	3597	1/1	0.94	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3161	1/1	0.94	0.12	50,50,50,50	0
56	MG	BA	3557	1/1	0.94	0.18	35,35,35,35	0
56	MG	AA	3170	1/1	0.94	0.16	83,83,83,83	0
56	MG	BA	3101	1/1	0.94	0.30	47,47,47,47	0
56	MG	BA	3725	1/1	0.94	0.06	29,29,29,29	0
56	MG	DA	3056	1/1	0.94	0.15	37,37,37,37	0
56	MG	BA	3234	1/1	0.94	0.19	48,48,48,48	0
56	MG	BA	3339	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3030	1/1	0.94	0.27	26,26,26,26	0
56	MG	BA	3577	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3290	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3295	1/1	0.94	0.11	31,31,31,31	0
56	MG	DA	3614	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3237	1/1	0.94	0.16	43,43,43,43	0
56	MG	DA	3298	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3037	1/1	0.94	0.24	39,39,39,39	0
56	MG	CA	3068	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3352	1/1	0.94	0.08	58,58,58,58	0
56	MG	DA	3067	1/1	0.94	0.19	35,35,35,35	0
56	MG	BA	3169	1/1	0.94	0.12	39,39,39,39	0
56	MG	DA	3623	1/1	0.94	0.08	63,63,63,63	0
56	MG	DA	3624	1/1	0.94	0.07	54,54,54,54	0
56	MG	DA	3626	1/1	0.94	0.08	63,63,63,63	0
56	MG	DA	3316	1/1	0.94	0.22	47,47,47,47	0
56	MG	DA	3317	1/1	0.94	0.13	34,34,34,34	0
56	MG	BA	3171	1/1	0.94	0.24	42,42,42,42	0
56	MG	DA	3320	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3634	1/1	0.94	0.12	33,33,33,33	0
56	MG	BA	3595	1/1	0.94	0.10	37,37,37,37	0
56	MG	AM	3001	1/1	0.94	0.05	76,76,76,76	0
56	MG	AA	3012	1/1	0.94	0.13	58,58,58,58	0
56	MG	BA	3361	1/1	0.94	0.06	39,39,39,39	0
56	MG	BB	3011	1/1	0.94	0.12	45,45,45,45	0
56	MG	CA	3080	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3644	1/1	0.94	0.19	50,50,50,50	0
56	MG	AA	3006	1/1	0.94	0.09	84,84,84,84	0
56	MG	AA	3059	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3648	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3602	1/1	0.94	0.08	44,44,44,44	0
56	MG	AA	3014	1/1	0.94	0.06	24,24,24,24	0
56	MG	BD	302	1/1	0.94	0.38	44,44,44,44	0
56	MG	BD	303	1/1	0.94	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3113	1/1	0.94	0.20	48,48,48,48	0
56	MG	AA	3201	1/1	0.94	0.12	76,76,76,76	0
56	MG	AA	3202	1/1	0.94	0.14	72,72,72,72	0
56	MG	DA	3364	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3383	1/1	0.94	0.16	51,51,51,51	0
56	MG	DA	3369	1/1	0.94	0.09	53,53,53,53	0
56	MG	BA	3613	1/1	0.94	0.15	47,47,47,47	0
56	MG	BE	306	1/1	0.94	0.24	38,38,38,38	0
56	MG	DD	304	1/1	0.94	0.22	40,40,40,40	0
56	MG	BA	3384	1/1	0.94	0.16	47,47,47,47	0
56	MG	BA	3385	1/1	0.94	0.07	56,56,56,56	0
56	MG	DE	304	1/1	0.94	0.09	30,30,30,30	0
56	MG	BA	3051	1/1	0.94	0.18	34,34,34,34	0
56	MG	DA	3385	1/1	0.94	0.21	58,58,58,58	0
56	MG	BA	3619	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3391	1/1	0.94	0.12	39,39,39,39	0
56	MG	BA	3256	1/1	0.94	0.21	60,60,60,60	0
56	MG	BA	3052	1/1	0.94	0.14	29,29,29,29	0
56	MG	DA	3103	1/1	0.94	0.11	52,52,52,52	0
56	MG	BN	3003	1/1	0.94	0.14	67,67,67,67	0
56	MG	BA	3056	1/1	0.94	0.23	39,39,39,39	0
56	MG	DR	5001	1/1	0.94	0.13	39,39,39,39	0
56	MG	BA	3404	1/1	0.94	0.05	42,42,42,42	0
56	MG	AA	3062	1/1	0.94	0.09	30,30,30,30	0
56	MG	AA	3151	1/1	0.94	0.07	49,49,49,49	0
56	MG	DA	3407	1/1	0.94	0.10	35,35,35,35	0
56	MG	BA	3428	1/1	0.94	0.17	36,36,36,36	0
56	MG	BA	3265	1/1	0.94	0.21	39,39,39,39	0
56	MG	AA	3206	1/1	0.94	0.15	79,79,79,79	0
56	MG	BA	3434	1/1	0.94	0.16	22,22,22,22	0
58	ZN	D4	501	1/1	0.94	0.10	155,155,155,155	0
56	MG	DA	3114	1/1	0.94	0.09	47,47,47,47	0
56	MG	DA	3422	1/1	0.94	0.19	45,45,45,45	0
56	MG	CA	3128	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3635	1/1	0.94	0.07	52,52,52,52	0
56	MG	BA	3558	1/1	0.95	0.12	47,47,47,47	0
56	MG	CA	3011	1/1	0.95	0.19	27,27,27,27	0
56	MG	DA	3446	1/1	0.95	0.14	46,46,46,46	0
56	MG	CA	3012	1/1	0.95	0.04	50,50,50,50	0
56	MG	BA	3559	1/1	0.95	0.16	29,29,29,29	0
56	MG	BA	3396	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3401	1/1	0.95	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3698	1/1	0.95	0.25	58,58,58,58	0
56	MG	CA	3166	1/1	0.95	0.09	71,71,71,71	0
56	MG	BA	3700	1/1	0.95	0.13	26,26,26,26	0
56	MG	BA	3165	1/1	0.95	0.29	44,44,44,44	0
56	MG	AA	3119	1/1	0.95	0.20	42,42,42,42	0
56	MG	DA	3459	1/1	0.95	0.09	43,43,43,43	0
56	MG	CA	3170	1/1	0.95	0.14	44,44,44,44	0
56	MG	BA	3406	1/1	0.95	0.19	54,54,54,54	0
56	MG	BA	3423	1/1	0.95	0.15	45,45,45,45	0
56	MG	DA	3463	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3424	1/1	0.95	0.11	44,44,44,44	0
56	MG	AA	3042	1/1	0.95	0.17	50,50,50,50	0
56	MG	DA	3466	1/1	0.95	0.07	43,43,43,43	0
56	MG	CF	3001	1/1	0.95	0.09	56,56,56,56	0
56	MG	DA	3472	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3020	1/1	0.95	0.28	43,43,43,43	0
56	MG	DA	3182	1/1	0.95	0.15	29,29,29,29	0
56	MG	AA	3058	1/1	0.95	0.25	59,59,59,59	0
56	MG	DA	3186	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3480	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3481	1/1	0.95	0.09	59,59,59,59	0
56	MG	BA	3712	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3713	1/1	0.95	0.07	49,49,49,49	0
56	MG	CX	104	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3430	1/1	0.95	0.11	47,47,47,47	0
56	MG	DA	3193	1/1	0.95	0.15	42,42,42,42	0
56	MG	BA	3594	1/1	0.95	0.16	55,55,55,55	0
56	MG	DA	3488	1/1	0.95	0.08	48,48,48,48	0
56	MG	BA	3073	1/1	0.95	0.05	43,43,43,43	0
56	MG	AA	3186	1/1	0.95	0.11	51,51,51,51	0
56	MG	DA	3197	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3007	1/1	0.95	0.15	43,43,43,43	0
56	MG	DA	3497	1/1	0.95	0.06	37,37,37,37	0
56	MG	AA	3008	1/1	0.95	0.11	61,61,61,61	0
56	MG	DA	3011	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3720	1/1	0.95	0.06	51,51,51,51	0
56	MG	BA	3121	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3438	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	3443	1/1	0.95	0.15	34,34,34,34	0
56	MG	DA	3210	1/1	0.95	0.14	46,46,46,46	0
56	MG	DA	3211	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3726	1/1	0.95	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3511	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3729	1/1	0.95	0.07	54,54,54,54	0
56	MG	BA	3302	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3217	1/1	0.95	0.17	33,33,33,33	0
56	MG	DA	3218	1/1	0.95	0.12	31,31,31,31	0
56	MG	DA	3021	1/1	0.95	0.18	43,43,43,43	0
56	MG	BA	3733	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3519	1/1	0.95	0.07	39,39,39,39	0
56	MG	CA	3046	1/1	0.95	0.22	52,52,52,52	0
56	MG	AA	3110	1/1	0.95	0.11	41,41,41,41	0
56	MG	BA	3451	1/1	0.95	0.09	31,31,31,31	0
56	MG	BA	3606	1/1	0.95	0.06	44,44,44,44	0
56	MG	AX	107	1/1	0.95	0.06	82,82,82,82	0
56	MG	DA	3228	1/1	0.95	0.19	49,49,49,49	0
56	MG	DA	3229	1/1	0.95	0.13	44,44,44,44	0
56	MG	CA	3051	1/1	0.95	0.11	77,77,77,77	0
56	MG	BA	3308	1/1	0.95	0.13	33,33,33,33	0
56	MG	BA	3239	1/1	0.95	0.06	33,33,33,33	0
56	MG	BA	3459	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3124	1/1	0.95	0.10	46,46,46,46	0
56	MG	BA	3615	1/1	0.95	0.16	55,55,55,55	0
56	MG	BA	3125	1/1	0.95	0.16	26,26,26,26	0
56	MG	DA	3242	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3243	1/1	0.95	0.10	43,43,43,43	0
56	MG	BB	3008	1/1	0.95	0.14	49,49,49,49	0
56	MG	DA	3245	1/1	0.95	0.16	43,43,43,43	0
56	MG	AA	3105	1/1	0.95	0.24	54,54,54,54	0
56	MG	BA	3128	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3031	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3548	1/1	0.95	0.13	60,60,60,60	0
56	MG	BA	3249	1/1	0.95	0.13	46,46,46,46	0
56	MG	BA	3132	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3050	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3085	1/1	0.95	0.19	35,35,35,35	0
56	MG	BA	3326	1/1	0.95	0.17	15,15,15,15	0
56	MG	BA	3134	1/1	0.95	0.13	34,34,34,34	0
56	MG	BA	3086	1/1	0.95	0.06	50,50,50,50	0
56	MG	DA	3561	1/1	0.95	0.11	40,40,40,40	0
56	MG	DA	3562	1/1	0.95	0.09	41,41,41,41	0
56	MG	AX	109	1/1	0.95	0.13	56,56,56,56	0
56	MG	DA	3267	1/1	0.95	0.11	40,40,40,40	0
56	MG	BD	306	1/1	0.95	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AX	110	1/1	0.95	0.10	45,45,45,45	0
56	MG	BD	310	1/1	0.95	0.12	48,48,48,48	0
56	MG	CA	3078	1/1	0.95	0.10	51,51,51,51	0
56	MG	BA	3089	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3092	1/1	0.95	0.08	28,28,28,28	0
56	MG	BA	3259	1/1	0.95	0.14	59,59,59,59	0
56	MG	BA	3341	1/1	0.95	0.11	31,31,31,31	0
56	MG	CA	3085	1/1	0.95	0.18	58,58,58,58	0
56	MG	DA	3583	1/1	0.95	0.12	35,35,35,35	0
56	MG	BF	302	1/1	0.95	0.18	49,49,49,49	0
56	MG	CA	3087	1/1	0.95	0.09	40,40,40,40	0
56	MG	BA	3501	1/1	0.95	0.10	35,35,35,35	0
56	MG	DA	3588	1/1	0.95	0.11	47,47,47,47	0
56	MG	CA	3089	1/1	0.95	0.11	54,54,54,54	0
56	MG	BF	304	1/1	0.95	0.21	30,30,30,30	0
56	MG	DA	3592	1/1	0.95	0.09	49,49,49,49	0
56	MG	DA	3593	1/1	0.95	0.13	62,62,62,62	0
56	MG	BA	3142	1/1	0.95	0.13	57,57,57,57	0
56	MG	DA	3294	1/1	0.95	0.15	30,30,30,30	0
56	MG	CA	3092	1/1	0.95	0.12	56,56,56,56	0
56	MG	CA	3093	1/1	0.95	0.11	65,65,65,65	0
56	MG	CA	3095	1/1	0.95	0.11	35,35,35,35	0
56	MG	DA	3599	1/1	0.95	0.16	69,69,69,69	0
56	MG	DA	3080	1/1	0.95	0.15	43,43,43,43	0
56	MG	AA	3221	1/1	0.95	0.21	52,52,52,52	0
56	MG	DA	3305	1/1	0.95	0.12	33,33,33,33	0
56	MG	CA	3100	1/1	0.95	0.13	72,72,72,72	0
56	MG	BA	3350	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3313	1/1	0.95	0.10	30,30,30,30	0
56	MG	BA	3040	1/1	0.95	0.09	40,40,40,40	0
56	MG	CA	3105	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3609	1/1	0.95	0.13	49,49,49,49	0
56	MG	DA	3610	1/1	0.95	0.06	49,49,49,49	0
56	MG	BN	3001	1/1	0.95	0.11	65,65,65,65	0
56	MG	BA	3264	1/1	0.95	0.10	29,29,29,29	0
56	MG	AA	3179	1/1	0.95	0.14	34,34,34,34	0
56	MG	BN	3004	1/1	0.95	0.20	69,69,69,69	0
56	MG	BA	3147	1/1	0.95	0.13	42,42,42,42	0
56	MG	BA	3650	1/1	0.95	0.09	44,44,44,44	0
56	MG	BP	204	1/1	0.95	0.08	53,53,53,53	0
56	MG	BQ	3001	1/1	0.95	0.21	38,38,38,38	0
56	MG	AA	3205	1/1	0.95	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3653	1/1	0.95	0.20	46,46,46,46	0
56	MG	BA	3360	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3339	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3270	1/1	0.95	0.12	29,29,29,29	0
56	MG	DA	3625	1/1	0.95	0.07	48,48,48,48	0
56	MG	BU	201	1/1	0.95	0.34	33,33,33,33	0
56	MG	DA	3347	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3516	1/1	0.95	0.09	64,64,64,64	0
56	MG	BA	3367	1/1	0.95	0.11	29,29,29,29	0
56	MG	BU	209	1/1	0.95	0.40	36,36,36,36	0
56	MG	DA	3358	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3635	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3107	1/1	0.95	0.12	50,50,50,50	0
56	MG	BV	3001	1/1	0.95	0.10	42,42,42,42	0
56	MG	BA	3659	1/1	0.95	0.06	42,42,42,42	0
56	MG	DA	3365	1/1	0.95	0.06	52,52,52,52	0
56	MG	DA	3366	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3005	1/1	0.95	0.11	43,43,43,43	0
56	MG	AA	3044	1/1	0.95	0.15	60,60,60,60	0
56	MG	BA	3527	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3371	1/1	0.95	0.07	37,37,37,37	0
56	MG	BA	3529	1/1	0.95	0.10	22,22,22,22	0
56	MG	DA	3377	1/1	0.95	0.13	32,32,32,32	0
56	MG	DA	3652	1/1	0.95	0.15	26,26,26,26	0
56	MG	DA	3654	1/1	0.95	0.07	50,50,50,50	0
56	MG	BA	3151	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3657	1/1	0.95	0.07	55,55,55,55	0
56	MG	DA	3379	1/1	0.95	0.08	63,63,63,63	0
56	MG	AK	3001	1/1	0.95	0.10	48,48,48,48	0
56	MG	BA	3102	1/1	0.95	0.18	45,45,45,45	0
56	MG	BA	3668	1/1	0.95	0.11	42,42,42,42	0
56	MG	B0	105	1/1	0.95	0.23	44,44,44,44	0
56	MG	CA	3137	1/1	0.95	0.13	59,59,59,59	0
56	MG	CA	3138	1/1	0.95	0.14	59,59,59,59	0
56	MG	AL	3001	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3009	1/1	0.95	0.12	36,36,36,36	0
56	MG	DD	302	1/1	0.95	0.29	48,48,48,48	0
56	MG	DA	3394	1/1	0.95	0.07	46,46,46,46	0
56	MG	DA	3125	1/1	0.95	0.09	55,55,55,55	0
56	MG	DD	305	1/1	0.95	0.11	73,73,73,73	0
56	MG	DE	301	1/1	0.95	0.18	51,51,51,51	0
56	MG	BA	3011	1/1	0.95	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3127	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3543	1/1	0.95	0.11	24,24,24,24	0
56	MG	BA	3285	1/1	0.95	0.14	44,44,44,44	0
56	MG	DF	301	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3130	1/1	0.95	0.06	34,34,34,34	0
56	MG	DF	305	1/1	0.95	0.22	55,55,55,55	0
56	MG	DA	3408	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3545	1/1	0.95	0.11	20,20,20,20	0
56	MG	DA	3413	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3387	1/1	0.95	0.09	49,49,49,49	0
56	MG	DQ	3001	1/1	0.95	0.16	40,40,40,40	0
56	MG	AA	3193	1/1	0.95	0.15	65,65,65,65	0
56	MG	DA	3417	1/1	0.95	0.12	54,54,54,54	0
56	MG	AA	3142	1/1	0.95	0.16	60,60,60,60	0
56	MG	BA	3162	1/1	0.95	0.08	43,43,43,43	0
56	MG	CA	3002	1/1	0.95	0.05	74,74,74,74	0
56	MG	DA	3139	1/1	0.95	0.11	47,47,47,47	0
56	MG	BA	3016	1/1	0.95	0.12	50,50,50,50	0
56	MG	DA	3428	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3683	1/1	0.95	0.19	37,37,37,37	0
56	MG	DA	3143	1/1	0.95	0.09	53,53,53,53	0
56	MG	D5	101	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3144	1/1	0.95	0.21	37,37,37,37	0
56	MG	DA	3145	1/1	0.95	0.11	52,52,52,52	0
56	MG	CA	3154	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3553	1/1	0.95	0.18	46,46,46,46	0
56	MG	BA	3554	1/1	0.95	0.16	25,25,25,25	0
56	MG	AA	3195	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3690	1/1	0.95	0.16	55,55,55,55	0
56	MG	BA	3623	1/1	0.96	0.12	43,43,43,43	0
56	MG	BB	3015	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3469	1/1	0.96	0.14	52,52,52,52	0
56	MG	DA	3470	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3484	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3269	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3486	1/1	0.96	0.12	55,55,55,55	0
56	MG	CA	3066	1/1	0.96	0.06	47,47,47,47	0
56	MG	DA	3213	1/1	0.96	0.15	48,48,48,48	0
56	MG	BA	3628	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3215	1/1	0.96	0.25	43,43,43,43	0
56	MG	DA	3037	1/1	0.96	0.19	37,37,37,37	0
56	MG	AA	3161	1/1	0.96	0.06	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3630	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3493	1/1	0.96	0.08	51,51,51,51	0
56	MG	BA	3496	1/1	0.96	0.20	21,21,21,21	0
56	MG	AA	3010	1/1	0.96	0.05	71,71,71,71	0
56	MG	AA	3050	1/1	0.96	0.08	50,50,50,50	0
56	MG	DA	3046	1/1	0.96	0.10	48,48,48,48	0
56	MG	DA	3047	1/1	0.96	0.09	36,36,36,36	0
56	MG	DA	3226	1/1	0.96	0.21	47,47,47,47	0
56	MG	BA	3048	1/1	0.96	0.20	33,33,33,33	0
56	MG	BA	3050	1/1	0.96	0.12	33,33,33,33	0
56	MG	CA	3076	1/1	0.96	0.14	48,48,48,48	0
56	MG	DA	3051	1/1	0.96	0.08	39,39,39,39	0
56	MG	BE	302	1/1	0.96	0.12	29,29,29,29	0
56	MG	DA	3501	1/1	0.96	0.16	67,67,67,67	0
56	MG	DA	3232	1/1	0.96	0.05	39,39,39,39	0
56	MG	BE	305	1/1	0.96	0.21	44,44,44,44	0
56	MG	BA	3090	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3218	1/1	0.96	0.09	58,58,58,58	0
56	MG	DA	3239	1/1	0.96	0.13	54,54,54,54	0
56	MG	BF	301	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3281	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3059	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3506	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3282	1/1	0.96	0.10	34,34,34,34	0
56	MG	BA	3372	1/1	0.96	0.08	42,42,42,42	0
56	MG	BA	3645	1/1	0.96	0.21	63,63,63,63	0
56	MG	DA	3247	1/1	0.96	0.17	34,34,34,34	0
56	MG	BA	3646	1/1	0.96	0.12	39,39,39,39	0
56	MG	BA	3170	1/1	0.96	0.21	34,34,34,34	0
56	MG	BA	3511	1/1	0.96	0.17	40,40,40,40	0
56	MG	AA	3104	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3129	1/1	0.96	0.28	44,44,44,44	0
56	MG	BA	3130	1/1	0.96	0.38	51,51,51,51	0
56	MG	BA	3652	1/1	0.96	0.18	54,54,54,54	0
56	MG	DA	3072	1/1	0.96	0.14	40,40,40,40	0
56	MG	BO	201	1/1	0.96	0.07	63,63,63,63	0
56	MG	DA	3261	1/1	0.96	0.13	44,44,44,44	0
56	MG	DA	3262	1/1	0.96	0.18	60,60,60,60	0
56	MG	AA	3167	1/1	0.96	0.16	78,78,78,78	0
56	MG	DA	3533	1/1	0.96	0.12	59,59,59,59	0
56	MG	DA	3264	1/1	0.96	0.07	38,38,38,38	0
56	MG	BP	203	1/1	0.96	0.55	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3076	1/1	0.96	0.24	38,38,38,38	0
56	MG	BA	3517	1/1	0.96	0.11	52,52,52,52	0
56	MG	DA	3538	1/1	0.96	0.13	37,37,37,37	0
56	MG	BA	3226	1/1	0.96	0.23	31,31,31,31	0
56	MG	BA	3290	1/1	0.96	0.07	35,35,35,35	0
56	MG	DA	3272	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3388	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3274	1/1	0.96	0.22	49,49,49,49	0
56	MG	DA	3546	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3525	1/1	0.96	0.09	31,31,31,31	0
56	MG	DA	3277	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3083	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3279	1/1	0.96	0.12	32,32,32,32	0
56	MG	DA	3280	1/1	0.96	0.11	46,46,46,46	0
56	MG	BA	3526	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3175	1/1	0.96	0.17	40,40,40,40	0
56	MG	DA	3283	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3055	1/1	0.96	0.21	44,44,44,44	0
56	MG	BU	207	1/1	0.96	0.13	38,38,38,38	0
56	MG	CA	3115	1/1	0.96	0.06	81,81,81,81	0
56	MG	BA	3095	1/1	0.96	0.21	55,55,55,55	0
56	MG	BA	3532	1/1	0.96	0.15	42,42,42,42	0
56	MG	CA	3118	1/1	0.96	0.08	39,39,39,39	0
56	MG	BA	3096	1/1	0.96	0.23	35,35,35,35	0
56	MG	BA	3232	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3025	1/1	0.96	0.09	48,48,48,48	0
56	MG	BW	3002	1/1	0.96	0.16	34,34,34,34	0
56	MG	BA	3400	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3136	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3576	1/1	0.96	0.09	57,57,57,57	0
56	MG	BA	3402	1/1	0.96	0.13	23,23,23,23	0
56	MG	DA	3580	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3581	1/1	0.96	0.10	41,41,41,41	0
56	MG	BA	3059	1/1	0.96	0.21	35,35,35,35	0
56	MG	AA	3138	1/1	0.96	0.21	38,38,38,38	0
56	MG	DA	3312	1/1	0.96	0.09	24,24,24,24	0
56	MG	AA	3212	1/1	0.96	0.10	36,36,36,36	0
56	MG	B0	103	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3407	1/1	0.96	0.17	35,35,35,35	0
56	MG	BA	3408	1/1	0.96	0.08	28,28,28,28	0
56	MG	DA	3590	1/1	0.96	0.07	39,39,39,39	0
56	MG	BA	3678	1/1	0.96	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3412	1/1	0.96	0.16	29,29,29,29	0
56	MG	BA	3551	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3419	1/1	0.96	0.30	36,36,36,36	0
56	MG	BA	3140	1/1	0.96	0.18	50,50,50,50	0
56	MG	BA	3241	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3329	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3330	1/1	0.96	0.06	30,30,30,30	0
56	MG	CA	3140	1/1	0.96	0.14	75,75,75,75	0
56	MG	BA	3556	1/1	0.96	0.07	25,25,25,25	0
56	MG	DA	3334	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3183	1/1	0.96	0.12	56,56,56,56	0
56	MG	CA	3143	1/1	0.96	0.11	91,91,91,91	0
56	MG	DA	3118	1/1	0.96	0.07	44,44,44,44	0
56	MG	BA	3688	1/1	0.96	0.07	58,58,58,58	0
56	MG	DA	3345	1/1	0.96	0.06	16,16,16,16	0
56	MG	DA	3120	1/1	0.96	0.39	50,50,50,50	0
56	MG	BA	3689	1/1	0.96	0.09	25,25,25,25	0
56	MG	CA	3001	1/1	0.96	0.06	48,48,48,48	0
56	MG	BA	3029	1/1	0.96	0.29	53,53,53,53	0
56	MG	DA	3354	1/1	0.96	0.05	39,39,39,39	0
56	MG	DA	3355	1/1	0.96	0.17	39,39,39,39	0
56	MG	BA	3692	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3244	1/1	0.96	0.22	46,46,46,46	0
56	MG	BA	3245	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3695	1/1	0.96	0.23	34,34,34,34	0
56	MG	BA	3067	1/1	0.96	0.28	55,55,55,55	0
56	MG	AA	3060	1/1	0.96	0.28	52,52,52,52	0
56	MG	BA	3069	1/1	0.96	0.12	33,33,33,33	0
56	MG	BA	3568	1/1	0.96	0.07	68,68,68,68	0
56	MG	BA	3106	1/1	0.96	0.22	52,52,52,52	0
56	MG	CA	3013	1/1	0.96	0.05	46,46,46,46	0
56	MG	BA	3576	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3703	1/1	0.96	0.09	44,44,44,44	0
56	MG	BA	3194	1/1	0.96	0.25	43,43,43,43	0
56	MG	CA	3017	1/1	0.96	0.17	54,54,54,54	0
56	MG	BA	3581	1/1	0.96	0.17	54,54,54,54	0
56	MG	AA	3199	1/1	0.96	0.08	62,62,62,62	0
56	MG	DA	3632	1/1	0.96	0.16	60,60,60,60	0
56	MG	BA	3033	1/1	0.96	0.24	54,54,54,54	0
56	MG	BA	3588	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3446	1/1	0.96	0.11	25,25,25,25	0
56	MG	BA	3197	1/1	0.96	0.21	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3147	1/1	0.96	0.15	46,46,46,46	0
56	MG	DA	3148	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3450	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3151	1/1	0.96	0.30	48,48,48,48	0
56	MG	BA	3110	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3398	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3715	1/1	0.96	0.13	44,44,44,44	0
56	MG	DA	3647	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3452	1/1	0.96	0.07	16,16,16,16	0
56	MG	DA	3402	1/1	0.96	0.14	33,33,33,33	0
56	MG	DA	3404	1/1	0.96	0.09	57,57,57,57	0
56	MG	BA	3036	1/1	0.96	0.13	25,25,25,25	0
56	MG	BA	3200	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3656	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3598	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3658	1/1	0.96	0.26	50,50,50,50	0
56	MG	DA	3158	1/1	0.96	0.28	47,47,47,47	0
56	MG	BA	3010	1/1	0.96	0.05	35,35,35,35	0
56	MG	BA	3332	1/1	0.96	0.13	52,52,52,52	0
56	MG	BA	3258	1/1	0.96	0.05	35,35,35,35	0
56	MG	DB	3005	1/1	0.96	0.14	41,41,41,41	0
56	MG	BA	3723	1/1	0.96	0.08	25,25,25,25	0
56	MG	DA	3165	1/1	0.96	0.28	48,48,48,48	0
56	MG	BA	3461	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3462	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3168	1/1	0.96	0.34	46,46,46,46	0
56	MG	DA	3423	1/1	0.96	0.07	29,29,29,29	0
56	MG	BA	3728	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3464	1/1	0.96	0.09	40,40,40,40	0
56	MG	AA	3066	1/1	0.96	0.17	41,41,41,41	0
56	MG	DA	3004	1/1	0.96	0.06	24,24,24,24	0
56	MG	BA	3260	1/1	0.96	0.11	47,47,47,47	0
56	MG	DA	3433	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3174	1/1	0.96	0.22	26,26,26,26	0
56	MG	BA	3608	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3609	1/1	0.96	0.16	29,29,29,29	0
56	MG	DF	303	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3009	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3010	1/1	0.96	0.07	42,42,42,42	0
56	MG	DA	3439	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3181	1/1	0.96	0.30	55,55,55,55	0
56	MG	AA	3091	1/1	0.96	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3443	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3183	1/1	0.96	0.11	42,42,42,42	0
56	MG	BA	3738	1/1	0.96	0.17	58,58,58,58	0
56	MG	DA	3185	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3611	1/1	0.96	0.07	61,61,61,61	0
56	MG	BA	3076	1/1	0.96	0.13	40,40,40,40	0
56	MG	AA	3024	1/1	0.96	0.12	49,49,49,49	0
56	MG	DU	3002	1/1	0.96	0.23	52,52,52,52	0
56	MG	DV	201	1/1	0.96	0.07	56,56,56,56	0
56	MG	DA	3016	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3041	1/1	0.96	0.24	45,45,45,45	0
56	MG	DW	201	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3192	1/1	0.96	0.15	48,48,48,48	0
56	MG	AA	3034	1/1	0.96	0.14	46,46,46,46	0
56	MG	BA	3344	1/1	0.96	0.06	65,65,65,65	0
56	MG	DA	3020	1/1	0.96	0.14	45,45,45,45	0
56	MG	D5	102	1/1	0.96	0.23	44,44,44,44	0
56	MG	BA	3346	1/1	0.96	0.07	33,33,33,33	0
56	MG	CA	3055	1/1	0.96	0.26	61,61,61,61	0
56	MG	BA	3349	1/1	0.96	0.07	31,31,31,31	0
56	MG	AA	3160	1/1	0.96	0.19	52,52,52,52	0
56	MG	BA	3210	1/1	0.96	0.20	39,39,39,39	0
56	MG	DA	3202	1/1	0.96	0.08	39,39,39,39	0
56	MG	BA	3355	1/1	0.96	0.07	39,39,39,39	0
56	MG	AA	3208	1/1	0.97	0.13	38,38,38,38	0
56	MG	DA	3311	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3699	1/1	0.97	0.08	23,23,23,23	0
56	MG	AA	3144	1/1	0.97	0.08	56,56,56,56	0
56	MG	AA	3103	1/1	0.97	0.15	43,43,43,43	0
56	MG	DA	3522	1/1	0.97	0.07	46,46,46,46	0
56	MG	DA	3315	1/1	0.97	0.10	39,39,39,39	0
56	MG	BA	3023	1/1	0.97	0.18	34,34,34,34	0
56	MG	BV	3003	1/1	0.97	0.14	27,27,27,27	0
56	MG	DA	3159	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3160	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3508	1/1	0.97	0.08	46,46,46,46	0
56	MG	BA	3216	1/1	0.97	0.09	46,46,46,46	0
56	MG	BA	3024	1/1	0.97	0.06	31,31,31,31	0
56	MG	DA	3327	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3706	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3707	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3426	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3427	1/1	0.97	0.07	20,20,20,20	0
56	MG	CA	3096	1/1	0.97	0.06	54,54,54,54	0
56	MG	CA	3097	1/1	0.97	0.09	60,60,60,60	0
56	MG	DA	3539	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3335	1/1	0.97	0.09	36,36,36,36	0
56	MG	AA	3049	1/1	0.97	0.18	46,46,46,46	0
56	MG	B0	102	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3042	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3342	1/1	0.97	0.09	31,31,31,31	0
56	MG	DA	3545	1/1	0.97	0.14	35,35,35,35	0
56	MG	BA	3617	1/1	0.97	0.16	30,30,30,30	0
56	MG	BA	3347	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3045	1/1	0.97	0.08	27,27,27,27	0
56	MG	BA	3220	1/1	0.97	0.18	27,27,27,27	0
56	MG	DA	3550	1/1	0.97	0.09	54,54,54,54	0
56	MG	DA	3350	1/1	0.97	0.11	21,21,21,21	0
56	MG	DA	3553	1/1	0.97	0.12	58,58,58,58	0
56	MG	DA	3177	1/1	0.97	0.13	30,30,30,30	0
56	MG	DA	3178	1/1	0.97	0.07	43,43,43,43	0
56	MG	DA	3556	1/1	0.97	0.07	35,35,35,35	0
56	MG	AA	3165	1/1	0.97	0.09	24,24,24,24	0
56	MG	BA	3354	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3521	1/1	0.97	0.10	38,38,38,38	0
56	MG	DA	3357	1/1	0.97	0.06	50,50,50,50	0
56	MG	B3	3401	1/1	0.97	0.10	24,24,24,24	0
56	MG	DA	3052	1/1	0.97	0.05	20,20,20,20	0
56	MG	B3	3402	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3522	1/1	0.97	0.12	42,42,42,42	0
56	MG	BA	3222	1/1	0.97	0.23	56,56,56,56	0
56	MG	B7	102	1/1	0.97	0.06	29,29,29,29	0
56	MG	AA	3031	1/1	0.97	0.19	41,41,41,41	0
56	MG	BA	3439	1/1	0.97	0.05	35,35,35,35	0
56	MG	AA	3214	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3574	1/1	0.97	0.11	22,22,22,22	0
56	MG	B8	5002	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3160	1/1	0.97	0.15	24,24,24,24	0
56	MG	DA	3577	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3374	1/1	0.97	0.10	40,40,40,40	0
56	MG	DA	3579	1/1	0.97	0.11	38,38,38,38	0
56	MG	DA	3376	1/1	0.97	0.08	42,42,42,42	0
56	MG	CA	3120	1/1	0.97	0.12	59,59,59,59	0
56	MG	DA	3063	1/1	0.97	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3158	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3531	1/1	0.97	0.11	28,28,28,28	0
56	MG	BA	3078	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3383	1/1	0.97	0.08	27,27,27,27	0
56	MG	DA	3199	1/1	0.97	0.15	46,46,46,46	0
56	MG	BA	3449	1/1	0.97	0.10	59,59,59,59	0
56	MG	BA	3730	1/1	0.97	0.06	43,43,43,43	0
56	MG	CA	3006	1/1	0.97	0.07	72,72,72,72	0
56	MG	BA	3731	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3204	1/1	0.97	0.23	44,44,44,44	0
56	MG	BA	3013	1/1	0.97	0.16	36,36,36,36	0
56	MG	BA	3364	1/1	0.97	0.08	30,30,30,30	0
56	MG	DA	3397	1/1	0.97	0.11	40,40,40,40	0
56	MG	DA	3207	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3303	1/1	0.97	0.11	11,11,11,11	0
56	MG	AA	3177	1/1	0.97	0.05	58,58,58,58	0
56	MG	BA	3542	1/1	0.97	0.11	37,37,37,37	0
56	MG	DA	3403	1/1	0.97	0.06	42,42,42,42	0
56	MG	CA	3133	1/1	0.97	0.04	45,45,45,45	0
56	MG	BA	3108	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3642	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3456	1/1	0.97	0.08	24,24,24,24	0
56	MG	BA	3457	1/1	0.97	0.06	25,25,25,25	0
56	MG	BA	3266	1/1	0.97	0.21	47,47,47,47	0
56	MG	DA	3410	1/1	0.97	0.05	40,40,40,40	0
56	MG	BA	3053	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3219	1/1	0.97	0.20	49,49,49,49	0
56	MG	BA	3233	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3085	1/1	0.97	0.07	35,35,35,35	0
56	MG	CA	3020	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3054	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3421	1/1	0.97	0.11	43,43,43,43	0
56	MG	DA	3088	1/1	0.97	0.06	47,47,47,47	0
56	MG	BA	3168	1/1	0.97	0.28	52,52,52,52	0
56	MG	CA	3023	1/1	0.97	0.14	37,37,37,37	0
56	MG	BB	3007	1/1	0.97	0.04	49,49,49,49	0
56	MG	DA	3426	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3377	1/1	0.97	0.04	27,27,27,27	0
56	MG	DA	3429	1/1	0.97	0.05	30,30,30,30	0
56	MG	CA	3026	1/1	0.97	0.04	52,52,52,52	0
56	MG	BA	3380	1/1	0.97	0.10	32,32,32,32	0
56	MG	BA	3381	1/1	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3382	1/1	0.97	0.12	21,21,21,21	0
56	MG	DA	3629	1/1	0.97	0.09	30,30,30,30	0
56	MG	DA	3233	1/1	0.97	0.08	58,58,58,58	0
56	MG	BA	3271	1/1	0.97	0.16	40,40,40,40	0
56	MG	BA	3655	1/1	0.97	0.11	44,44,44,44	0
56	MG	DA	3237	1/1	0.97	0.15	37,37,37,37	0
56	MG	AA	3149	1/1	0.97	0.05	49,49,49,49	0
56	MG	DA	3440	1/1	0.97	0.05	48,48,48,48	0
56	MG	BA	3034	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3101	1/1	0.97	0.13	59,59,59,59	0
56	MG	BA	3560	1/1	0.97	0.14	24,24,24,24	0
56	MG	BA	3471	1/1	0.97	0.05	28,28,28,28	0
56	MG	DA	3641	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3562	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3472	1/1	0.97	0.07	53,53,53,53	0
56	MG	BA	3662	1/1	0.97	0.08	46,46,46,46	0
56	MG	BD	308	1/1	0.97	0.15	21,21,21,21	0
56	MG	BA	3386	1/1	0.97	0.07	29,29,29,29	0
56	MG	DA	3451	1/1	0.97	0.03	68,68,68,68	0
56	MG	DA	3649	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3566	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3453	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3653	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3474	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3058	1/1	0.97	0.20	41,41,41,41	0
56	MG	BA	3569	1/1	0.97	0.09	55,55,55,55	0
56	MG	BE	304	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3321	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3573	1/1	0.97	0.06	53,53,53,53	0
56	MG	BA	3670	1/1	0.97	0.08	55,55,55,55	0
56	MG	DA	3258	1/1	0.97	0.14	39,39,39,39	0
56	MG	BE	308	1/1	0.97	0.14	27,27,27,27	0
56	MG	BE	309	1/1	0.97	0.06	37,37,37,37	0
56	MG	BA	3389	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3276	1/1	0.97	0.15	9,9,9,9	0
56	MG	DB	3008	1/1	0.97	0.09	36,36,36,36	0
56	MG	DB	3009	1/1	0.97	0.27	41,41,41,41	0
56	MG	BA	3580	1/1	0.97	0.10	58,58,58,58	0
56	MG	DA	3467	1/1	0.97	0.12	48,48,48,48	0
56	MG	DA	3265	1/1	0.97	0.13	44,44,44,44	0
56	MG	DD	301	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3035	1/1	0.97	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BF	305	1/1	0.97	0.15	38,38,38,38	0
56	MG	DA	3471	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3278	1/1	0.97	0.19	53,53,53,53	0
56	MG	BA	3115	1/1	0.97	0.14	28,28,28,28	0
56	MG	BA	3587	1/1	0.97	0.12	23,23,23,23	0
56	MG	CA	3059	1/1	0.97	0.18	51,51,51,51	0
56	MG	BA	3329	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3479	1/1	0.97	0.11	35,35,35,35	0
56	MG	BA	3330	1/1	0.97	0.07	35,35,35,35	0
56	MG	DF	302	1/1	0.97	0.07	47,47,47,47	0
56	MG	AA	3057	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3489	1/1	0.97	0.06	50,50,50,50	0
56	MG	BA	3490	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3133	1/1	0.97	0.12	31,31,31,31	0
56	MG	DA	3006	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3492	1/1	0.97	0.12	48,48,48,48	0
56	MG	BN	3006	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3003	1/1	0.97	0.08	24,24,24,24	0
56	MG	BP	201	1/1	0.97	0.23	37,37,37,37	0
56	MG	DA	3492	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3494	1/1	0.97	0.09	28,28,28,28	0
56	MG	DA	3494	1/1	0.97	0.07	50,50,50,50	0
56	MG	DA	3286	1/1	0.97	0.05	26,26,26,26	0
56	MG	BA	3334	1/1	0.97	0.08	41,41,41,41	0
56	MG	DA	3142	1/1	0.97	0.19	33,33,33,33	0
56	MG	BA	3497	1/1	0.97	0.21	28,28,28,28	0
56	MG	BA	3403	1/1	0.97	0.07	28,28,28,28	0
56	MG	DA	3292	1/1	0.97	0.06	34,34,34,34	0
56	MG	AV	101	1/1	0.97	0.15	51,51,51,51	0
56	MG	BA	3500	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3603	1/1	0.97	0.11	40,40,40,40	0
56	MG	DA	3297	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3146	1/1	0.97	0.23	56,56,56,56	0
56	MG	CA	3077	1/1	0.97	0.24	51,51,51,51	0
56	MG	DA	3300	1/1	0.97	0.07	47,47,47,47	0
56	MG	DA	3301	1/1	0.97	0.12	30,30,30,30	0
56	MG	DA	3150	1/1	0.97	0.05	57,57,57,57	0
56	MG	BA	3337	1/1	0.97	0.12	48,48,48,48	0
56	MG	BA	3065	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3309	1/1	0.97	0.08	25,25,25,25	0
56	MG	DA	3308	1/1	0.98	0.05	32,32,32,32	0
56	MG	AA	3172	1/1	0.98	0.04	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3312	1/1	0.98	0.05	43,43,43,43	0
56	MG	BA	3584	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3585	1/1	0.98	0.10	25,25,25,25	0
56	MG	DA	3208	1/1	0.98	0.16	46,46,46,46	0
56	MG	DA	3025	1/1	0.98	0.21	38,38,38,38	0
56	MG	DA	3026	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3584	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3409	1/1	0.98	0.07	40,40,40,40	0
56	MG	DA	3028	1/1	0.98	0.06	34,34,34,34	0
56	MG	DA	3450	1/1	0.98	0.06	47,47,47,47	0
56	MG	BA	3519	1/1	0.98	0.04	57,57,57,57	0
56	MG	DA	3319	1/1	0.98	0.05	31,31,31,31	0
56	MG	BA	3589	1/1	0.98	0.12	34,34,34,34	0
56	MG	DA	3322	1/1	0.98	0.09	41,41,41,41	0
56	MG	BA	3032	1/1	0.98	0.15	36,36,36,36	0
56	MG	DA	3324	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3724	1/1	0.98	0.11	22,22,22,22	0
56	MG	BA	3413	1/1	0.98	0.05	19,19,19,19	0
56	MG	BQ	3003	1/1	0.98	0.07	15,15,15,15	0
56	MG	BA	3592	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3727	1/1	0.98	0.10	27,27,27,27	0
56	MG	BR	202	1/1	0.98	0.09	25,25,25,25	0
56	MG	BA	3416	1/1	0.98	0.08	25,25,25,25	0
56	MG	DA	3332	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3418	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3077	1/1	0.98	0.03	20,20,20,20	0
56	MG	BU	203	1/1	0.98	0.10	26,26,26,26	0
56	MG	DA	3605	1/1	0.98	0.04	58,58,58,58	0
56	MG	BU	204	1/1	0.98	0.10	49,49,49,49	0
56	MG	BU	205	1/1	0.98	0.09	39,39,39,39	0
56	MG	BU	206	1/1	0.98	0.15	41,41,41,41	0
56	MG	DA	3341	1/1	0.98	0.03	40,40,40,40	0
56	MG	DA	3136	1/1	0.98	0.05	39,39,39,39	0
56	MG	DA	3343	1/1	0.98	0.07	37,37,37,37	0
56	MG	DA	3474	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3422	1/1	0.98	0.08	23,23,23,23	0
56	MG	DA	3476	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3236	1/1	0.98	0.11	37,37,37,37	0
56	MG	BA	3528	1/1	0.98	0.09	44,44,44,44	0
56	MG	AA	3137	1/1	0.98	0.14	40,40,40,40	0
56	MG	DA	3348	1/1	0.98	0.05	39,39,39,39	0
56	MG	BA	3475	1/1	0.98	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3736	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3352	1/1	0.98	0.06	24,24,24,24	0
56	MG	BA	3378	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3379	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3345	1/1	0.98	0.03	37,37,37,37	0
56	MG	BA	3534	1/1	0.98	0.11	36,36,36,36	0
56	MG	BA	3188	1/1	0.98	0.05	49,49,49,49	0
56	MG	DA	3489	1/1	0.98	0.04	36,36,36,36	0
56	MG	DA	3490	1/1	0.98	0.04	46,46,46,46	0
56	MG	BA	3536	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3320	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3362	1/1	0.98	0.19	42,42,42,42	0
56	MG	BA	3275	1/1	0.98	0.20	28,28,28,28	0
56	MG	BA	3483	1/1	0.98	0.09	18,18,18,18	0
56	MG	BA	3541	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3431	1/1	0.98	0.18	54,54,54,54	0
56	MG	BA	3432	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3368	1/1	0.98	0.06	34,34,34,34	0
56	MG	BA	3323	1/1	0.98	0.06	25,25,25,25	0
56	MG	BB	3010	1/1	0.98	0.10	44,44,44,44	0
56	MG	BA	3679	1/1	0.98	0.05	39,39,39,39	0
56	MG	DA	3643	1/1	0.98	0.13	18,18,18,18	0
56	MG	BB	3012	1/1	0.98	0.08	42,42,42,42	0
56	MG	DA	3253	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3375	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3351	1/1	0.98	0.10	21,21,21,21	0
56	MG	BA	3079	1/1	0.98	0.10	50,50,50,50	0
56	MG	DA	3510	1/1	0.98	0.05	67,67,67,67	0
56	MG	BA	3353	1/1	0.98	0.11	31,31,31,31	0
56	MG	DA	3512	1/1	0.98	0.08	37,37,37,37	0
56	MG	B5	502	1/1	0.98	0.05	56,56,56,56	0
56	MG	BA	3491	1/1	0.98	0.08	38,38,38,38	0
56	MG	DA	3260	1/1	0.98	0.03	32,32,32,32	0
56	MG	DA	3382	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3206	1/1	0.98	0.09	32,32,32,32	0
56	MG	DA	3384	1/1	0.98	0.05	24,24,24,24	0
56	MG	BD	301	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3386	1/1	0.98	0.06	18,18,18,18	0
56	MG	BA	3091	1/1	0.98	0.15	55,55,55,55	0
56	MG	DA	3388	1/1	0.98	0.07	25,25,25,25	0
56	MG	BA	3440	1/1	0.98	0.05	40,40,40,40	0
56	MG	BA	3495	1/1	0.98	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3266	1/1	0.98	0.08	32,32,32,32	0
56	MG	DA	3526	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3442	1/1	0.98	0.12	33,33,33,33	0
56	MG	CA	3082	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3555	1/1	0.98	0.17	31,31,31,31	0
56	MG	BD	307	1/1	0.98	0.05	36,36,36,36	0
56	MG	DA	3082	1/1	0.98	0.04	7,7,7,7	0
56	MG	BA	3176	1/1	0.98	0.10	50,50,50,50	0
56	MG	BA	3062	1/1	0.98	0.28	46,46,46,46	0
56	MG	BA	3626	1/1	0.98	0.05	50,50,50,50	0
56	MG	DA	3275	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3445	1/1	0.98	0.10	16,16,16,16	0
56	MG	BA	3063	1/1	0.98	0.08	34,34,34,34	0
56	MG	BA	3393	1/1	0.98	0.07	27,27,27,27	0
56	MG	BA	3127	1/1	0.98	0.12	42,42,42,42	0
56	MG	BA	3228	1/1	0.98	0.05	23,23,23,23	0
56	MG	DE	306	1/1	0.98	0.07	44,44,44,44	0
56	MG	CA	3094	1/1	0.98	0.19	37,37,37,37	0
56	MG	BA	3049	1/1	0.98	0.15	17,17,17,17	0
56	MG	DA	3411	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	3412	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3564	1/1	0.98	0.09	26,26,26,26	0
56	MG	BA	3397	1/1	0.98	0.04	44,44,44,44	0
56	MG	DA	3415	1/1	0.98	0.04	22,22,22,22	0
56	MG	DO	5001	1/1	0.98	0.05	33,33,33,33	0
56	MG	CA	3098	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3398	1/1	0.98	0.07	36,36,36,36	0
56	MG	BA	3399	1/1	0.98	0.09	22,22,22,22	0
56	MG	CA	3101	1/1	0.98	0.07	58,58,58,58	0
56	MG	DA	3420	1/1	0.98	0.04	43,43,43,43	0
56	MG	CA	3102	1/1	0.98	0.04	55,55,55,55	0
56	MG	DA	3191	1/1	0.98	0.07	31,31,31,31	0
56	MG	DA	3291	1/1	0.98	0.11	42,42,42,42	0
56	MG	BA	3363	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3153	1/1	0.98	0.08	47,47,47,47	0
56	MG	BA	3639	1/1	0.98	0.05	35,35,35,35	0
56	MG	DA	3560	1/1	0.98	0.05	57,57,57,57	0
56	MG	DA	3427	1/1	0.98	0.04	29,29,29,29	0
56	MG	BA	3365	1/1	0.98	0.05	63,63,63,63	0
56	MG	AA	3156	1/1	0.98	0.07	31,31,31,31	0
56	MG	DA	3564	1/1	0.98	0.03	29,29,29,29	0
56	MG	BG	3001	1/1	0.98	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3574	1/1	0.98	0.05	52,52,52,52	0
56	MG	BA	3287	1/1	0.98	0.07	11,11,11,11	0
57	SF4	CD	501	8/8	0.98	0.03	63,76,87,96	0
56	MG	AA	3040	1/1	0.98	0.05	46,46,46,46	0
58	ZN	CN	501	1/1	0.98	0.04	104,104,104,104	0
58	ZN	DY	501	1/1	0.98	0.04	90,90,90,90	0
56	MG	BA	3579	1/1	0.98	0.12	21,21,21,21	0
56	MG	DA	3303	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3370	1/1	0.98	0.03	39,39,39,39	0
56	MG	BA	3515	1/1	0.98	0.12	46,46,46,46	0
56	MG	DA	3307	1/1	0.98	0.08	40,40,40,40	0
56	MG	BA	3572	1/1	0.99	0.09	23,23,23,23	0
56	MG	DA	3650	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3192	1/1	0.99	0.04	48,48,48,48	0
56	MG	BA	3333	1/1	0.99	0.10	27,27,27,27	0
56	MG	BA	3575	1/1	0.99	0.07	26,26,26,26	0
56	MG	DA	3337	1/1	0.99	0.08	50,50,50,50	0
56	MG	DA	3396	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3537	1/1	0.99	0.07	45,45,45,45	0
56	MG	CA	3083	1/1	0.99	0.05	30,30,30,30	0
56	MG	DA	3340	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3045	1/1	0.99	0.12	49,49,49,49	0
56	MG	DA	3401	1/1	0.99	0.11	41,41,41,41	0
56	MG	BA	3437	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3578	1/1	0.99	0.09	47,47,47,47	0
56	MG	BA	3410	1/1	0.99	0.05	21,21,21,21	0
56	MG	BA	3411	1/1	0.99	0.09	21,21,21,21	0
56	MG	BA	3080	1/1	0.99	0.03	12,12,12,12	0
56	MG	DA	3293	1/1	0.99	0.04	34,34,34,34	0
56	MG	BA	3441	1/1	0.99	0.09	29,29,29,29	0
56	MG	DA	3349	1/1	0.99	0.04	27,27,27,27	0
56	MG	AA	3157	1/1	0.99	0.03	26,26,26,26	0
56	MG	BA	3414	1/1	0.99	0.12	51,51,51,51	0
56	MG	BB	3013	1/1	0.99	0.07	31,31,31,31	0
56	MG	BA	3415	1/1	0.99	0.06	28,28,28,28	0
56	MG	BA	3586	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3319	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3547	1/1	0.99	0.10	30,30,30,30	0
56	MG	BA	3417	1/1	0.99	0.07	21,21,21,21	0
56	MG	BA	3306	1/1	0.99	0.05	19,19,19,19	0
56	MG	DA	3359	1/1	0.99	0.07	21,21,21,21	0
56	MG	DA	3360	1/1	0.99	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3304	1/1	0.99	0.04	44,44,44,44	0
56	MG	BA	3448	1/1	0.99	0.10	23,23,23,23	0
56	MG	BA	3374	1/1	0.99	0.11	26,26,26,26	0
56	MG	BA	3420	1/1	0.99	0.10	13,13,13,13	0
56	MG	DA	3257	1/1	0.99	0.08	25,25,25,25	0
56	MG	DA	3616	1/1	0.99	0.04	41,41,41,41	0
56	MG	BA	3421	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3057	1/1	0.99	0.16	36,36,36,36	0
56	MG	DA	3552	1/1	0.99	0.05	42,42,42,42	0
56	MG	BA	3322	1/1	0.99	0.05	46,46,46,46	0
56	MG	BA	3454	1/1	0.99	0.07	20,20,20,20	0
56	MG	DA	3430	1/1	0.99	0.11	75,75,75,75	0
56	MG	BA	3488	1/1	0.99	0.14	43,43,43,43	0
56	MG	BA	3015	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3372	1/1	0.99	0.03	37,37,37,37	0
56	MG	BA	3523	1/1	0.99	0.09	32,32,32,32	0
56	MG	AA	3145	1/1	0.99	0.10	63,63,63,63	0
56	MG	BE	301	1/1	0.99	0.14	28,28,28,28	0
56	MG	BA	3684	1/1	0.99	0.12	44,44,44,44	0
56	MG	BE	303	1/1	0.99	0.04	39,39,39,39	0
56	MG	AA	3220	1/1	0.99	0.06	42,42,42,42	0
56	MG	AA	3152	1/1	0.99	0.07	29,29,29,29	0
56	MG	DA	3633	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3159	1/1	0.99	0.10	47,47,47,47	0
56	MG	BA	3362	1/1	0.99	0.05	23,23,23,23	0
56	MG	AA	3163	1/1	0.99	0.10	23,23,23,23	0
56	MG	DA	3505	1/1	0.99	0.06	24,24,24,24	0
56	MG	BA	3314	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3691	1/1	0.99	0.10	40,40,40,40	0
57	SF4	AD	501	8/8	0.99	0.04	62,75,82,88	0
56	MG	DA	3572	1/1	0.99	0.05	39,39,39,39	0
58	ZN	AN	102	1/1	0.99	0.02	88,88,88,88	0
58	ZN	BY	501	1/1	0.99	0.03	67,67,67,67	0
56	MG	DA	3573	1/1	0.99	0.10	32,32,32,32	0
58	ZN	B5	501	1/1	0.99	0.02	49,49,49,49	0
56	MG	DA	3508	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3463	1/1	0.99	0.05	32,32,32,32	0
56	MG	AA	3192	1/1	0.99	0.08	73,73,73,73	0
58	ZN	D5	103	1/1	0.99	0.02	61,61,61,61	0
58	ZN	D6	501	1/1	0.99	0.03	65,65,65,65	0
58	ZN	D9	501	1/1	0.99	0.04	63,63,63,63	0
56	MG	BA	3366	1/1	0.99	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3570	1/1	0.99	0.10	33,33,33,33	0
56	MG	DA	3389	1/1	0.99	0.07	32,32,32,32	0
56	MG	BA	3348	1/1	0.99	0.06	29,29,29,29	0
58	ZN	B6	501	1/1	1.00	0.03	51,51,51,51	0
58	ZN	B9	501	1/1	1.00	0.02	49,49,49,49	0
56	MG	BA	3327	1/1	1.00	0.05	21,21,21,21	0
56	MG	BA	3480	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3321	1/1	1.00	0.03	31,31,31,31	0
56	MG	BX	101	1/1	1.00	0.04	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.