



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 12:25 PM EDT

PDB ID : 4W2F
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

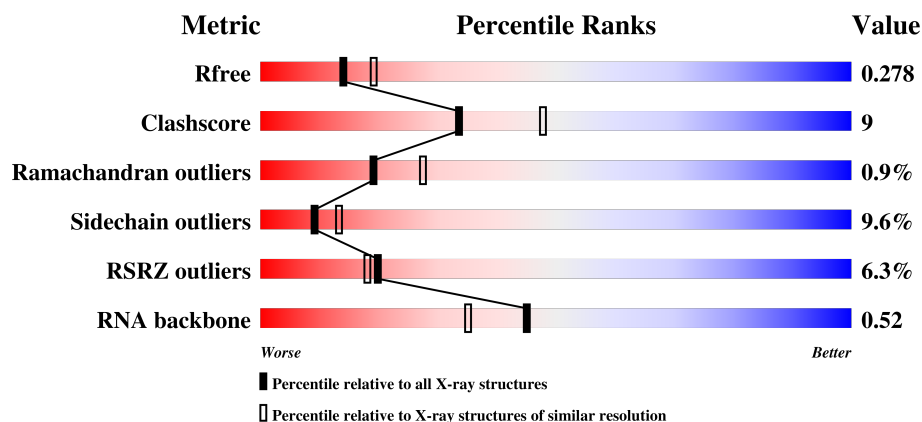
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)
RNA backbone	2636	1023 (2.80-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1521	
1	CA	1521	
2	AB	256	
2	CB	256	

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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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	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	

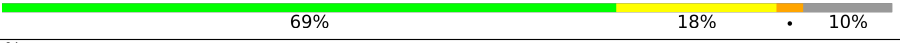










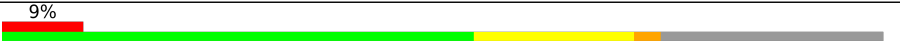
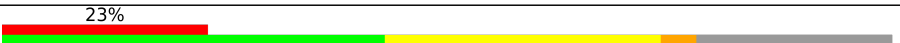



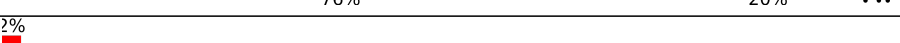
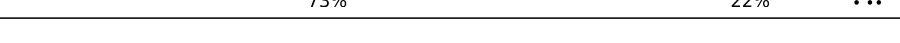



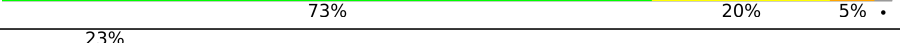

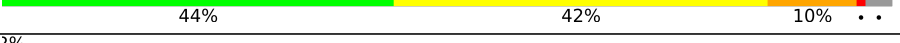

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	

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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298643 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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5967	10397	1497			
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
			1548	973	301	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
			1655	1038	326	284	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
			810	514	144	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	C	N	O			
			714	445	138	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	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2871	Total	C	N	O	P	0	0	0
			61844	27523	11572	19878	2871			
25	DA	2800	Total	C	N	O	P	0	0	0
			60314	26840	11284	19390	2800			

- 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
			2577	1146	476	835	120			
26	DB	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			1429	916	256	253	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1097	701	191	204	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			873	550	174	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			
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	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
45	DZ	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			552	349	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	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
			517	331	102	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CR	1	Total	Mg	0	0
			1	1		
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	906	Total	Mg	0	0
			906	906		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	AB	2	Total	Mg	0	0
			2	2		
56	DF	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CV	1	Total 1	Mg 1	0	0
56	B8	3	Total 3	Mg 3	0	0
56	BE	12	Total 12	Mg 12	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	4	Total 4	Mg 4	0	0
56	B1	2	Total 2	Mg 2	0	0
56	DY	1	Total 1	Mg 1	0	0
56	AN	1	Total 1	Mg 1	0	0
56	BP	6	Total 6	Mg 6	0	0
56	AX	13	Total 13	Mg 13	0	0
56	DR	1	Total 1	Mg 1	0	0
56	BI	1	Total 1	Mg 1	0	0
56	CA	201	Total 201	Mg 201	0	0
56	B5	4	Total 4	Mg 4	0	0
56	BB	30	Total 30	Mg 30	0	0
56	BT	2	Total 2	Mg 2	0	0
56	D8	2	Total 2	Mg 2	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DB	21	Total 21	Mg 21	0	0
56	CF	2	Total 2	Mg 2	0	0
56	DT	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B9	1	Total 1	Mg 1	0	0
56	BF	15	Total 15	Mg 15	0	0
56	BX	6	Total 6	Mg 6	0	0
56	B2	2	Total 2	Mg 2	0	0
56	AA	233	Total 233	Mg 233	0	0
56	BQ	7	Total 7	Mg 7	0	0
56	CQ	2	Total 2	Mg 2	0	0
56	D0	1	Total 1	Mg 1	0	0
56	AR	1	Total 1	Mg 1	0	0
56	DV	2	Total 2	Mg 2	0	0
56	B6	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	10	Total 10	Mg 10	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	4	Total 4	Mg 4	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CG	1	Total 1	Mg 1	0	0
56	BG	6	Total 6	Mg 6	0	0
56	BY	3	Total 3	Mg 3	0	0
56	DE	7	Total 7	Mg 7	0	0
56	B3	2	Total 2	Mg 2	0	0

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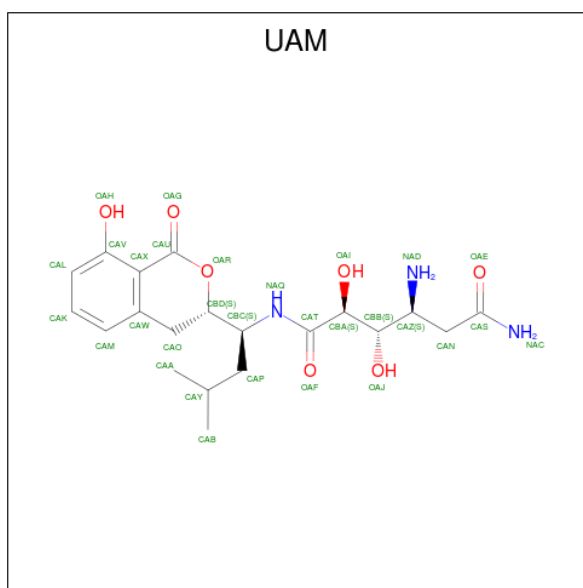
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CJ	2	Total 2	Mg 2	0	0
56	BR	3	Total 3	Mg 3	0	0
56	CP	1	Total 1	Mg 1	0	0
56	DA	673	Total 673	Mg 673	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DW	3	Total 3	Mg 3	0	0
56	D5	2	Total 2	Mg 2	0	0
56	B7	3	Total 3	Mg 3	0	0
56	AL	1	Total 1	Mg 1	0	0
56	BV	5	Total 5	Mg 5	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	5	Total 5	Mg 5	0	0
56	CX	6	Total 6	Mg 6	0	0
56	D1	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	AH	1	Total 1	Mg 1	0	0
56	BZ	3	Total 3	Mg 3	0	0
56	DZ	1	Total 1	Mg 1	0	0
56	BS	3	Total 3	Mg 3	0	0
56	CW	4	Total 4	Mg 4	0	0
56	DG	1	Total 1	Mg 1	0	0

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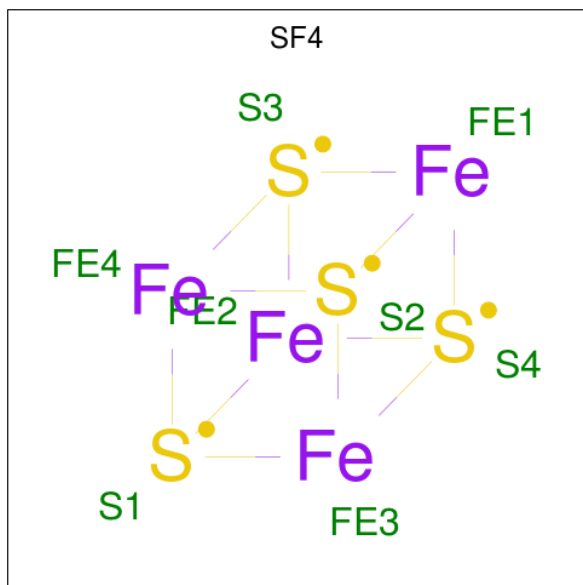
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CD	2	Total 2	Mg 2	0	0
56	BD	13	Total 13	Mg 13	0	0
56	AT	1	Total 1	Mg 1	0	0
56	CL	2	Total 2	Mg 2	0	0
56	B0	7	Total 7	Mg 7	0	0
56	CE	1	Total 1	Mg 1	0	0
56	BW	5	Total 5	Mg 5	0	0
56	AY	2	Total 2	Mg 2	0	0
56	DD	6	Total 6	Mg 6	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	BH	1	Total 1	Mg 1	0	0

- Molecule 57 is Amicoumacin A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			30	20	3	7		
57	CA	1	Total	C	N	O	0	0
			30	20	3	7		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D5	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	D6	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	B6	1	Total	Zn	0	0
			1	1		

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	264	Total	O	0	0
			264	264		
61	AB	1	Total	O	0	0
			1	1		
61	AE	2	Total	O	0	0
			2	2		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	4	Total	O	0	0
			4	4		
61	AM	1	Total	O	0	0
			1	1		
61	AQ	1	Total	O	0	0
			1	1		
61	AV	4	Total	O	0	0
			4	4		
61	AW	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AX	11	Total 11	O 11	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1486	Total 1486	O 1486	0	0
61	BB	43	Total 43	O 43	0	0
61	BD	19	Total 19	O 19	0	0
61	BE	20	Total 20	O 20	0	0
61	BF	14	Total 14	O 14	0	0
61	BG	5	Total 5	O 5	0	0
61	BH	1	Total 1	O 1	0	0
61	BI	2	Total 2	O 2	0	0
61	BN	2	Total 2	O 2	0	0
61	BO	7	Total 7	O 7	0	0
61	BP	19	Total 19	O 19	0	0
61	BQ	5	Total 5	O 5	0	0
61	BR	5	Total 5	O 5	0	0
61	BS	5	Total 5	O 5	0	0
61	BT	5	Total 5	O 5	0	0
61	BU	8	Total 8	O 8	0	0
61	BV	6	Total 6	O 6	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BY	3	Total 3	O 3	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	8	Total 8	O 8	0	0
61	B1	3	Total 3	O 3	0	0
61	B2	4	Total 4	O 4	0	0
61	B3	3	Total 3	O 3	0	0
61	B4	1	Total 1	O 1	0	0
61	B5	4	Total 4	O 4	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	4	Total 4	O 4	0	0
61	B8	8	Total 8	O 8	0	0
61	CA	204	Total 204	O 204	0	0
61	CD	1	Total 1	O 1	0	0
61	CG	1	Total 1	O 1	0	0
61	CI	1	Total 1	O 1	0	0
61	CJ	4	Total 4	O 4	0	0
61	CL	4	Total 4	O 4	0	0
61	CO	1	Total 1	O 1	0	0
61	CP	1	Total 1	O 1	0	0
61	CR	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0

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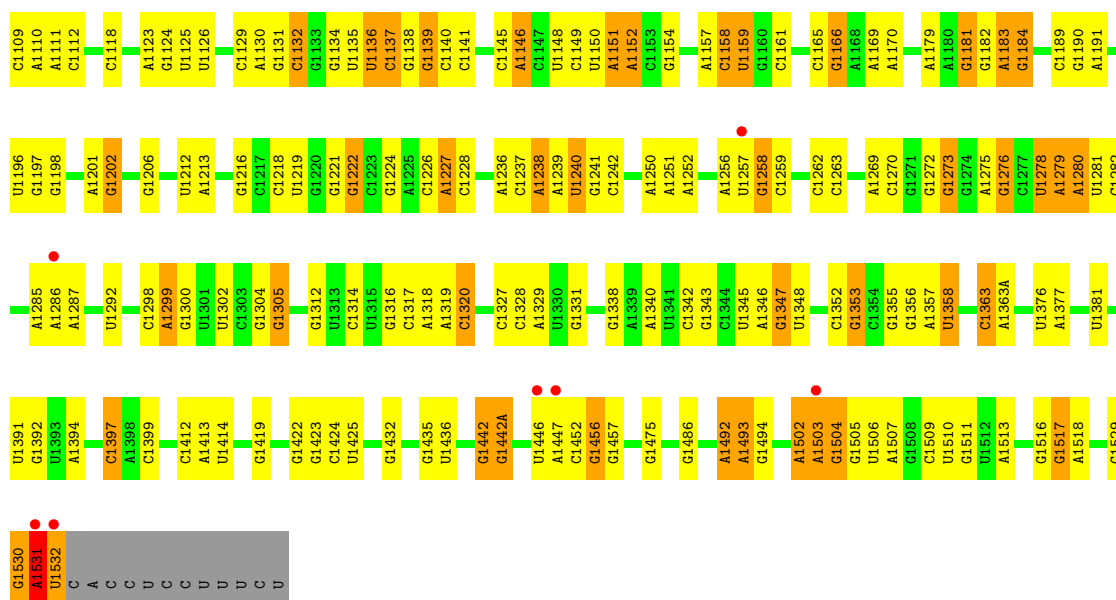
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	2	Total	O	0	0
			2	2		
61	CX	6	Total	O	0	0
			6	6		
61	DA	1039	Total	O	0	0
			1039	1039		
61	DB	10	Total	O	0	0
			10	10		
61	DD	17	Total	O	0	0
			17	17		
61	DE	8	Total	O	0	0
			8	8		
61	DF	6	Total	O	0	0
			6	6		
61	DI	2	Total	O	0	0
			2	2		
61	DN	1	Total	O	0	0
			1	1		
61	DO	3	Total	O	0	0
			3	3		
61	DP	12	Total	O	0	0
			12	12		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	3	Total	O	0	0
			3	3		
61	DT	3	Total	O	0	0
			3	3		
61	DU	1	Total	O	0	0
			1	1		
61	DV	1	Total	O	0	0
			1	1		
61	DW	2	Total	O	0	0
			2	2		
61	DX	2	Total	O	0	0
			2	2		
61	DY	1	Total	O	0	0
			1	1		
61	DZ	2	Total	O	0	0
			2	2		
61	D0	4	Total	O	0	0
			4	4		

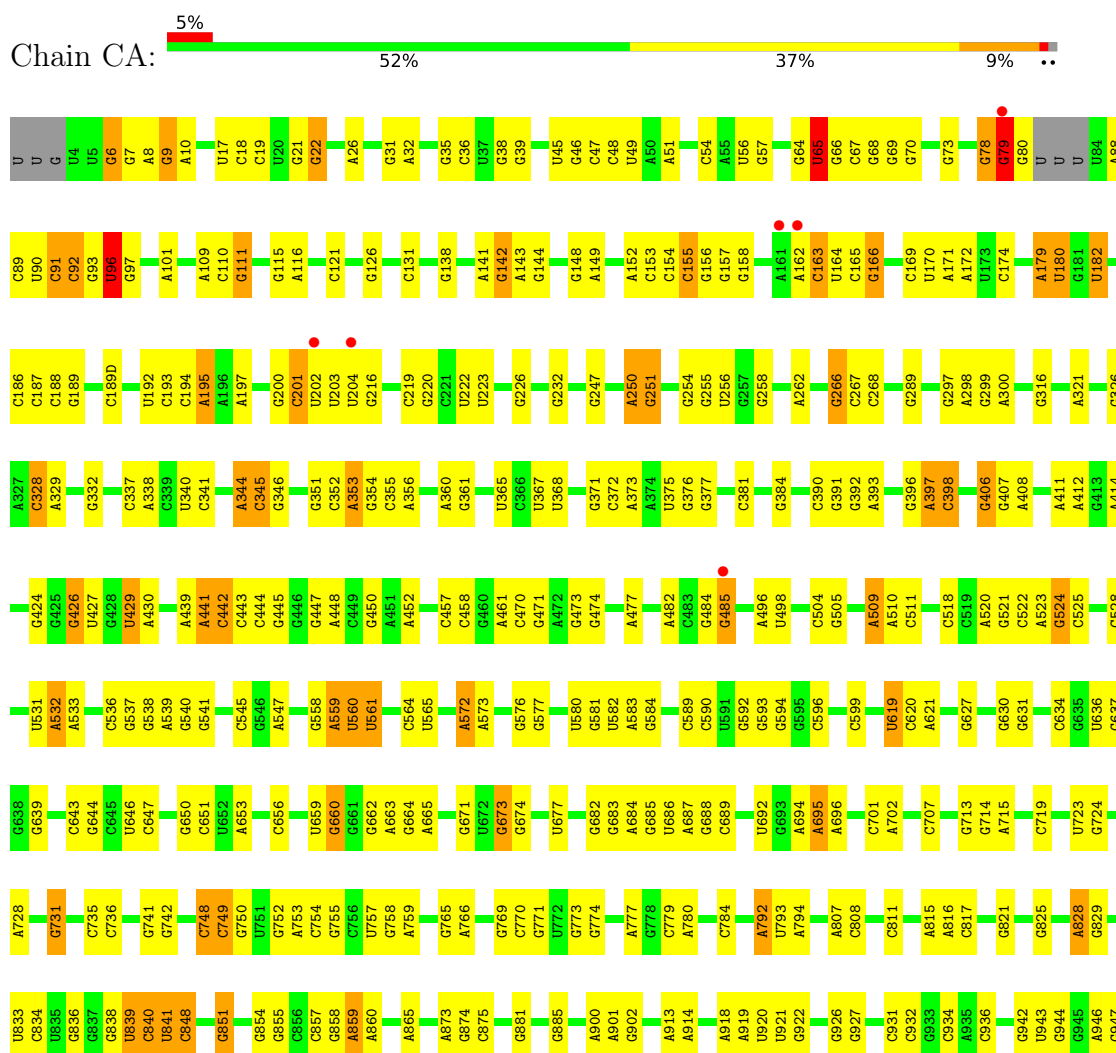
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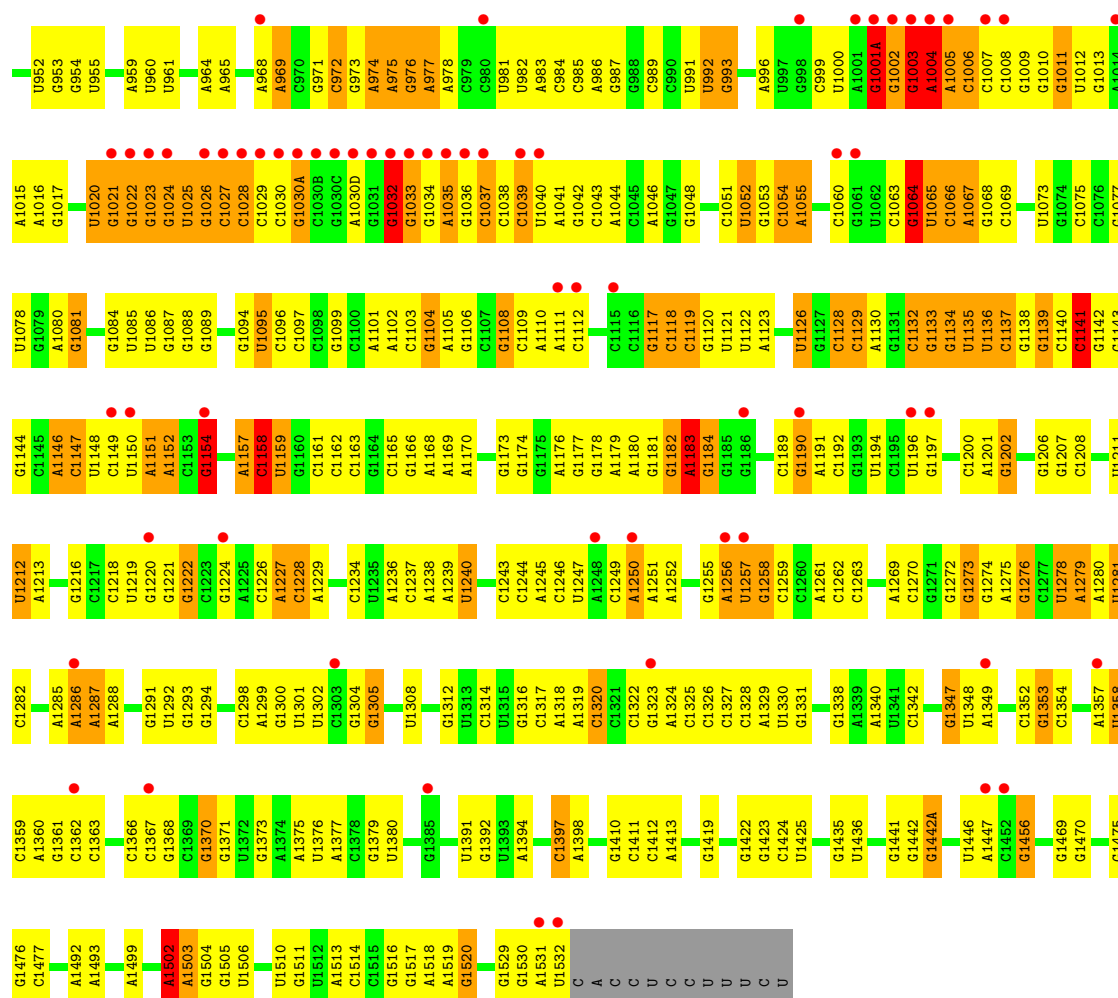
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	D2	1	Total 1	O 1	0	0
61	D3	1	Total 1	O 1	0	0
61	D5	2	Total 2	O 2	0	0
61	D7	5	Total 5	O 5	0	0
61	D8	5	Total 5	O 5	0	0
61	D9	1	Total 1	O 1	0	0

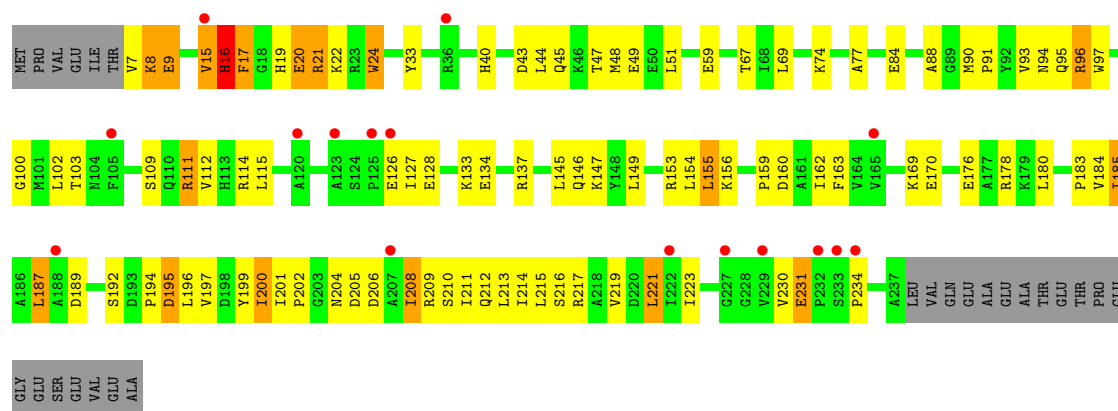


• Molecule 1: 16S Ribosomal RNA



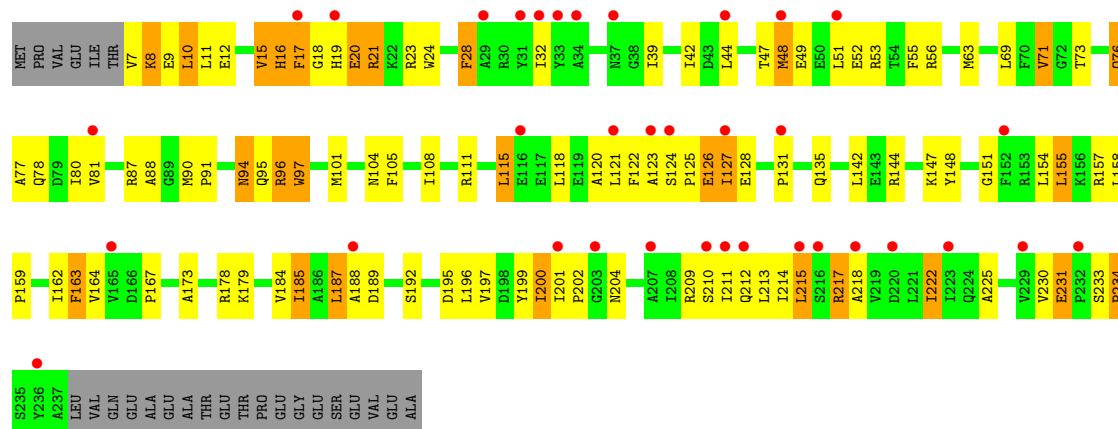


• Molecule 2: 30S Ribosomal Protein S2

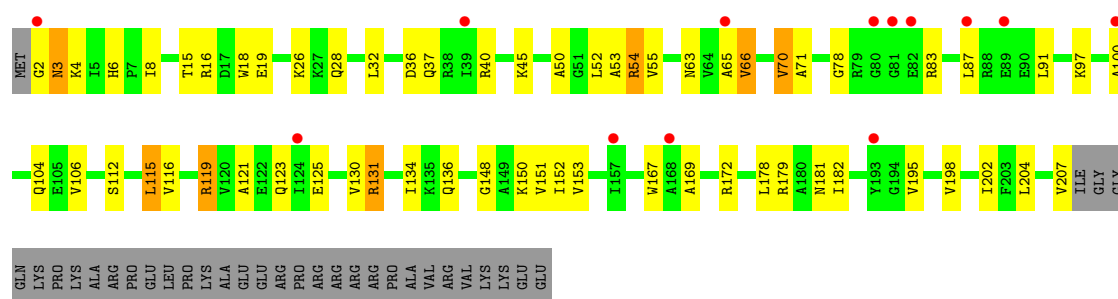


• Molecule 2: 30S Ribosomal Protein S2

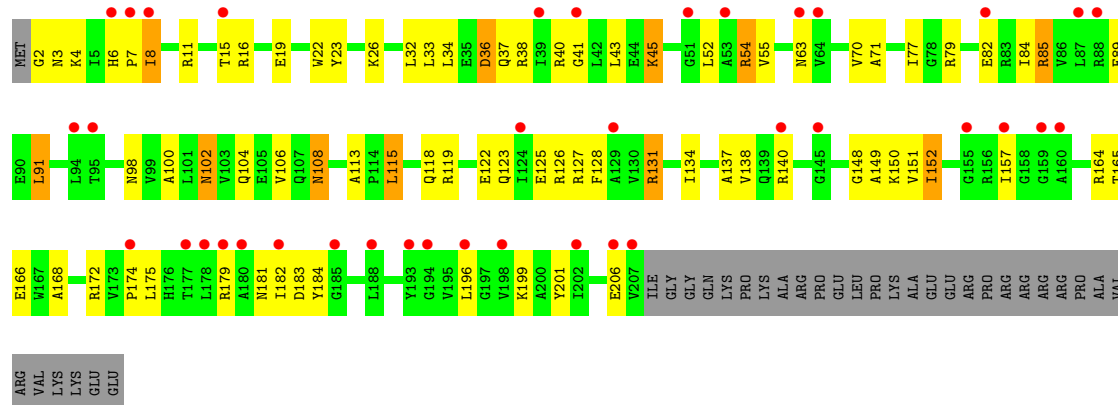




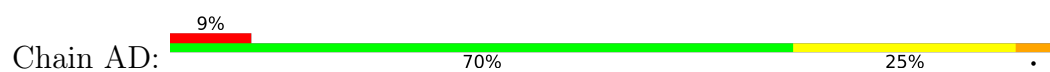
• Molecule 3: 30S Ribosomal Protein S3

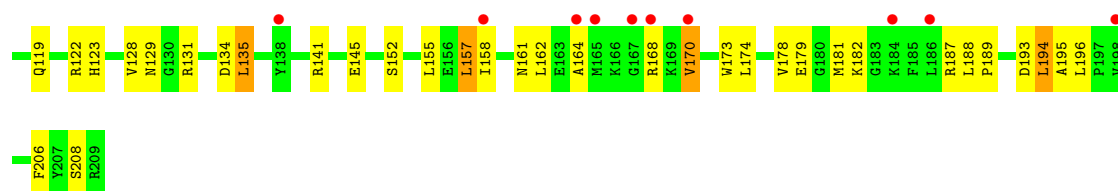


• Molecule 3: 30S Ribosomal Protein S3

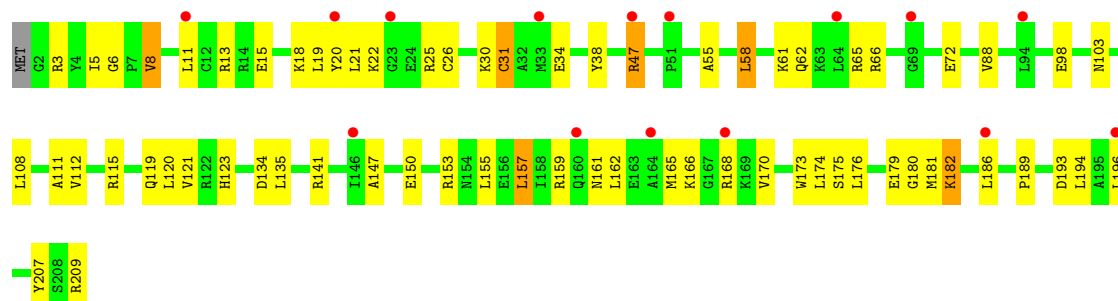


• Molecule 4: 30S Ribosomal Protein S4

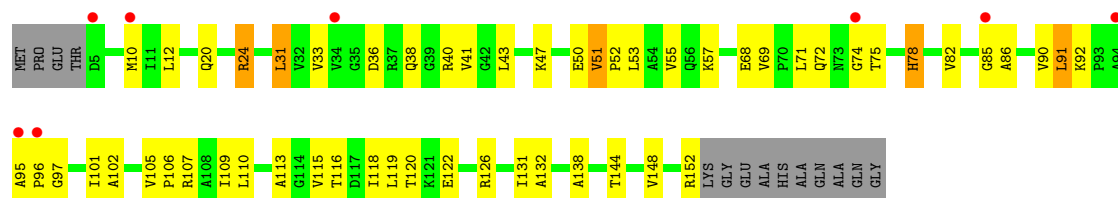




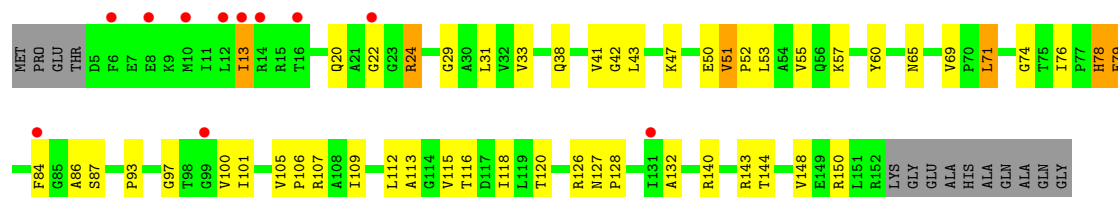
• Molecule 4: 30S Ribosomal Protein S4



• Molecule 5: 30S Ribosomal Protein S5



• Molecule 5: 30S Ribosomal Protein S5



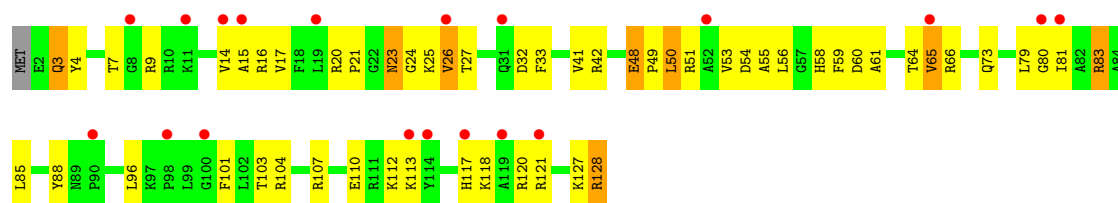
• Molecule 6: 30S Ribosomal Protein S6



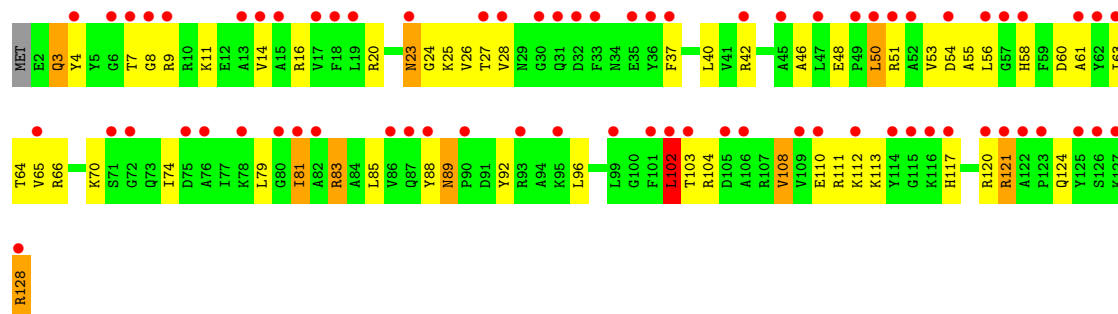
• Molecule 6: 30S Ribosomal Protein S6



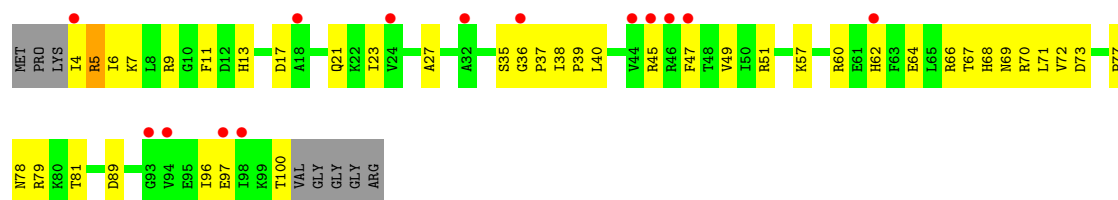




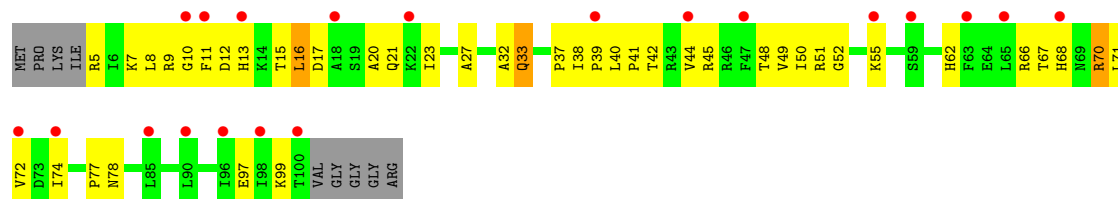
• Molecule 9: 30S Ribosomal Protein S9



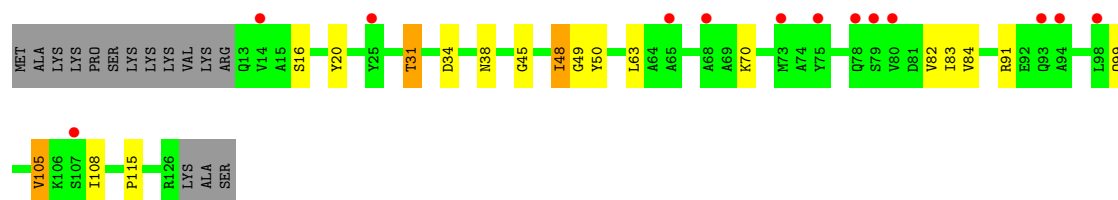
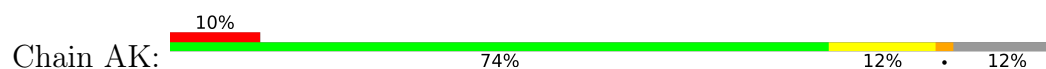
• Molecule 10: 30S Ribosomal Protein S10



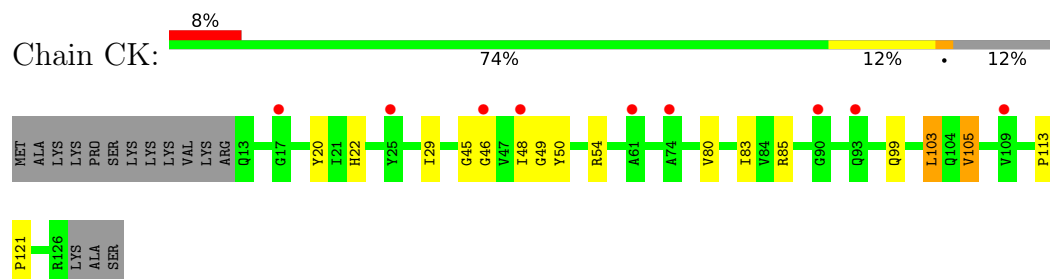
• Molecule 10: 30S Ribosomal Protein S10



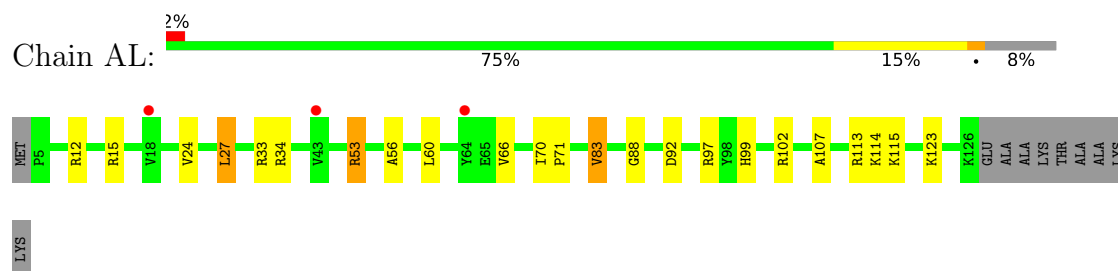
• Molecule 11: 30S Ribosomal Protein S11



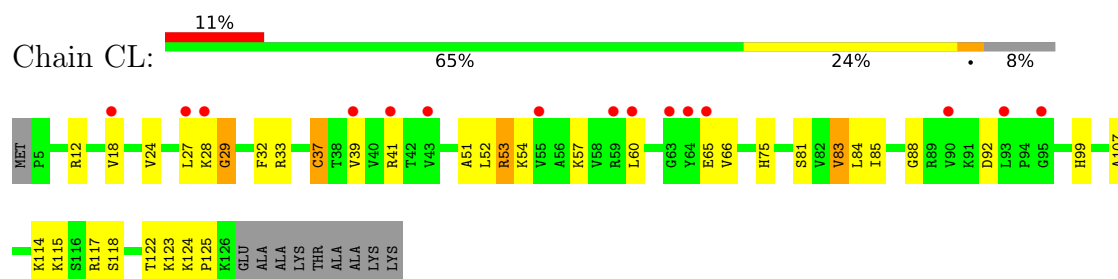
● Molecule 11: 30S Ribosomal Protein S11



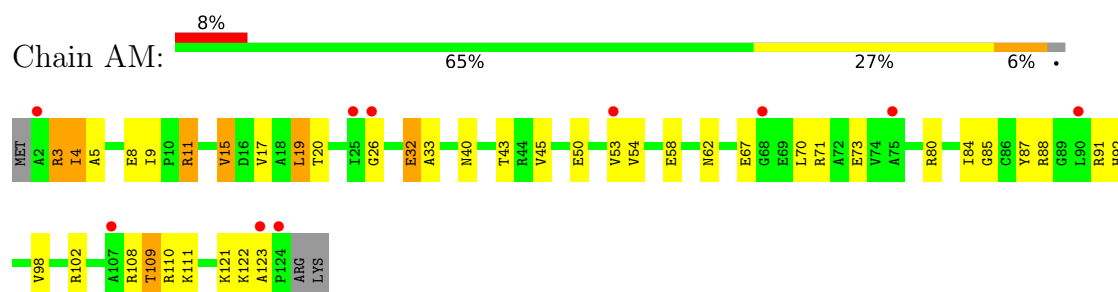
● Molecule 12: 30S Ribosomal Protein S12



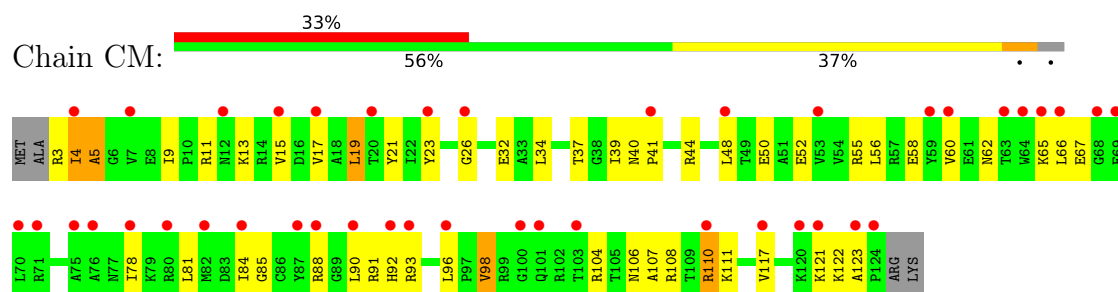
● Molecule 12: 30S Ribosomal Protein S12



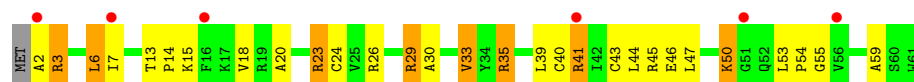
● Molecule 13: 30S Ribosomal Protein S13



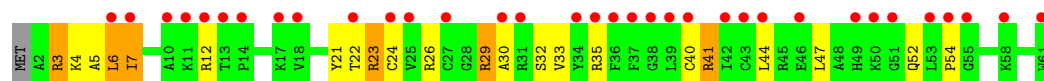
● Molecule 13: 30S Ribosomal Protein S13



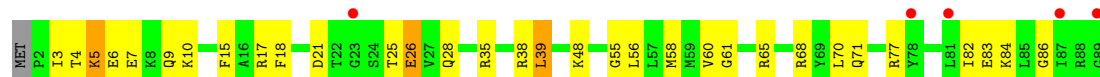
• Molecule 14: 30S Ribosomal Protein S14



• Molecule 14: 30S Ribosomal Protein S14



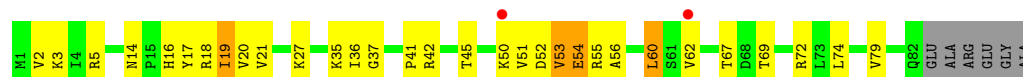
• Molecule 15: 30S Ribosomal Protein S15



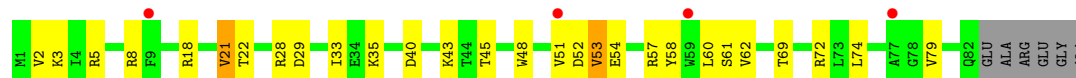
• Molecule 15: 30S Ribosomal Protein S15



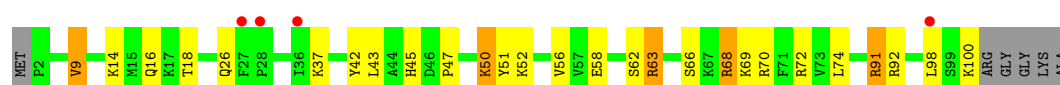
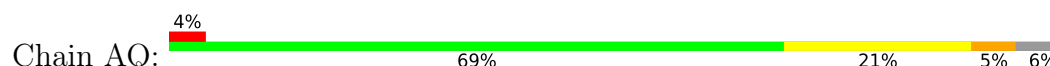
• Molecule 16: 30S Ribosomal Protein S16



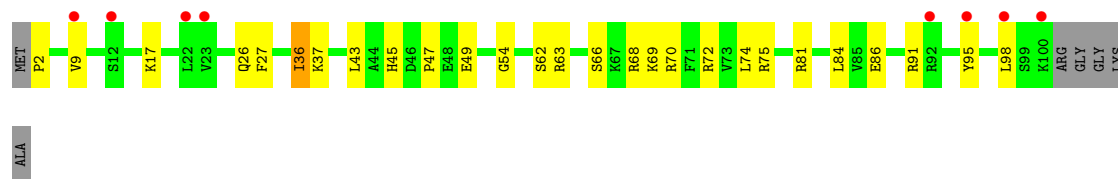
• Molecule 16: 30S Ribosomal Protein S16



• Molecule 17: 30S Ribosomal Protein S17



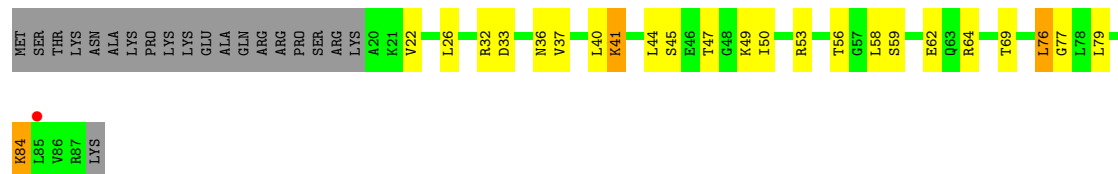
• Molecule 17: 30S Ribosomal Protein S17



• Molecule 18: 30S Ribosomal Protein S18



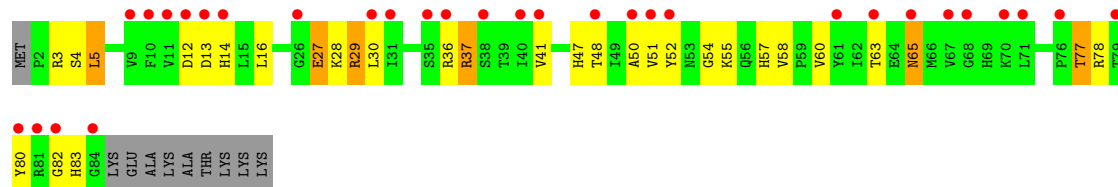
• Molecule 18: 30S Ribosomal Protein S18



• Molecule 19: 30S Ribosomal Protein S19

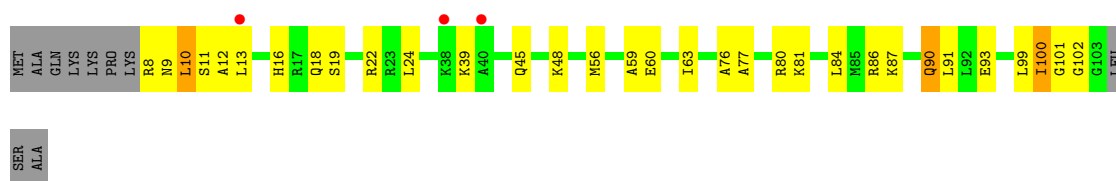


• Molecule 19: 30S Ribosomal Protein S19

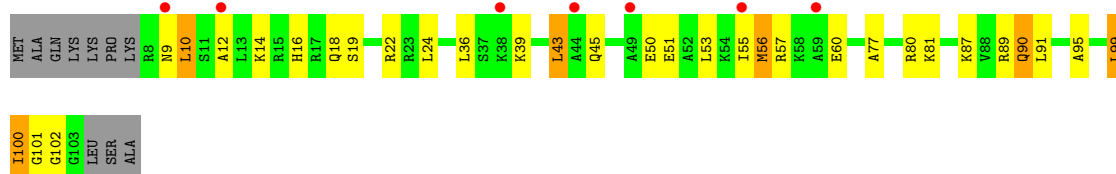


• Molecule 20: 30S Ribosomal Protein S20

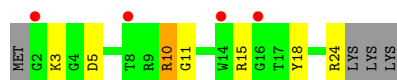




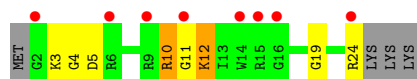
- Molecule 20: 30S Ribosomal Protein S20



- Molecule 21: 30S Ribosomal Protein THX



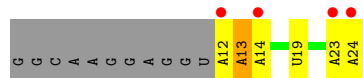
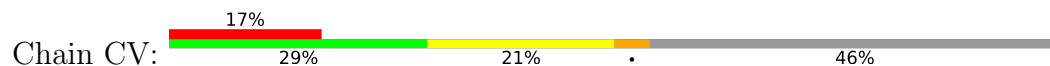
- Molecule 21: 30S Ribosomal Protein THX



- Molecule 22: mRNA



- Molecule 22: mRNA

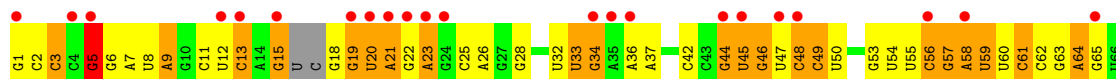
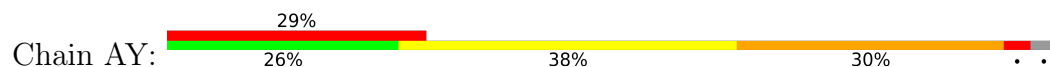


- Molecule 23: A/P-site tRNA

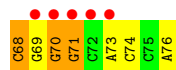
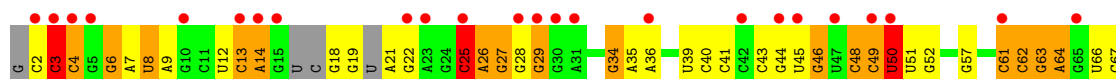




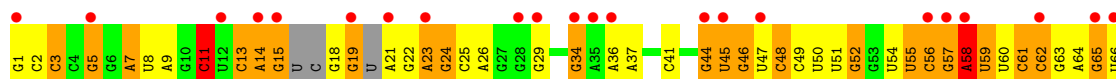
- Molecule 23: A/P-site tRNA



- Molecule 23: A/P-site tRNA



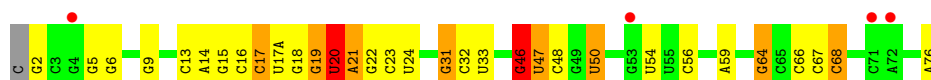
- Molecule 23: A/P-site tRNA



- Molecule 24: E-site tRNA

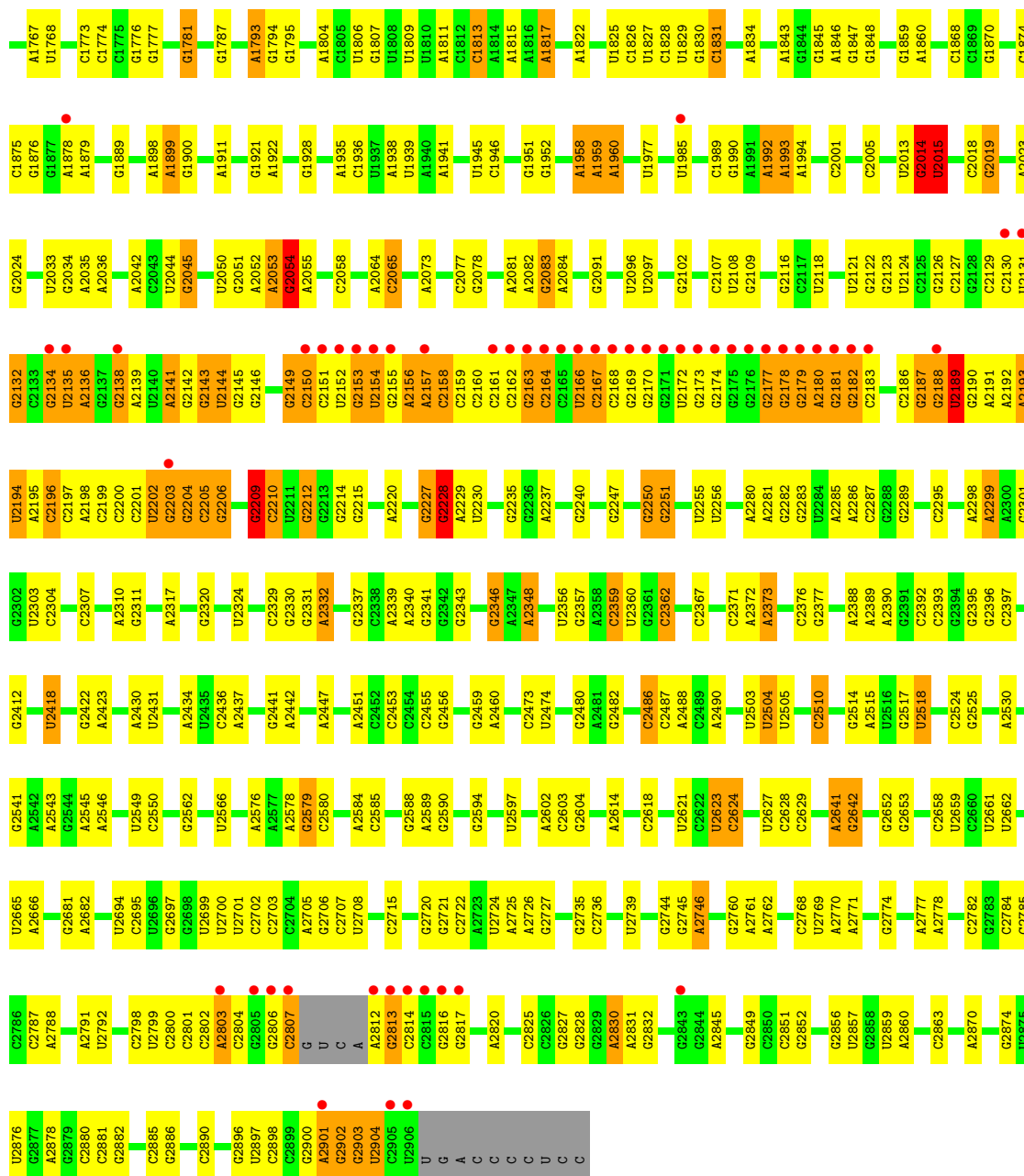


- Molecule 24: E-site tRNA

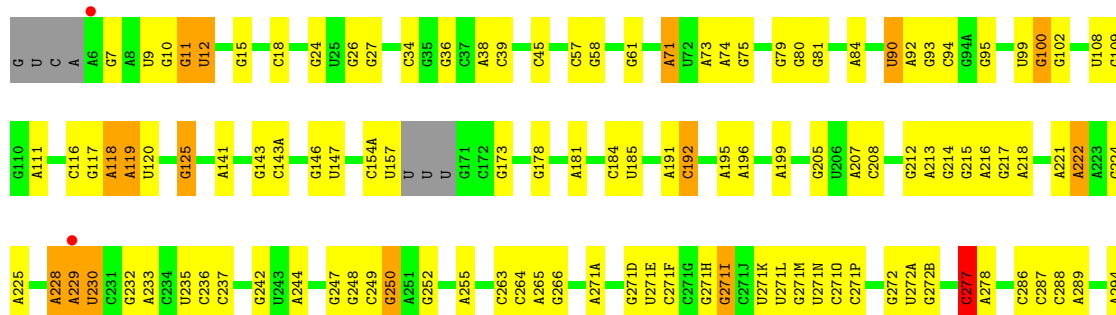


- Molecule 25: 23S Ribosomal RNA





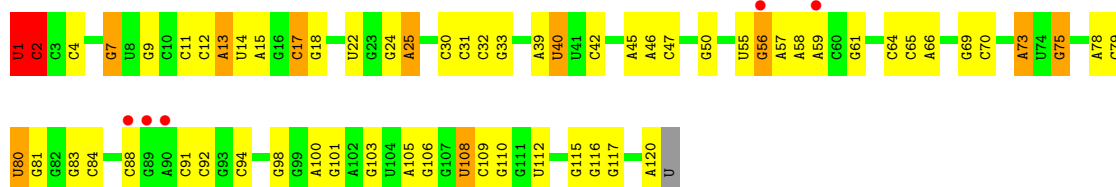
• Molecule 25: 23S Ribosomal RNA





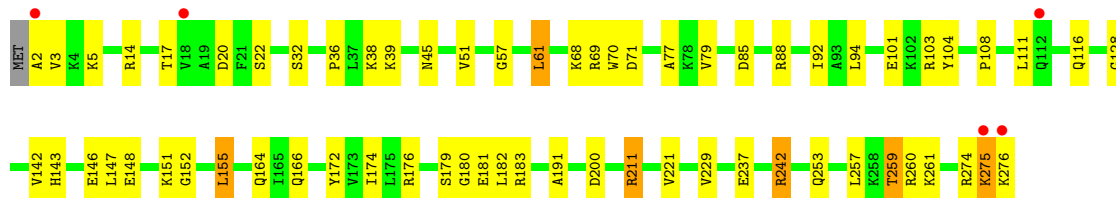


Chain DB:



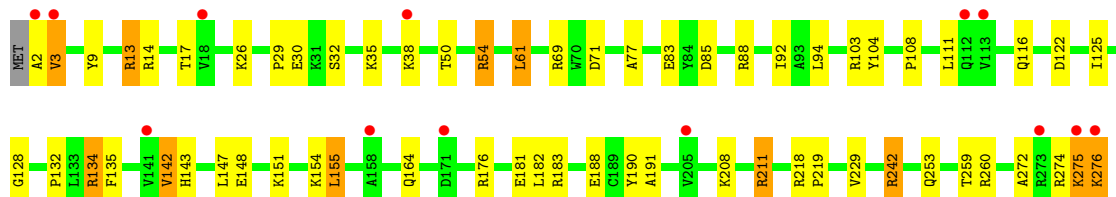
• Molecule 27: 50S Ribosomal Protein L2

Chain BD:



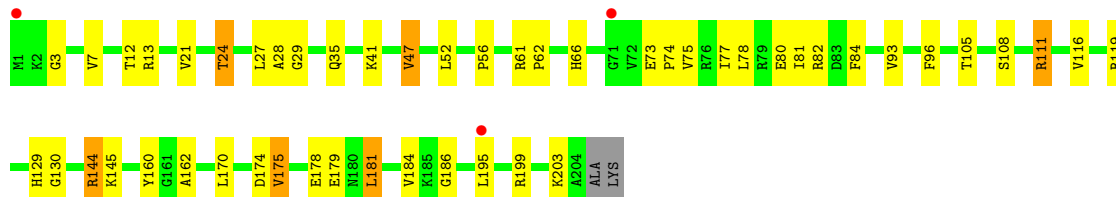
• Molecule 27: 50S Ribosomal Protein L2

Chain DD:



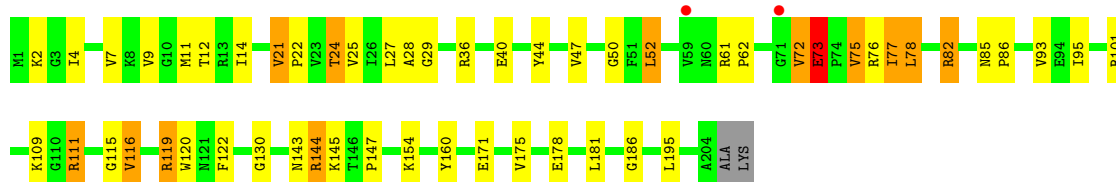
• Molecule 28: 50S Ribosomal Protein L3

Chain BE:

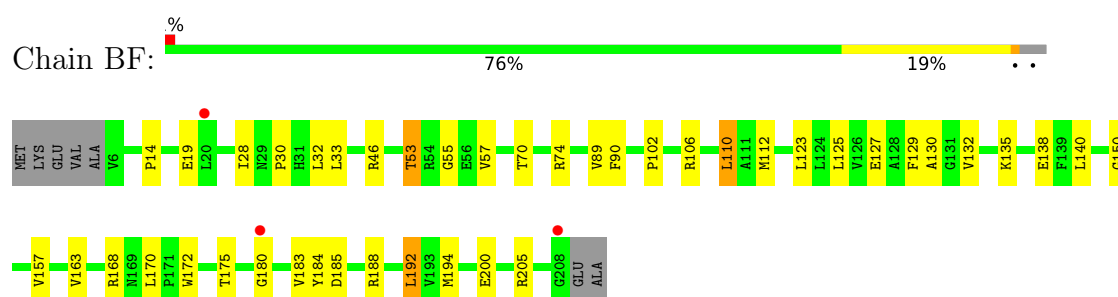


• Molecule 28: 50S Ribosomal Protein L3

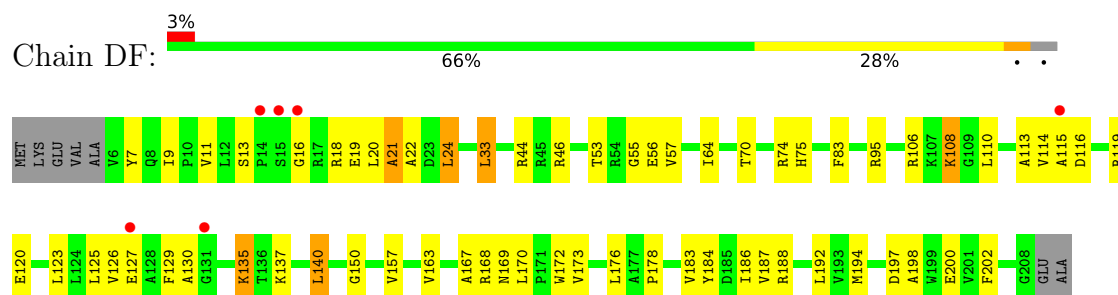
Chain DE:



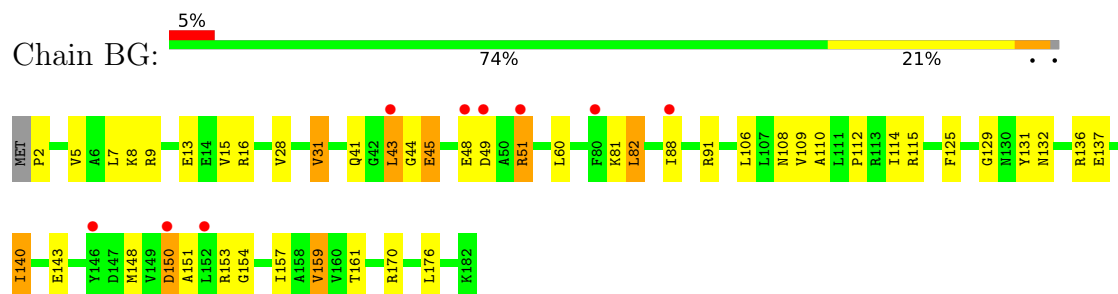
• Molecule 29: 50S Ribosomal Protein L4



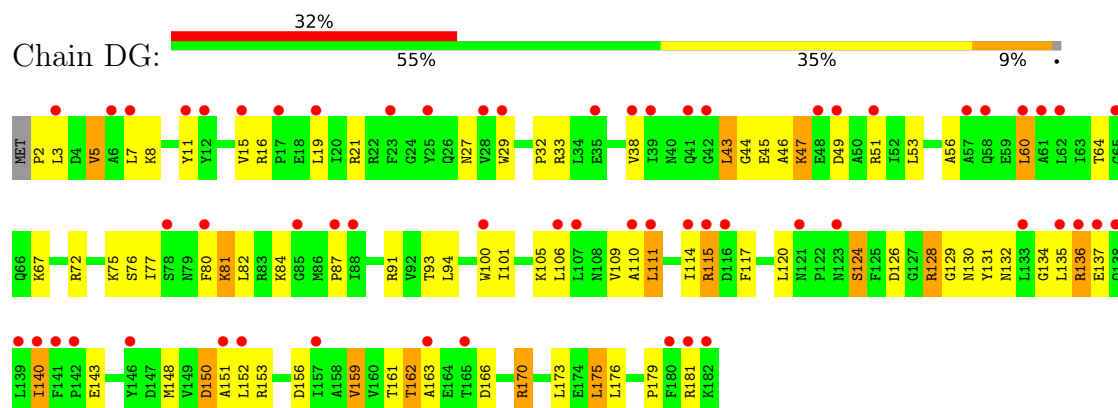
• Molecule 29: 50S Ribosomal Protein L4



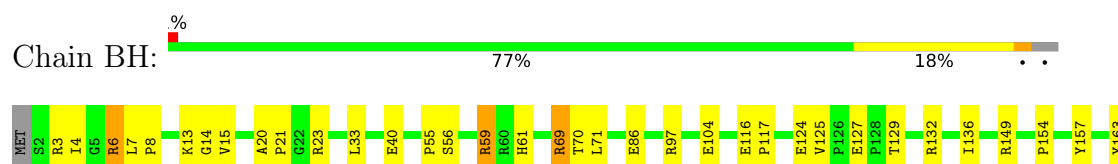
• Molecule 30: 50S Ribosomal Protein L5

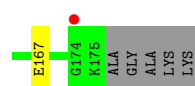


• Molecule 30: 50S Ribosomal Protein L5

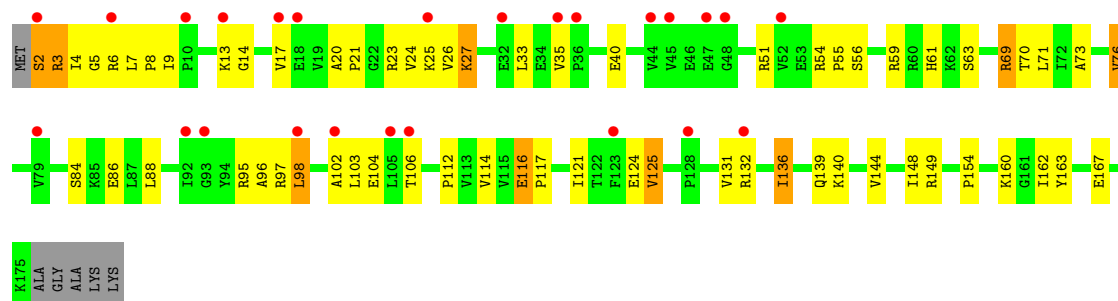


• Molecule 31: 50S Ribosomal Protein L6

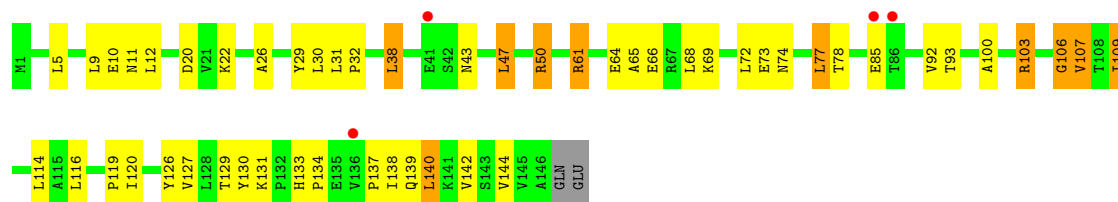




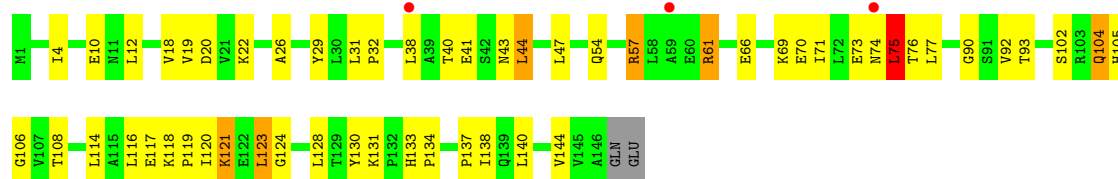
• Molecule 31: 50S Ribosomal Protein L6



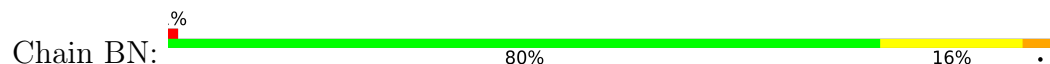
• Molecule 32: 50S Ribosomal Protein L9



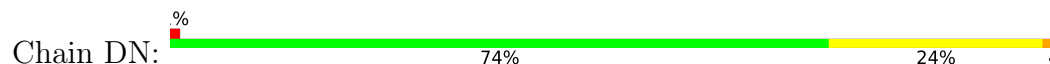
• Molecule 32: 50S Ribosomal Protein L9

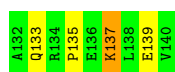


• Molecule 33: 50S Ribosomal Protein L13



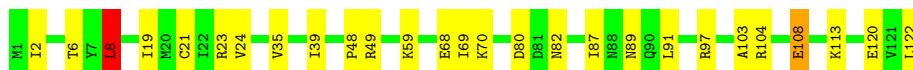
• Molecule 33: 50S Ribosomal Protein L13





• Molecule 34: 50S Ribosomal Protein L14

Chain BO: 78% 20% ..



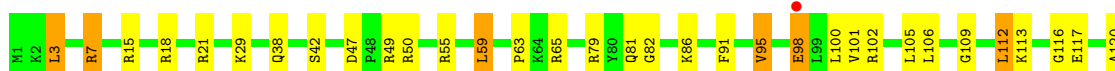
• Molecule 34: 50S Ribosomal Protein L14

Chain DO: 75% 24% .



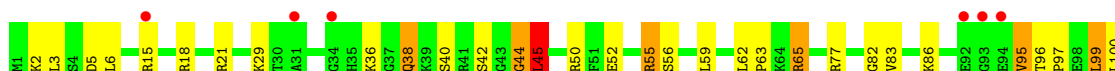
• Molecule 35: 50S Ribosomal Protein L15

Chain BP: % 70% 24% 5% .



• Molecule 35: 50S Ribosomal Protein L15

Chain DP: 5% 67% 27% 5% ..



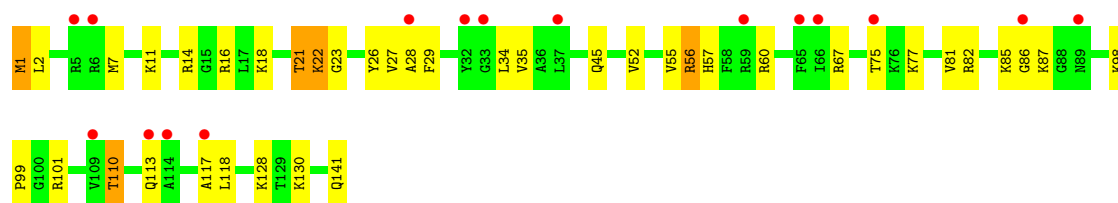
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ: % 75% 23% .



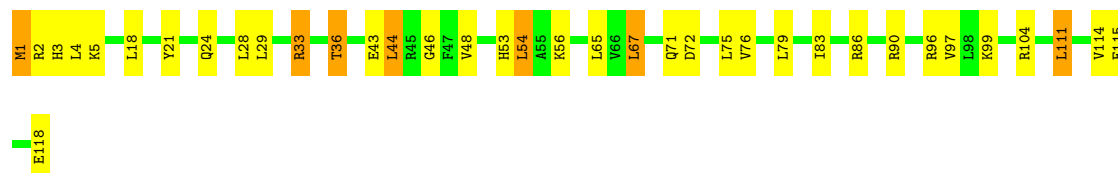
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ: 11% 72% 25% .



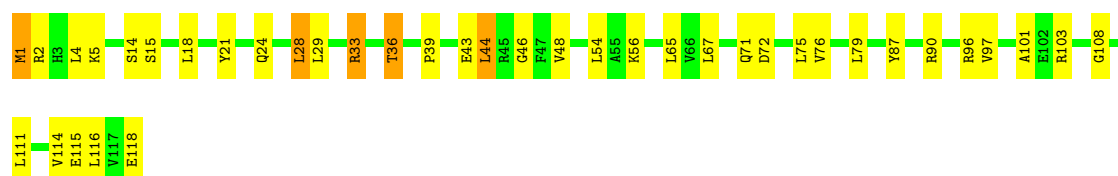
• Molecule 37: 50S Ribosomal Protein L17

Chain BR: 69% 25% 6%



• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 67% 29%



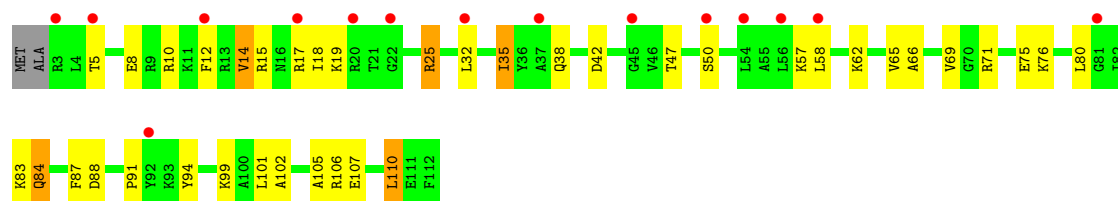
• Molecule 38: 50S Ribosomal Protein L18

Chain BS: 2% 71% 24%



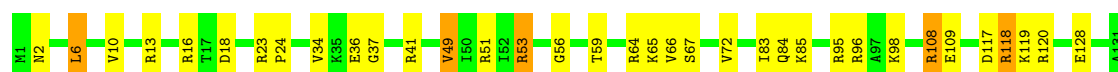
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 13% 63% 30%



• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 66% 21% 10%



LYS
GLU
GLU
ALA
GLN
LYS
ALA
GLN
GLU
PRO
LYS
LYS
ALA
SER
GLN
GLU


• Molecule 39: 50S Ribosomal Protein L19

Chain DT:  69% 18% • 10%

M1 L6 E11 S12 R10 R13 R14 V15 R16 R17 T17 D18 R23 P24 V28 R41 V49 T50 R51 T52 R53 G56 T59 T62 T68 L78 L86 R91 R95 R96 A97 K98 K113 D117 R118 R119 R120 I121 A131 LYS GLU GLU ALA GLN LYS


ALA
GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

• Molecule 40: 50S Ribosomal Protein L20

Chain BU:  % 77% 17% • •


MET P2 V8 V9 R10 R11 R12 I17 F32 R36 L39 G43 R50 R53 R54 R55 R58 R59 L60 W61 L74 W75 Y76 I80 I86 E89 R92 R95 V100 Q104 E108 R112 A116 Q117 GLY

• Molecule 40: 50S Ribosomal Protein L20

Chain DU:  % 74% 23% • •

MET P2 R3 K15 K19 L27 S31 R36 H49 R52 R53 K54 R55 R58 W61 L74 Y76 F79 L83 R84 K85 A86 G87 I88 E89 R92 K93 V100 R101 Q104 V105 F106 A107 E108 L109 R112 A116 Q117 GLY

• Molecule 41: 50S Ribosomal Protein L21

Chain BV:  76% 19% 5%


M1 K10 L18 K19 E23 L40 E43 V46 T49 P50 V51 V52 A55 L62 V72 K76 A77 K78 V79 P80 Y81 K85 Q89 P90 L95 R100 G101

• Molecule 41: 50S Ribosomal Protein L21

Chain DV:  5% 68% 27% 5%


M1 T4 V5 K6 V14 E15 R21 L25 G30 A31 V37 L38 L39 L40 E43 V46 V47 G48 T49 P50 V51 V52 E60 V61 L62 L71 L72 W76 K79 Q80 Y81 K84 K85 Q89 P90 Y91 L95 I96 K97 E98 T99 R100 G101

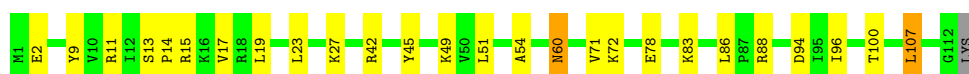
• Molecule 42: 50S Ribosomal Protein L22

Chain BW:  % 82% 16% • •

M1 E2 R11 I12 S13 P14 R15 R16 V17 R18 L19 R25 R42 L51 R68 K72 A73 A74 Y75 E78 R92 T104 L107 G112 LYS

• Molecule 42: 50S Ribosomal Protein L22

Chain DW:  76% 21% • •



• Molecule 43: 50S Ribosomal Protein L23

Chain BX: 79% 19% ..



• Molecule 43: 50S Ribosomal Protein L23

Chain DX: 5% 72% 26% ..



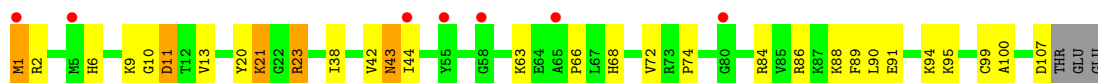
• Molecule 44: 50S Ribosomal Protein L24

Chain BY: 2% 65% 31% ..



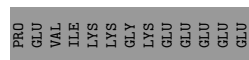
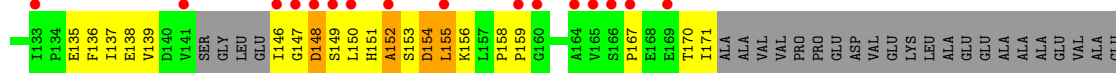
• Molecule 44: 50S Ribosomal Protein L24

Chain DY: 6% 70% 23% 5% .



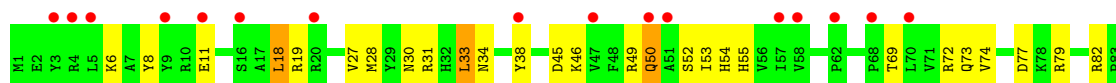
• Molecule 45: 50S Ribosomal Protein L25

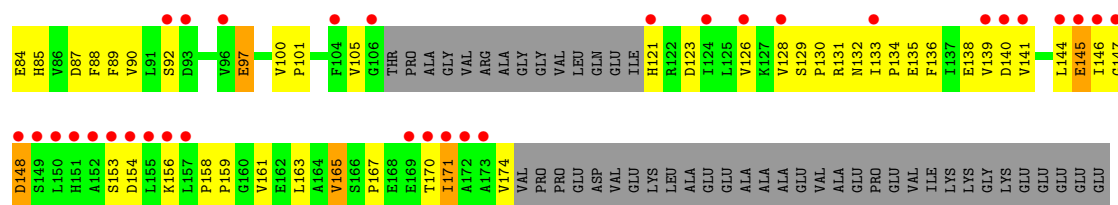
Chain BZ: 9% 53% 18% 25%



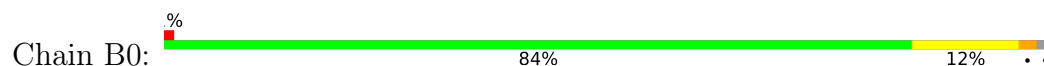
• Molecule 45: 50S Ribosomal Protein L25

Chain DZ: 23% 43% 31% 22%

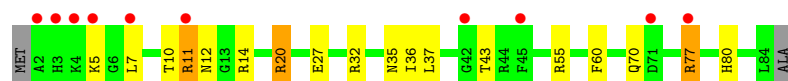
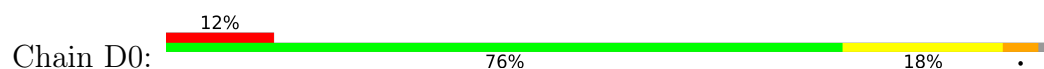




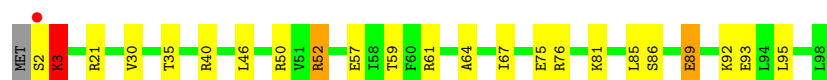
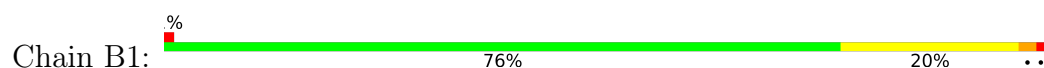
• Molecule 46: 50S Ribosomal Protein L27



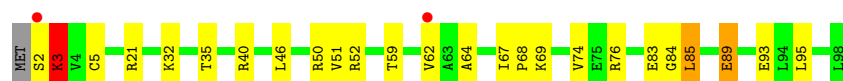
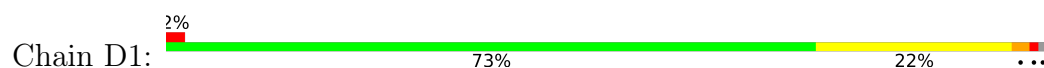
• Molecule 46: 50S Ribosomal Protein L27



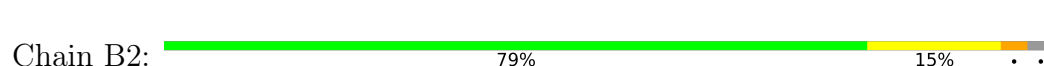
• Molecule 47: 50S Ribosomal Protein L28



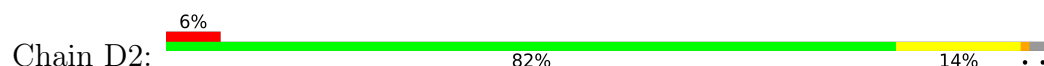
• Molecule 47: 50S Ribosomal Protein L28




• Molecule 48: 50S Ribosomal Protein L29



• Molecule 48: 50S Ribosomal Protein L29




• Molecule 49: 50S Ribosomal Protein L30

Chain B3:  80% 18% .



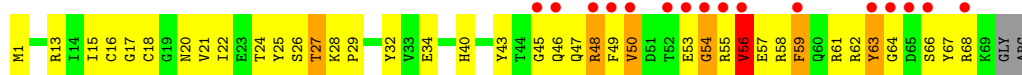
- Molecule 49: 50S Ribosomal Protein L30

Chain D3:  8% 73% 20% 5% .



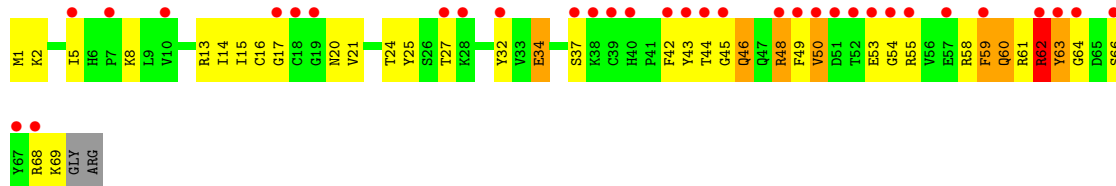
- Molecule 50: 50S Ribosomal Protein L31

Chain B4:  23% 42% 45% 8% . .




- Molecule 50: 50S Ribosomal Protein L31

Chain D4:  46% 44% 42% 10% . .




- Molecule 51: 50S Ribosomal Protein L32

Chain B5:  2% 85% 10% . .



- Molecule 51: 50S Ribosomal Protein L32

Chain D5:  77% 18% . .

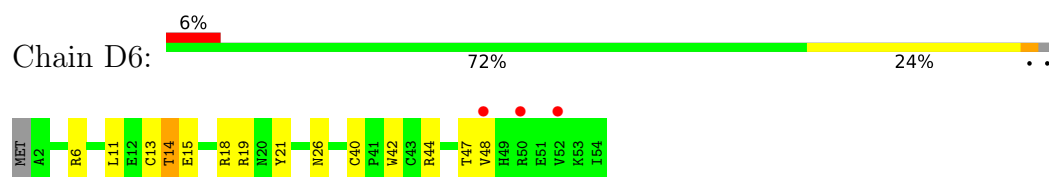


- Molecule 52: 50S Ribosomal Protein L33

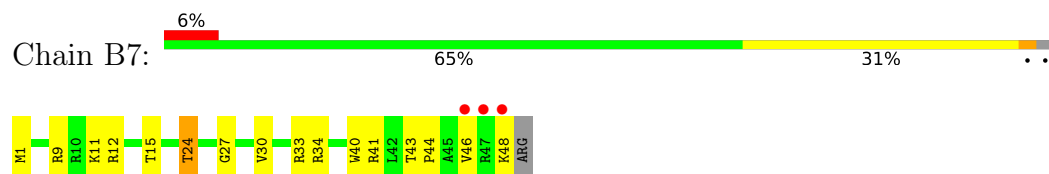
Chain B6:  70% 24% . .



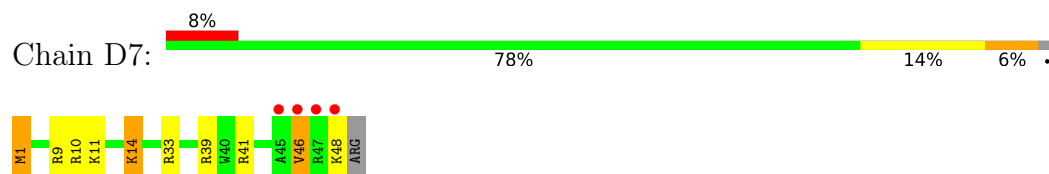
- Molecule 52: 50S Ribosomal Protein L33



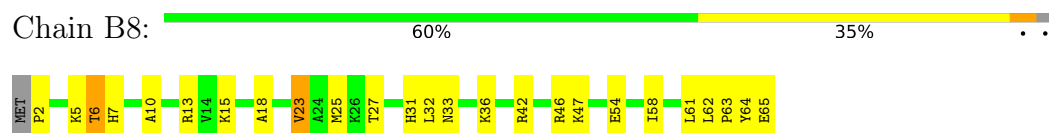
● Molecule 53: 50S Ribosomal Protein L34



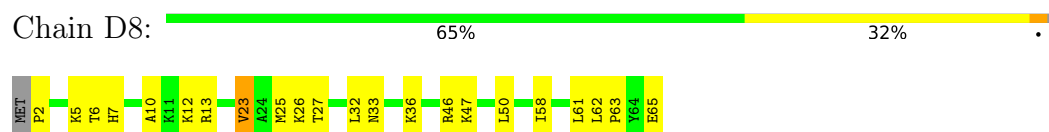
● Molecule 53: 50S Ribosomal Protein L34



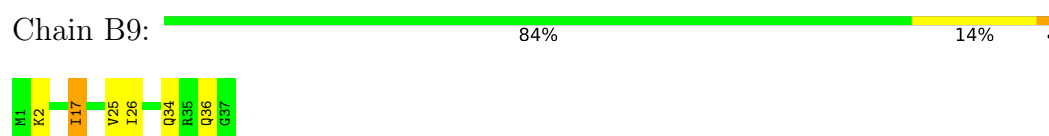
● Molecule 54: 50S Ribosomal Protein L35



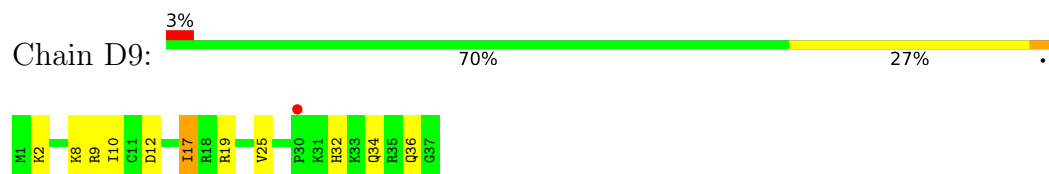
● Molecule 54: 50S Ribosomal Protein L35



● Molecule 55: 50S Ribosomal Protein L36



● Molecule 55: 50S Ribosomal Protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40 311.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (256.12-2.40) 99.6 (311.98-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.237 , 0.277 0.237 , 0.278	Depositor DCC
R_{free} test set	113081 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	298643	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.38	0/36027	0.90	45/56227 (0.1%)
1	CA	0.37	1/36170 (0.0%)	0.91	47/56452 (0.1%)
2	AB	0.30	0/1881	0.58	0/2542
2	CB	0.30	0/1860	0.61	1/2518 (0.0%)
3	AC	0.28	0/1572	0.50	0/2126
3	CC	0.30	0/1566	0.56	0/2119
4	AD	0.29	0/1685	0.49	0/2262
4	CD	0.29	0/1704	0.50	0/2284
5	AE	0.29	0/1145	0.52	0/1543
5	CE	0.31	0/1149	0.57	0/1548
6	AF	0.30	0/823	0.49	0/1115
6	CF	0.30	0/829	0.51	0/1123
7	AG	0.28	0/1250	0.54	0/1679
7	CG	0.27	0/1254	0.53	0/1683
8	AH	0.28	0/1108	0.51	0/1494
8	CH	0.27	0/1108	0.49	0/1494
9	AI	0.29	0/1002	0.56	0/1346
9	CI	0.28	0/997	0.53	1/1343 (0.1%)
10	AJ	0.28	0/722	0.57	0/982
10	CJ	0.29	0/727	0.55	0/988
11	AK	0.29	0/844	0.50	0/1145
11	CK	0.28	0/848	0.51	0/1149
12	AL	0.30	0/946	0.51	0/1274
12	CL	0.29	0/946	0.56	1/1274 (0.1%)
13	AM	0.28	0/969	0.56	0/1302
13	CM	0.28	0/961	0.55	0/1291
14	AN	0.29	0/501	0.48	0/664
14	CN	0.30	0/501	0.55	0/664
15	AO	0.28	0/739	0.51	0/985
15	CO	0.29	0/739	0.52	0/985
16	AP	0.27	0/697	0.51	0/939
16	CP	0.28	0/693	0.50	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/836	0.53	0/1117
17	CQ	0.27	0/836	0.48	0/1117
18	AR	0.30	0/560	0.51	0/746
18	CR	0.26	0/560	0.49	0/746
19	AS	0.27	0/667	0.53	0/900
19	CS	0.31	0/661	0.64	0/893
20	AT	0.26	0/730	0.55	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.27	0/203	0.48	0/266
21	CU	0.30	0/203	0.51	0/266
22	AV	0.36	0/310	0.84	0/480
22	CV	0.40	0/310	0.89	1/480 (0.2%)
23	AW	0.53	1/1606 (0.1%)	1.13	2/2497 (0.1%)
23	AY	0.53	1/1606 (0.1%)	1.13	8/2497 (0.3%)
23	CW	0.51	0/1556	1.23	9/2418 (0.4%)
23	CY	0.56	1/1583 (0.1%)	1.22	12/2459 (0.5%)
24	AX	0.50	2/1725 (0.1%)	1.13	14/2689 (0.5%)
24	CX	0.49	0/1725	1.13	14/2689 (0.5%)
25	BA	0.50	5/69261 (0.0%)	0.96	91/108110 (0.1%)
25	DA	0.42	0/67545	0.92	63/105432 (0.1%)
26	BB	0.43	1/2882 (0.0%)	0.83	1/4494 (0.0%)
26	DB	0.47	1/2879 (0.0%)	0.91	2/4487 (0.0%)
27	BD	0.36	0/2186	0.60	1/2944 (0.0%)
27	DD	0.34	0/2186	0.56	0/2944
28	BE	0.36	0/1592	0.56	0/2149
28	DE	0.34	0/1592	0.61	1/2149 (0.0%)
29	BF	0.35	0/1619	0.54	0/2193
29	DF	0.33	0/1615	0.55	0/2188
30	BG	0.29	0/1454	0.51	0/1964
30	DG	0.29	0/1453	0.52	0/1963
31	BH	0.31	0/1356	0.56	0/1834
31	DH	0.30	0/1356	0.54	0/1834
32	BI	0.29	0/1112	0.56	0/1514
32	DI	0.27	0/1079	0.55	1/1475 (0.1%)
33	BN	0.33	0/1144	0.54	0/1543
33	DN	0.32	0/1144	0.53	0/1543
34	BO	0.34	0/943	0.54	1/1269 (0.1%)
34	DO	0.32	0/943	0.56	1/1269 (0.1%)
35	BP	0.32	0/1152	0.57	0/1533
35	DP	0.32	0/1152	0.59	1/1533 (0.1%)
36	BQ	0.34	0/1143	0.53	0/1527
36	DQ	0.32	0/1143	0.53	0/1527
37	BR	0.36	0/982	0.61	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DR	0.34	0/982	0.55	0/1312
38	BS	0.31	0/883	0.52	0/1176
38	DS	0.31	0/880	0.53	0/1172
39	BT	0.33	0/1105	0.56	0/1477
39	DT	0.30	0/1097	0.53	0/1468
40	BU	0.38	0/977	0.58	0/1301
40	DU	0.34	0/977	0.53	0/1301
41	BV	0.41	0/782	0.62	0/1049
41	DV	0.29	0/782	0.54	0/1049
42	BW	0.38	0/897	0.57	0/1205
42	DW	0.33	0/897	0.55	0/1205
43	BX	0.37	0/764	0.63	1/1025 (0.1%)
43	DX	0.34	0/764	0.53	1/1025 (0.1%)
44	BY	0.34	0/819	0.56	0/1095
44	DY	0.33	0/819	0.54	0/1095
45	BZ	0.31	0/1267	0.57	0/1717
45	DZ	0.30	0/1299	0.55	0/1763
46	B0	0.35	0/662	0.60	0/881
46	D0	0.30	0/662	0.49	0/881
47	B1	0.32	0/762	0.52	0/1014
47	D1	0.33	0/762	0.52	0/1014
48	B2	0.32	0/590	0.56	0/781
48	D2	0.28	0/590	0.47	0/781
49	B3	0.37	0/474	0.60	0/635
49	D3	0.27	0/469	0.50	0/630
50	B4	0.34	0/565	0.63	0/761
50	D4	0.33	0/545	0.65	0/737
51	B5	0.36	0/469	0.54	0/635
51	D5	0.33	0/469	0.59	0/635
52	B6	0.36	0/460	0.57	0/613
52	D6	0.29	0/456	0.49	0/608
53	B7	0.39	0/426	0.59	0/561
53	D7	0.34	0/426	0.54	0/561
54	B8	0.36	0/525	0.58	0/691
54	D8	0.30	0/525	0.51	0/691
55	B9	0.34	0/310	0.49	0/407
55	D9	0.31	0/310	0.53	0/407
All	All	0.41	13/317730 (0.0%)	0.85	320/475754 (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	1
7	AG	0	1
7	CG	0	1
50	B4	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	1	G	OP3-P	-10.51	1.48	1.61
26	BB	1	U	OP3-P	-10.37	1.48	1.61
23	CY	1	G	OP3-P	-10.36	1.48	1.61
26	DB	1	U	OP3-P	-10.22	1.48	1.61
23	AW	1	G	OP3-P	-9.85	1.49	1.61

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1154	G	C5-C6-O6	12.79	136.28	128.60
24	AX	46	G	C6-N1-C2	-10.27	118.94	125.10
24	AX	14	A	C4-C5-C6	10.10	122.05	117.00
25	BA	1807	G	O5'-P-OP2	-9.98	96.71	105.70
1	AA	1002	G	N3-C4-N9	9.53	131.72	126.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
50	B4	59	PHE	Peptide
50	B4	67	TYR	Peptide
7	CG	79	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32185	0	16243	436	0
1	CA	32312	0	16307	518	0
2	AB	1846	0	1867	71	0
2	CB	1825	0	1828	83	0
3	AC	1548	0	1535	40	0
3	CC	1542	0	1517	55	0
4	AD	1655	0	1672	48	0
4	CD	1674	0	1714	43	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	38	0
6	AF	810	0	804	18	0
6	CF	816	0	808	12	0
7	AG	1231	0	1238	29	0
7	CG	1235	0	1249	32	0
8	AH	1088	0	1126	28	0
8	CH	1088	0	1126	39	0
9	AI	983	0	986	40	0
9	CI	978	0	966	46	0
10	AJ	709	0	650	27	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	12	0
11	CK	833	0	836	10	0
12	AL	930	0	980	15	0
12	CL	930	0	980	23	0
13	AM	958	0	1002	29	0
13	CM	950	0	988	38	0
14	AN	492	0	529	23	0
14	CN	492	0	529	17	0
15	AO	728	0	760	21	0
15	CO	728	0	760	23	0
16	AP	681	0	697	17	0
16	CP	677	0	686	18	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	14	0
18	AR	555	0	618	18	0
18	CR	555	0	618	17	0
19	AS	652	0	662	27	0
19	CS	646	0	644	29	0
20	AT	728	0	798	17	0
20	CT	727	0	796	21	0
21	AU	199	0	208	4	0
21	CU	199	0	208	5	0
22	AV	277	0	140	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	277	0	140	6	0
23	AW	1592	0	819	29	0
23	AY	1585	0	804	55	0
23	CW	1544	0	788	39	0
23	CY	1565	0	795	61	0
24	AX	1625	0	828	15	0
24	CX	1625	0	828	19	0
25	BA	61844	0	31181	611	0
25	DA	60314	0	30412	734	0
26	BB	2577	0	1305	15	0
26	DB	2575	0	1303	51	0
27	BD	2136	0	2218	51	0
27	DD	2136	0	2218	54	0
28	BE	1559	0	1618	31	0
28	DE	1559	0	1617	38	0
29	BF	1584	0	1625	22	0
29	DF	1580	0	1619	42	0
30	BG	1429	0	1447	25	0
30	DG	1428	0	1438	55	0
31	BH	1330	0	1407	22	0
31	DH	1330	0	1407	41	0
32	BI	1097	0	1140	32	0
32	DI	1064	0	1082	29	0
33	BN	1117	0	1184	16	0
33	DN	1117	0	1184	21	0
34	BO	933	0	996	18	0
34	DO	933	0	996	17	0
35	BP	1135	0	1212	29	0
35	DP	1135	0	1212	47	0
36	BQ	1122	0	1179	20	0
36	DQ	1122	0	1179	31	0
37	BR	968	0	1033	24	0
37	DR	968	0	1033	32	0
38	BS	873	0	927	23	0
38	DS	870	0	923	23	0
39	BT	1091	0	1151	26	0
39	DT	1083	0	1136	21	0
40	BU	959	0	1019	19	0
40	DU	959	0	1019	21	0
41	BV	771	0	830	15	0
41	DV	771	0	830	18	0
42	BW	886	0	940	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DW	886	0	940	15	0
43	BX	750	0	814	13	0
43	DX	750	0	814	18	0
44	BY	806	0	881	19	0
44	DY	806	0	881	18	0
45	BZ	1240	0	1240	24	0
45	DZ	1271	0	1273	52	0
46	B0	653	0	674	10	0
46	D0	653	0	674	18	0
47	B1	755	0	826	15	0
47	D1	755	0	826	14	0
48	B2	588	0	643	7	0
48	D2	588	0	643	5	0
49	B3	469	0	518	5	0
49	D3	464	0	514	9	0
50	B4	552	0	533	26	0
50	D4	532	0	503	30	0
51	B5	455	0	465	6	0
51	D5	455	0	465	8	0
52	B6	453	0	473	8	0
52	D6	449	0	469	11	0
53	B7	418	0	467	9	0
53	D7	418	0	467	11	0
54	B8	517	0	582	18	0
54	D8	517	0	582	23	0
55	B9	307	0	335	4	0
55	D9	307	0	335	9	0
56	AA	233	0	0	0	0
56	AB	2	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AH	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AR	1	0	0	0	0
56	AT	1	0	0	0	0
56	AW	4	0	0	0	0
56	AX	13	0	0	0	0
56	AY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B0	7	0	0	0	0
56	B1	2	0	0	0	0
56	B2	2	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	3	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	906	0	0	0	0
56	BB	30	0	0	0	0
56	BD	13	0	0	0	0
56	BE	12	0	0	0	0
56	BF	15	0	0	0	0
56	BG	6	0	0	0	0
56	BH	1	0	0	0	0
56	BI	1	0	0	0	0
56	BN	4	0	0	0	0
56	BO	5	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	7	0	0	0	0
56	BR	3	0	0	0	0
56	BS	3	0	0	0	0
56	BT	2	0	0	0	0
56	BU	10	0	0	0	0
56	BV	5	0	0	0	0
56	BW	5	0	0	0	0
56	BX	6	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	3	0	0	0	0
56	CA	201	0	0	0	0
56	CD	2	0	0	0	0
56	CE	1	0	0	0	0
56	CF	2	0	0	0	0
56	CG	1	0	0	0	0
56	CJ	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	2	0	0	0	0
56	CR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	4	0	0	0	0
56	CX	6	0	0	0	0
56	D0	1	0	0	0	0
56	D1	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	2	0	0	0	0
56	DA	673	0	0	0	0
56	DB	21	0	0	0	0
56	DD	6	0	0	0	0
56	DE	7	0	0	0	0
56	DF	7	0	0	0	0
56	DG	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0
56	DU	4	0	0	0	0
56	DV	2	0	0	0	0
56	DW	3	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
56	DZ	1	0	0	0	0
57	AA	30	0	28	1	0
57	CA	30	0	29	1	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	264	0	0	16	0
61	AB	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	4	0	0	0	0
61	AM	1	0	0	0	0
61	AQ	1	0	0	0	0
61	AV	4	0	0	0	0
61	AW	2	0	0	0	0
61	AX	11	0	0	2	0
61	AY	1	0	0	0	0
61	B0	8	0	0	0	0
61	B1	3	0	0	0	0
61	B2	4	0	0	2	0
61	B3	3	0	0	0	0
61	B4	1	0	0	0	0
61	B5	4	0	0	0	0
61	B6	1	0	0	0	0
61	B7	4	0	0	1	0
61	B8	8	0	0	0	0
61	BA	1486	0	0	44	0
61	BB	43	0	0	2	0
61	BD	19	0	0	2	0
61	BE	20	0	0	1	0
61	BF	14	0	0	1	0
61	BG	5	0	0	1	0
61	BH	1	0	0	0	0
61	BI	2	0	0	0	0
61	BN	2	0	0	0	0
61	BO	7	0	0	0	0
61	BP	19	0	0	1	0
61	BQ	5	0	0	1	0
61	BR	5	0	0	0	0
61	BS	5	0	0	0	0
61	BT	5	0	0	0	0
61	BU	8	0	0	1	0
61	BV	6	0	0	0	0
61	BW	1	0	0	0	0
61	BX	2	0	0	0	0
61	BY	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BZ	1	0	0	0	0
61	CA	204	0	0	12	0
61	CD	1	0	0	0	0
61	CG	1	0	0	1	0
61	CI	1	0	0	0	0
61	CJ	4	0	0	0	0
61	CL	4	0	0	0	0
61	CO	1	0	0	0	0
61	CP	1	0	0	0	0
61	CR	1	0	0	0	0
61	CT	1	0	0	0	0
61	CW	2	0	0	0	0
61	CX	6	0	0	0	0
61	D0	4	0	0	0	0
61	D1	4	0	0	1	0
61	D2	1	0	0	0	0
61	D3	1	0	0	0	0
61	D5	2	0	0	0	0
61	D7	5	0	0	0	0
61	D8	5	0	0	0	0
61	D9	1	0	0	0	0
61	DA	1039	0	0	58	0
61	DB	10	0	0	1	0
61	DD	17	0	0	0	0
61	DE	8	0	0	1	0
61	DF	6	0	0	0	0
61	DI	2	0	0	0	0
61	DN	1	0	0	0	0
61	DO	3	0	0	0	0
61	DP	12	0	0	3	0
61	DQ	1	0	0	0	0
61	DR	3	0	0	0	0
61	DT	3	0	0	0	0
61	DU	1	0	0	0	0
61	DV	1	0	0	0	0
61	DW	2	0	0	0	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0
61	DZ	2	0	0	0	0
All	All	298643	0	196646	4377	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 9.

The worst 5 of 4377 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:1027:C:N3	1:AA:1034:G:C6	2.18	1.10
1:CA:1002:G:H1	1:CA:1038:C:N4	1.51	1.08
23:AW:6:G:H1	23:AW:67:C:N4	1.49	1.07
1:CA:1028:C:N3	1:CA:1033:G:C6	2.23	1.06
1:AA:78:G:C6	1:AA:91:C:N4	2.29	1.00

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%)	204 (89%)	19 (8%)	6 (3%)	6	6
2	CB	229/256 (90%)	201 (88%)	16 (7%)	12 (5%)	2	1
3	AC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	31	44
3	CC	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	11	15
4	AD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	31	44
4	CD	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	AE	146/162 (90%)	140 (96%)	3 (2%)	3 (2%)	8	9
5	CE	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	24	35
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	AG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
7	CG	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	13	18
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	125/128 (98%)	114 (91%)	8 (6%)	3 (2%)	6	7
9	CI	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	21	31
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	4	3
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	8	9
11	AK	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	9	11
11	CK	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	9	11
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	4 (3%)	2 (2%)	10	13
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	14	20
16	AP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	13	18
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	13	18
17	AQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
17	CQ	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	14	20
20	AT	94/106 (89%)	87 (93%)	4 (4%)	3 (3%)	4	3
20	CT	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	2	1
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
27	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	36	51
27	DD	273/276 (99%)	265 (97%)	7 (3%)	1 (0%)	36	51
28	BE	202/206 (98%)	198 (98%)	3 (2%)	1 (0%)	31	44
28	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	17	25
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	31	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	201/210 (96%)	198 (98%)	1 (0%)	2 (1%)	17	25
30	BG	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
30	DG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	16	22
31	BH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
31	DH	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	5	5
32	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	24	35
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	136 (99%)	1 (1%)	1 (1%)	24	35
34	BO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	24	35
35	DP	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	8	9
36	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
36	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	24	35
37	BR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
37	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
38	BS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
38	DS	108/112 (96%)	106 (98%)	1 (1%)	1 (1%)	19	27
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	21	31
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	17	25
41	DV	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	17	25
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
43	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	16	22
44	BY	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	148/206 (72%)	140 (95%)	6 (4%)	2 (1%)	12	17
45	DZ	156/206 (76%)	149 (96%)	6 (4%)	1 (1%)	27	39
46	B0	81/85 (95%)	80 (99%)	0	1 (1%)	14	20
46	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
47	B1	95/98 (97%)	94 (99%)	0	1 (1%)	16	22
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	16	22
48	B2	68/72 (94%)	67 (98%)	0	1 (2%)	11	15
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%)	55 (96%)	2 (4%)	0	100	100
50	B4	67/71 (94%)	57 (85%)	4 (6%)	6 (9%)	1	0
50	D4	67/71 (94%)	55 (82%)	6 (9%)	6 (9%)	1	0
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	57 (100%)	0	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	50 (98%)	1 (2%)	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%)	7	8
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11372/12128 (94%)	10883 (96%)	387 (3%)	102 (1%)	19	27

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
9	AI	54	ASP
27	BD	275	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	170 (88%)	22 (12%)	6	8
2	CB	187/220 (85%)	158 (84%)	29 (16%)	3	3
3	AC	142/188 (76%)	128 (90%)	14 (10%)	8	12
3	CC	140/188 (74%)	125 (89%)	15 (11%)	7	10
4	AD	169/181 (93%)	154 (91%)	15 (9%)	11	16
4	CD	173/181 (96%)	158 (91%)	15 (9%)	11	17
5	AE	113/123 (92%)	103 (91%)	10 (9%)	11	16
5	CE	114/123 (93%)	101 (89%)	13 (11%)	6	8
6	AF	84/90 (93%)	77 (92%)	7 (8%)	12	18
6	CF	85/90 (94%)	77 (91%)	8 (9%)	9	14
7	AG	119/127 (94%)	106 (89%)	13 (11%)	7	9
7	CG	120/127 (94%)	102 (85%)	18 (15%)	3	4
8	AH	114/119 (96%)	106 (93%)	8 (7%)	16	26
8	CH	114/119 (96%)	100 (88%)	14 (12%)	5	6
9	AI	90/99 (91%)	77 (86%)	13 (14%)	3	4
9	CI	89/99 (90%)	74 (83%)	15 (17%)	2	2
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	20	32
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	16	25
11	AK	82/99 (83%)	79 (96%)	3 (4%)	37	56
11	CK	83/99 (84%)	81 (98%)	2 (2%)	52	72
12	AL	97/109 (89%)	92 (95%)	5 (5%)	25	41
12	CL	97/109 (89%)	92 (95%)	5 (5%)	25	41
13	AM	93/101 (92%)	81 (87%)	12 (13%)	5	5
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	5
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	0
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	71 (91%)	7 (9%)	10	15
15	CO	78/80 (98%)	68 (87%)	10 (13%)	5	5
16	AP	69/74 (93%)	59 (86%)	10 (14%)	3	4
16	CP	68/74 (92%)	63 (93%)	5 (7%)	15	23
17	AQ	94/97 (97%)	84 (89%)	10 (11%)	7	10
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	19	30
18	AR	59/77 (77%)	52 (88%)	7 (12%)	6	7
18	CR	59/77 (77%)	54 (92%)	5 (8%)	12	18
19	AS	69/80 (86%)	63 (91%)	6 (9%)	11	17
19	CS	67/80 (84%)	61 (91%)	6 (9%)	10	15
20	AT	70/82 (85%)	62 (89%)	8 (11%)	6	8
20	CT	70/82 (85%)	63 (90%)	7 (10%)	8	12
21	AU	18/22 (82%)	16 (89%)	2 (11%)	7	9
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	2
27	BD	215/218 (99%)	204 (95%)	11 (5%)	26	42
27	DD	215/218 (99%)	201 (94%)	14 (6%)	19	29
28	BE	164/166 (99%)	149 (91%)	15 (9%)	10	15
28	DE	164/166 (99%)	147 (90%)	17 (10%)	8	11
29	BF	160/166 (96%)	145 (91%)	15 (9%)	9	14
29	DF	159/166 (96%)	144 (91%)	15 (9%)	9	14
30	BG	144/156 (92%)	128 (89%)	16 (11%)	7	9
30	DG	143/156 (92%)	119 (83%)	24 (17%)	2	2
31	BH	144/148 (97%)	136 (94%)	8 (6%)	23	37
31	DH	144/148 (97%)	129 (90%)	15 (10%)	8	11
32	BI	113/124 (91%)	96 (85%)	17 (15%)	3	4
32	DI	105/124 (85%)	88 (84%)	17 (16%)	2	3
33	BN	118/119 (99%)	107 (91%)	11 (9%)	10	14
33	DN	118/119 (99%)	106 (90%)	12 (10%)	8	11
34	BO	100/100 (100%)	94 (94%)	6 (6%)	21	33
34	DO	100/100 (100%)	97 (97%)	3 (3%)	44	65
35	BP	115/116 (99%)	102 (89%)	13 (11%)	6	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DP	115/116 (99%)	106 (92%)	9 (8%)	14	21
36	BQ	111/111 (100%)	101 (91%)	10 (9%)	10	15
36	DQ	111/111 (100%)	101 (91%)	10 (9%)	10	15
37	BR	101/101 (100%)	87 (86%)	14 (14%)	4	4
37	DR	101/101 (100%)	88 (87%)	13 (13%)	5	5
38	BS	86/88 (98%)	78 (91%)	8 (9%)	10	14
38	DS	85/88 (97%)	76 (89%)	9 (11%)	7	10
39	BT	115/127 (91%)	108 (94%)	7 (6%)	20	32
39	DT	113/127 (89%)	105 (93%)	8 (7%)	16	25
40	BU	93/94 (99%)	86 (92%)	7 (8%)	15	23
40	DU	93/94 (99%)	88 (95%)	5 (5%)	24	38
41	BV	80/82 (98%)	71 (89%)	9 (11%)	6	8
41	DV	80/82 (98%)	71 (89%)	9 (11%)	6	8
42	BW	90/92 (98%)	85 (94%)	5 (6%)	23	37
42	DW	90/92 (98%)	84 (93%)	6 (7%)	18	28
43	BX	77/78 (99%)	75 (97%)	2 (3%)	49	70
43	DX	77/78 (99%)	74 (96%)	3 (4%)	35	54
44	BY	85/91 (93%)	76 (89%)	9 (11%)	7	10
44	DY	85/91 (93%)	76 (89%)	9 (11%)	7	10
45	BZ	135/179 (75%)	119 (88%)	16 (12%)	6	7
45	DZ	137/179 (76%)	123 (90%)	14 (10%)	8	11
46	B0	65/67 (97%)	62 (95%)	3 (5%)	29	46
46	D0	65/67 (97%)	62 (95%)	3 (5%)	29	46
47	B1	80/83 (96%)	71 (89%)	9 (11%)	6	8
47	D1	80/83 (96%)	72 (90%)	8 (10%)	8	12
48	B2	65/67 (97%)	60 (92%)	5 (8%)	14	22
48	D2	65/67 (97%)	60 (92%)	5 (8%)	14	22
49	B3	51/52 (98%)	48 (94%)	3 (6%)	21	34
49	D3	50/52 (96%)	45 (90%)	5 (10%)	8	12
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	2
50	D4	53/63 (84%)	39 (74%)	14 (26%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B5	50/52 (96%)	46 (92%)	4 (8%)	13	20
51	D5	50/52 (96%)	45 (90%)	5 (10%)	8	12
52	B6	51/52 (98%)	48 (94%)	3 (6%)	21	34
52	D6	50/52 (96%)	49 (98%)	1 (2%)	58	77
53	B7	41/42 (98%)	36 (88%)	5 (12%)	5	6
53	D7	41/42 (98%)	38 (93%)	3 (7%)	15	24
54	B8	54/55 (98%)	49 (91%)	5 (9%)	10	14
54	D8	54/55 (98%)	52 (96%)	2 (4%)	37	56
55	B9	34/34 (100%)	33 (97%)	1 (3%)	45	66
55	D9	34/34 (100%)	33 (97%)	1 (3%)	45	66
All	All	9306/10066 (92%)	8408 (90%)	898 (10%)	9	13

5 of 898 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B3	23	LEU
5	CE	57	LYS
44	DY	11	ASP
51	B5	6	VAL
2	CB	157	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
50	B4	46	GLN
4	CD	125	HIS
37	DR	71	GLN
50	B4	60	GLN
3	CC	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	297 (19%)	24 (1%)
1	CA	1501/1521 (98%)	306 (20%)	23 (1%)
22	AV	12/24 (50%)	2 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	CV	12/24 (50%)	1 (8%)	0
23	AW	71/76 (93%)	30 (42%)	2 (2%)
23	AY	71/76 (93%)	29 (40%)	1 (1%)
23	CW	68/76 (89%)	27 (39%)	1 (1%)
23	CY	69/76 (90%)	28 (40%)	3 (4%)
24	AX	75/77 (97%)	15 (20%)	1 (1%)
24	CX	75/77 (97%)	16 (21%)	1 (1%)
25	BA	2864/2915 (98%)	446 (15%)	39 (1%)
25	DA	2791/2915 (95%)	485 (17%)	29 (1%)
26	BB	120/121 (99%)	19 (15%)	1 (0%)
26	DB	119/121 (98%)	20 (16%)	1 (0%)
All	All	9342/9620 (97%)	1721 (18%)	126 (1%)

5 of 1721 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2166	U
1	CA	250	A
25	DA	1653	G
25	BA	2192	A
25	BA	2623	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	AW	32	23	16,21,22	1.35	1 (6%)	20,30,33	3.10	6 (30%)
23	MIA	AW	37	23	22,31,32	2.43	3 (13%)	26,44,47	2.42	10 (38%)
23	PSU	AW	39	23	16,21,22	1.41	2 (12%)	20,30,33	3.15	6 (30%)
23	7MG	AW	46	23	20,26,27	1.91	3 (15%)	24,39,42	2.67	6 (25%)
23	5MU	AW	54	23	13,22,23	0.80	0	14,32,35	2.01	1 (7%)
23	PSU	AW	55	23	16,21,22	1.27	2 (12%)	20,30,33	3.35	6 (30%)
23	4SU	AW	8	23	13,21,22	1.33	1 (7%)	14,30,33	1.82	2 (14%)
24	5MC	AX	32	24	14,22,23	1.54	1 (7%)	17,32,35	1.47	3 (17%)
24	5MU	AX	54	24,56	13,22,23	0.82	0	14,32,35	2.16	2 (14%)
24	PSU	AX	55	24	16,21,22	1.60	1 (6%)	20,30,33	3.24	7 (35%)
24	4SU	AX	8	24	13,21,22	1.51	2 (15%)	14,30,33	2.89	2 (14%)
23	PSU	AY	32	23	16,21,22	1.32	1 (6%)	20,30,33	3.21	6 (30%)
23	MIA	AY	37	23	17,24,32	1.30	2 (11%)	16,35,47	1.27	2 (12%)
23	PSU	AY	39	23	16,21,22	1.28	1 (6%)	20,30,33	3.28	6 (30%)
23	7MG	AY	46	23	20,26,27	2.06	3 (15%)	24,39,42	2.80	8 (33%)
23	5MU	AY	54	23	13,22,23	0.85	1 (7%)	14,32,35	1.81	2 (14%)
23	PSU	AY	55	23	16,21,22	1.32	2 (12%)	20,30,33	2.98	5 (25%)
23	4SU	AY	8	23	13,21,22	1.34	1 (7%)	14,30,33	1.54	2 (14%)
23	PSU	CW	32	23	16,21,22	1.29	1 (6%)	20,30,33	3.19	6 (30%)
23	MIA	CW	37	23	19,27,32	1.84	3 (15%)	21,39,47	1.96	7 (33%)
23	PSU	CW	39	23	16,21,22	1.31	1 (6%)	20,30,33	3.32	6 (30%)
23	7MG	CW	46	23	20,26,27	1.99	3 (15%)	24,39,42	2.56	6 (25%)
23	5MU	CW	54	23	13,22,23	0.73	0	14,32,35	2.15	1 (7%)
23	PSU	CW	55	23	16,21,22	1.19	1 (6%)	20,30,33	3.27	6 (30%)
23	4SU	CW	8	23	13,21,22	1.36	1 (7%)	14,30,33	1.67	2 (14%)
24	5MC	CX	32	24	14,22,23	1.55	1 (7%)	17,32,35	1.38	3 (17%)
24	5MU	CX	54	24	13,22,23	0.86	1 (7%)	14,32,35	1.90	2 (14%)
24	PSU	CX	55	24	16,21,22	1.23	1 (6%)	20,30,33	3.08	5 (25%)
24	4SU	CX	8	24	13,21,22	1.46	2 (15%)	14,30,33	2.70	2 (14%)
23	PSU	CY	32	23	16,21,22	1.29	1 (6%)	20,30,33	3.17	6 (30%)
23	MIA	CY	37	23	17,24,32	1.25	2 (11%)	16,35,47	1.29	2 (12%)
23	PSU	CY	39	23	16,21,22	1.45	1 (6%)	20,30,33	3.43	6 (30%)
23	7MG	CY	46	23	20,26,27	1.83	3 (15%)	24,39,42	3.20	9 (37%)
23	5MU	CY	54	23	13,22,23	0.80	0	14,32,35	1.94	2 (14%)
23	PSU	CY	55	23	16,21,22	1.46	4 (25%)	20,30,33	3.12	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	4SU	CY	8	23	13,21,22	1.40	1 (7%)	14,30,33	1.44	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	4/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	1/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	2/3/25/34	0/3/3/3
23	PSU	AY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	1/7/37/38	0/3/3/3
23	5MU	AY	54	23	-	3/3/25/26	0/2/2/2
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	1/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	3/7/29/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	2/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	2/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	CY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	2/3/25/34	0/3/3/3
23	PSU	CY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	4/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	CY	54	23	-	2/3/25/26	0/2/2/2
23	PSU	CY	55	23	-	5/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-7.24	1.69	1.75
23	AW	37	MIA	C13-C14	7.12	1.53	1.32
23	CW	46	7MG	C6-C5	6.25	1.48	1.41
23	CW	37	MIA	C2-S10	-6.13	1.70	1.75
23	AY	46	7MG	C6-C5	6.06	1.48	1.41

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	46	7MG	N3-C4-N9	10.46	140.70	126.94
24	AX	8	4SU	C2-N3-C4	9.47	128.89	115.15
23	AY	39	PSU	N1-C2-N3	-9.24	121.08	128.43
23	AY	46	7MG	N3-C4-N9	9.19	139.04	126.94
23	CW	39	PSU	N1-C2-N3	-9.17	121.14	128.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AY	54	5MU	O4'-C4'-C5'-O5'
23	CY	54	5MU	C3'-C4'-C5'-O5'
23	CY	54	5MU	O4'-C4'-C5'-O5'
23	CY	55	PSU	C2'-C1'-C5-C4
23	CY	55	PSU	C2'-C1'-C5-C6

There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	46	7MG	1	0
23	AW	55	PSU	1	0
24	AX	8	4SU	2	0
23	AY	32	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AY	37	MIA	2	0
23	AY	46	7MG	1	0
23	AY	55	PSU	2	0
23	AY	8	4SU	3	0
23	CW	39	PSU	1	0
23	CW	46	7MG	1	0
23	CW	8	4SU	2	0
24	CX	32	5MC	3	0
23	CY	37	MIA	1	0
23	CY	46	7MG	3	0
23	CY	55	PSU	6	0
23	CY	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2325 ligands modelled in this entry, 2321 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	$\# Z > 2$
57	UAM	AA	3232	56	31,31,31	1.45	2 (6%)	38,44,44	1.22	3 (7%)
58	SF4	AD	501	4	0,12,12	0.00	-	-		
57	UAM	CA	3202	-	31,31,31	1.47	2 (6%)	38,44,44	1.29	6 (15%)
58	SF4	CD	501	4	0,12,12	0.00	-	-		

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
57	UAM	AA	3232	56	-	5/28/40/40	0/2/2/2
58	SF4	AD	501	4	-	-	0/6/5/5
57	UAM	CA	3202	-	-	5/28/40/40	0/2/2/2
58	SF4	CD	501	4	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3232	UAM	CAO-CAW	-6.92	1.39	1.51
57	CA	3202	UAM	CAO-CAW	-6.67	1.39	1.51
57	CA	3202	UAM	CAX-CAU	-3.21	1.38	1.46
57	AA	3232	UAM	CAX-CAU	-2.66	1.39	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3232	UAM	CBD-OAR-CAU	-3.55	113.28	118.94
57	AA	3232	UAM	CAY-CAP-CBC	-3.43	108.39	115.83
57	CA	3202	UAM	CBD-OAR-CAU	-3.28	113.71	118.94
57	CA	3202	UAM	OAR-CAU-OAG	3.26	121.32	117.58
57	AA	3232	UAM	OAR-CAU-OAG	2.95	120.96	117.58

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CA	3202	UAM	CAY-CAP-CBC-CBD
57	CA	3202	UAM	CBD-CBC-NAQ-CAT
57	CA	3202	UAM	CAP-CBC-NAQ-CAT
57	AA	3232	UAM	CAZ-CAN-CAS-OAE
57	AA	3232	UAM	CAZ-CAN-CAS-NAC

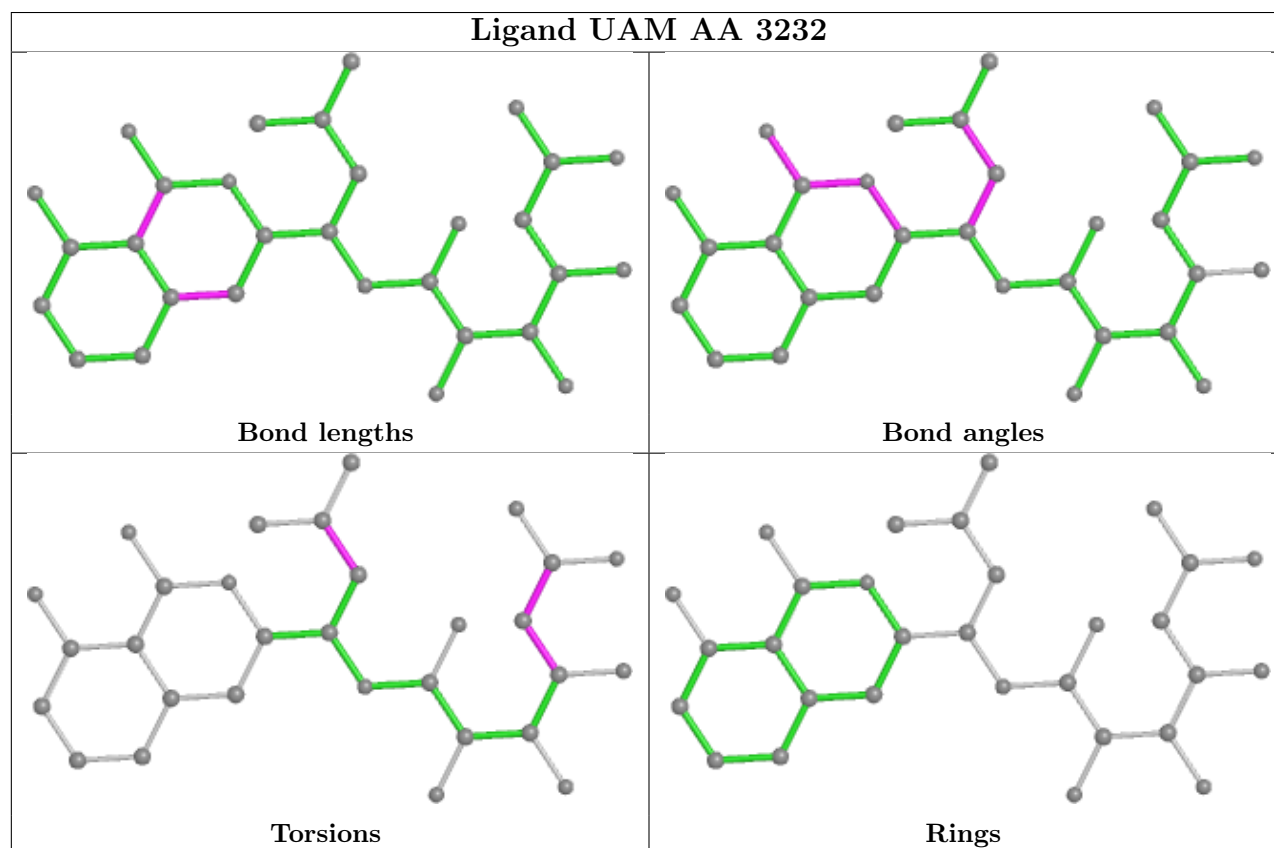
There are no ring outliers.

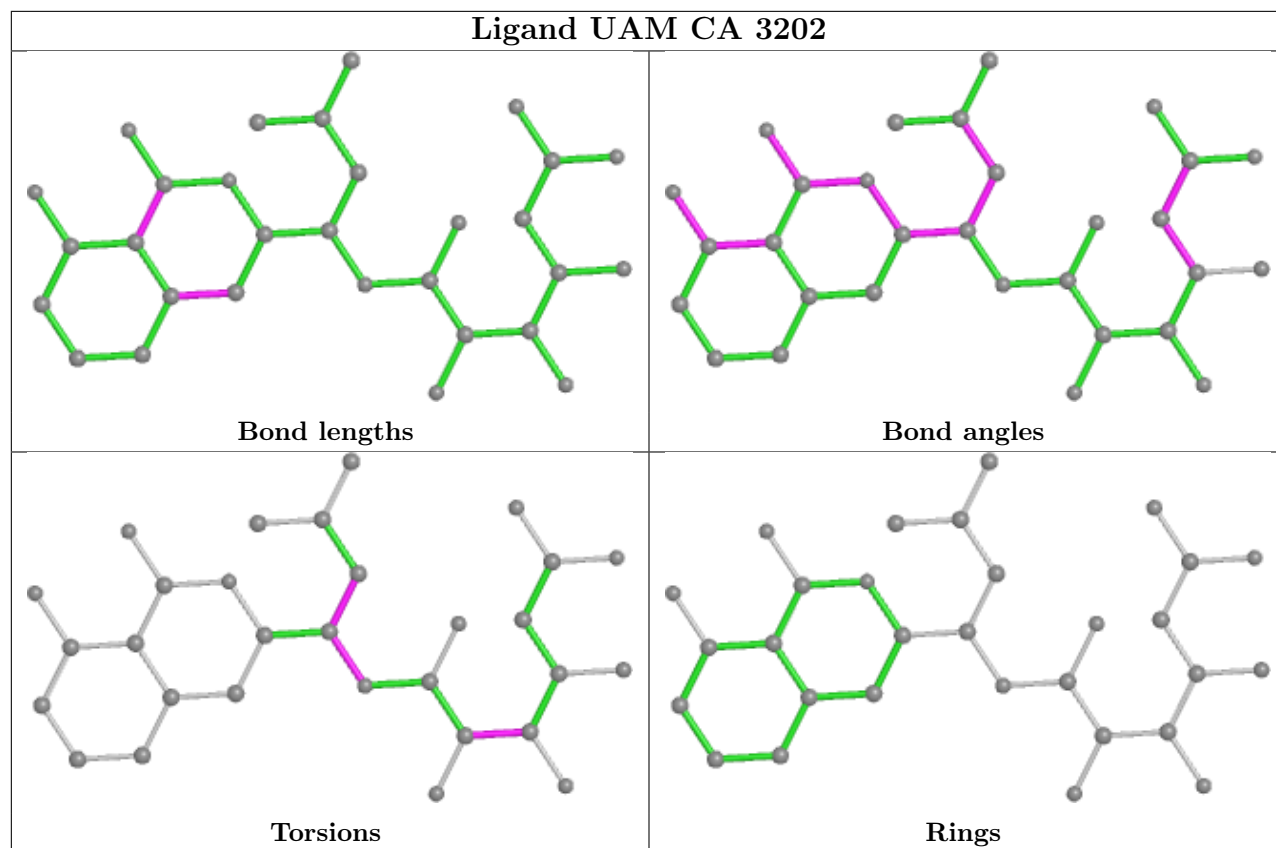
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3232	UAM	1	0
57	CA	3202	UAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1497/1521 (98%)	0.22	33 (2%) 62 59	36, 63, 86, 100	0
1	CA	1503/1521 (98%)	0.30	70 (4%) 31 29	38, 65, 87, 100	0
2	AB	231/256 (90%)	0.51	16 (6%) 17 15	62, 75, 84, 89	0
2	CB	231/256 (90%)	0.80	35 (15%) 2 1	64, 77, 84, 90	0
3	AC	206/239 (86%)	0.77	13 (6%) 20 18	59, 70, 80, 85	0
3	CC	206/239 (86%)	1.24	38 (18%) 1 1	61, 72, 81, 86	0
4	AD	208/209 (99%)	0.77	18 (8%) 10 9	48, 63, 72, 77	0
4	CD	208/209 (99%)	0.78	15 (7%) 15 14	49, 63, 72, 76	0
5	AE	148/162 (91%)	0.70	8 (5%) 26 24	49, 63, 73, 80	0
5	CE	148/162 (91%)	0.68	11 (7%) 14 13	49, 65, 74, 80	0
6	AF	100/101 (99%)	0.36	0 100 100	50, 60, 69, 74	0
6	CF	100/101 (99%)	0.40	3 (3%) 50 48	49, 61, 70, 75	0
7	AG	155/156 (99%)	0.55	7 (4%) 33 31	54, 66, 76, 83	0
7	CG	155/156 (99%)	1.22	32 (20%) 1 0	55, 68, 77, 85	0
8	AH	137/138 (99%)	0.53	3 (2%) 62 59	53, 64, 71, 78	0
8	CH	137/138 (99%)	0.58	8 (5%) 23 21	54, 66, 72, 78	0
9	AI	127/128 (99%)	1.04	19 (14%) 2 1	49, 72, 79, 83	0
9	CI	127/128 (99%)	2.16	71 (55%) 0 0	55, 74, 81, 84	0
10	AJ	97/105 (92%)	0.98	14 (14%) 2 2	46, 69, 84, 88	0
10	CJ	96/105 (91%)	1.51	20 (20%) 1 0	59, 78, 87, 91	0
11	AK	114/129 (88%)	0.91	13 (11%) 5 4	42, 61, 72, 76	0
11	CK	114/129 (88%)	0.97	10 (8%) 10 9	43, 63, 73, 77	0
12	AL	122/132 (92%)	0.40	3 (2%) 57 55	43, 54, 65, 72	0
12	CL	122/132 (92%)	0.79	15 (12%) 4 3	46, 56, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	AM	123/126 (97%)	0.80	10 (8%)	12	10	51, 66, 73, 77	0
13	CM	122/126 (96%)	1.68	42 (34%)	0	0	53, 69, 74, 79	0
14	AN	60/61 (98%)	1.09	6 (10%)	7	6	60, 67, 74, 76	0
14	CN	60/61 (98%)	2.69	34 (56%)	0	0	61, 70, 76, 79	0
15	AO	88/89 (98%)	0.58	5 (5%)	24	22	41, 61, 70, 75	0
15	CO	88/89 (98%)	0.57	4 (4%)	33	31	45, 61, 71, 77	0
16	AP	82/88 (93%)	0.54	2 (2%)	59	56	53, 62, 72, 74	0
16	CP	82/88 (93%)	0.57	4 (4%)	29	28	52, 62, 71, 74	0
17	AQ	99/105 (94%)	0.64	4 (4%)	38	37	50, 62, 72, 74	0
17	CQ	99/105 (94%)	0.73	8 (8%)	12	10	50, 63, 73, 75	0
18	AR	68/88 (77%)	0.63	7 (10%)	6	6	45, 57, 70, 73	0
18	CR	68/88 (77%)	0.29	1 (1%)	73	71	51, 64, 72, 77	0
19	AS	83/93 (89%)	0.77	6 (7%)	15	14	60, 70, 78, 85	0
19	CS	83/93 (89%)	1.67	31 (37%)	0	0	64, 72, 80, 87	0
20	AT	96/106 (90%)	0.47	3 (3%)	49	47	53, 64, 75, 76	0
20	CT	96/106 (90%)	0.68	7 (7%)	15	13	53, 63, 76, 78	0
21	AU	23/27 (85%)	1.05	4 (17%)	1	1	58, 64, 67, 70	0
21	CU	23/27 (85%)	1.57	8 (34%)	0	0	60, 66, 70, 74	0
22	AV	13/24 (54%)	0.96	2 (15%)	2	1	50, 59, 78, 86	0
22	CV	13/24 (54%)	1.67	4 (30%)	0	0	54, 62, 81, 88	0
23	AW	67/76 (88%)	1.47	16 (23%)	0	0	42, 83, 94, 98	0
23	AY	67/76 (88%)	1.57	22 (32%)	0	0	36, 88, 94, 99	0
23	CW	65/76 (85%)	2.27	29 (44%)	0	0	45, 84, 94, 99	0
23	CY	66/76 (86%)	1.64	24 (36%)	0	0	39, 88, 94, 96	0
24	AX	72/77 (93%)	0.63	5 (6%)	17	15	35, 66, 80, 89	0
24	CX	72/77 (93%)	0.42	4 (5%)	24	23	38, 69, 81, 90	0
25	BA	2871/2915 (98%)	0.69	107 (3%)	41	40	19, 38, 88, 103	0
25	DA	2800/2915 (96%)	0.13	93 (3%)	46	44	24, 42, 84, 100	0
26	BB	120/121 (99%)	0.47	0	100	100	36, 56, 68, 86	0
26	DB	120/121 (99%)	0.20	5 (4%)	36	34	42, 60, 71, 88	0
27	BD	275/276 (99%)	0.64	5 (1%)	68	66	21, 36, 51, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	275/276 (99%)	0.56	13 (4%) 31 29	22, 38, 53, 75	0
28	BE	204/206 (99%)	0.67	3 (1%) 73 71	21, 42, 59, 72	0
28	DE	204/206 (99%)	0.28	2 (0%) 82 80	23, 45, 62, 74	0
29	BF	203/210 (96%)	0.76	3 (1%) 73 71	20, 46, 69, 82	0
29	DF	203/210 (96%)	0.38	6 (2%) 50 48	23, 52, 69, 83	0
30	BG	181/182 (99%)	0.80	9 (4%) 29 27	45, 61, 73, 84	0
30	DG	181/182 (99%)	1.64	59 (32%) 0 0	50, 63, 75, 84	0
31	BH	174/180 (96%)	0.59	1 (0%) 89 87	47, 60, 69, 77	0
31	DH	174/180 (96%)	0.87	25 (14%) 2 2	51, 65, 73, 78	0
32	BI	146/148 (98%)	0.35	4 (2%) 54 52	43, 66, 77, 81	0
32	DI	146/148 (98%)	0.33	3 (2%) 63 60	43, 67, 77, 81	0
33	BN	140/140 (100%)	0.79	1 (0%) 87 86	29, 42, 62, 72	0
33	DN	140/140 (100%)	0.21	2 (1%) 75 73	34, 47, 66, 74	0
34	BO	122/122 (100%)	0.63	0 100 100	31, 42, 59, 65	0
34	DO	122/122 (100%)	0.32	0 100 100	35, 45, 60, 67	0
35	BP	149/150 (99%)	0.56	1 (0%) 87 86	22, 51, 68, 76	0
35	DP	149/150 (99%)	0.43	7 (4%) 31 29	25, 54, 70, 77	0
36	BQ	141/141 (100%)	0.79	2 (1%) 75 73	29, 45, 62, 70	0
36	DQ	141/141 (100%)	0.84	16 (11%) 5 4	34, 50, 66, 71	0
37	BR	118/118 (100%)	0.72	0 100 100	24, 35, 46, 56	0
37	DR	118/118 (100%)	0.12	0 100 100	26, 38, 49, 58	0
38	BS	110/112 (98%)	0.73	2 (1%) 68 66	41, 54, 66, 71	0
38	DS	110/112 (98%)	1.05	15 (13%) 3 2	45, 58, 68, 73	0
39	BT	131/146 (89%)	0.56	0 100 100	34, 46, 66, 75	0
39	DT	131/146 (89%)	0.31	0 100 100	38, 50, 70, 76	0
40	BU	116/118 (98%)	0.78	1 (0%) 84 82	23, 33, 52, 64	0
40	DU	116/118 (98%)	0.33	1 (0%) 84 82	29, 39, 56, 66	0
41	BV	101/101 (100%)	0.36	0 100 100	15, 31, 49, 71	0
41	DV	101/101 (100%)	0.57	5 (4%) 29 27	40, 66, 74, 84	0
42	BW	112/113 (99%)	0.71	1 (0%) 84 82	23, 31, 50, 75	0
42	DW	112/113 (99%)	0.35	0 100 100	27, 35, 54, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
43	BX	95/96 (98%)	0.67	0	100 100	28, 40, 61, 75	0
43	DX	95/96 (98%)	0.60	5 (5%)	26 25	30, 44, 62, 75	0
44	BY	107/110 (97%)	0.67	2 (1%)	66 64	36, 52, 68, 76	0
44	DY	107/110 (97%)	0.62	7 (6%)	19 17	38, 56, 70, 76	0
45	BZ	154/206 (74%)	0.95	19 (12%)	4 3	34, 59, 80, 89	0
45	DZ	160/206 (77%)	1.69	48 (30%)	0 0	62, 77, 87, 97	0
46	B0	83/85 (97%)	0.61	1 (1%)	79 77	25, 33, 50, 61	0
46	D0	83/85 (97%)	1.13	10 (12%)	4 3	42, 61, 69, 73	0
47	B1	97/98 (98%)	0.45	1 (1%)	82 80	27, 43, 66, 70	0
47	D1	97/98 (98%)	0.50	2 (2%)	63 60	30, 44, 66, 73	0
48	B2	70/72 (97%)	0.29	0	100 100	25, 42, 57, 67	0
48	D2	70/72 (97%)	0.60	4 (5%)	24 22	51, 64, 70, 72	0
49	B3	59/60 (98%)	0.37	0	100 100	16, 29, 52, 70	0
49	D3	59/60 (98%)	0.88	5 (8%)	11 9	49, 63, 74, 78	0
50	B4	69/71 (97%)	1.18	16 (23%)	0 0	55, 71, 83, 88	0
50	D4	69/71 (97%)	2.29	33 (47%)	0 0	61, 74, 85, 89	0
51	B5	59/60 (98%)	0.74	1 (1%)	70 67	19, 32, 48, 58	0
51	D5	59/60 (98%)	0.20	0	100 100	25, 35, 52, 59	0
52	B6	53/54 (98%)	0.59	0	100 100	22, 38, 55, 57	0
52	D6	53/54 (98%)	0.49	3 (5%)	24 22	42, 56, 67, 73	0
53	B7	48/49 (97%)	0.77	3 (6%)	20 18	15, 26, 50, 64	0
53	D7	48/49 (97%)	0.87	4 (8%)	11 10	25, 37, 63, 68	0
54	B8	64/65 (98%)	0.42	0	100 100	21, 28, 35, 52	0
54	D8	64/65 (98%)	0.70	0	100 100	39, 51, 58, 64	0
55	B9	37/37 (100%)	0.67	0	100 100	26, 44, 62, 69	0
55	D9	37/37 (100%)	0.51	1 (2%)	54 52	39, 49, 64, 73	0
All	All	20920/21748 (96%)	0.59	1324 (6%)	20 18	15, 56, 82, 103	0

The worst 5 of 1324 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	1030(B)	C	11.7
50	D4	49	PHE	11.1

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Mol	Chain	Res	Type	RSRZ
23	CW	71	G	11.1
23	AW	71	G	9.7
25	BA	936	C	8.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	7MG	CY	46	24/25	0.65	0.24	84,93,103,111	0
23	4SU	CY	8	20/21	0.69	0.19	76,90,105,117	0
23	5MU	CY	54	21/22	0.70	0.24	78,87,97,118	0
23	7MG	AY	46	24/25	0.71	0.27	76,92,102,121	0
23	PSU	CY	32	20/21	0.72	0.25	71,78,92,94	0
23	4SU	CW	8	20/21	0.72	0.30	78,89,106,119	0
23	5MU	AY	54	21/22	0.75	0.28	70,85,94,111	0
23	7MG	CW	46	24/25	0.76	0.33	81,92,99,121	0
23	4SU	AY	8	20/21	0.77	0.20	77,91,110,118	0
23	PSU	CY	55	20/21	0.77	0.27	80,91,104,111	0
23	PSU	AY	55	20/21	0.78	0.30	82,92,102,111	0
23	7MG	AW	46	24/25	0.80	0.25	66,84,103,129	0
23	MIA	CY	37	22/30	0.81	0.33	65,78,95,107	0
23	PSU	AW	55	20/21	0.82	0.22	62,70,81,83	0
23	MIA	AY	37	22/30	0.83	0.30	69,78,88,91	0
23	PSU	AY	32	20/21	0.84	0.17	71,79,89,91	0
23	PSU	CW	55	20/21	0.85	0.20	64,74,85,87	0
23	4SU	AW	8	20/21	0.85	0.18	56,80,91,93	0
24	PSU	CX	55	20/21	0.87	0.19	48,69,86,88	0
23	5MU	CW	54	21/22	0.87	0.18	65,75,84,86	0
23	PSU	AW	32	20/21	0.88	0.19	61,69,75,77	0
23	PSU	CY	39	20/21	0.89	0.23	64,74,81,84	0
24	4SU	CX	8	20/21	0.89	0.14	65,74,85,85	0
23	MIA	CW	37	25/30	0.89	0.20	36,64,70,71	0
24	5MU	CX	54	21/22	0.90	0.26	70,78,82,89	0
23	PSU	AY	39	20/21	0.92	0.20	67,73,79,81	0
24	PSU	AX	55	20/21	0.92	0.20	45,66,84,85	0
23	PSU	CW	32	20/21	0.92	0.28	66,72,78,78	0
23	PSU	CW	39	20/21	0.93	0.27	57,65,69,71	0
23	MIA	AW	37	29/30	0.93	0.18	37,49,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	4SU	AX	8	20/21	0.93	0.17	53,60,66,68	0
23	PSU	AW	39	20/21	0.94	0.20	55,62,65,67	0
24	5MU	AX	54	21/22	0.94	0.20	54,66,74,75	0
23	5MU	AW	54	21/22	0.94	0.16	38,59,67,72	0
24	5MC	CX	32	21/22	0.94	0.17	51,66,72,75	0
24	5MC	AX	32	21/22	0.96	0.19	43,51,61,70	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3720	1/1	0.33	0.24	73,73,73,73	0
56	MG	DA	3404	1/1	0.39	0.20	49,49,49,49	0
56	MG	AA	3054	1/1	0.42	0.22	68,68,68,68	0
56	MG	DE	305	1/1	0.52	0.23	49,49,49,49	0
56	MG	BA	3372	1/1	0.52	0.13	55,55,55,55	0
56	MG	DA	3449	1/1	0.55	0.13	45,45,45,45	0
56	MG	AA	3139	1/1	0.56	0.20	82,82,82,82	0
56	MG	AA	3122	1/1	0.59	0.14	61,61,61,61	0
56	MG	BA	3469	1/1	0.59	0.17	61,61,61,61	0
56	MG	BA	3640	1/1	0.59	0.16	60,60,60,60	0
56	MG	BA	3694	1/1	0.59	0.23	62,62,62,62	0
56	MG	DA	3500	1/1	0.60	0.19	67,67,67,67	0
56	MG	BA	3617	1/1	0.60	0.12	44,44,44,44	0
56	MG	BA	3793	1/1	0.60	0.17	64,64,64,64	0
56	MG	BA	3759	1/1	0.61	0.12	44,44,44,44	0
56	MG	BA	3784	1/1	0.62	0.20	49,49,49,49	0
56	MG	DA	3582	1/1	0.62	0.19	52,52,52,52	0
56	MG	CA	3058	1/1	0.62	0.21	63,63,63,63	0
56	MG	DA	3247	1/1	0.62	0.12	63,63,63,63	0
56	MG	BA	3714	1/1	0.62	0.09	58,58,58,58	0
56	MG	DA	3621	1/1	0.63	0.16	48,48,48,48	0
56	MG	DA	3383	1/1	0.65	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3454	1/1	0.65	0.19	39,39,39,39	0
56	MG	BA	3766	1/1	0.65	0.09	48,48,48,48	0
56	MG	BA	3643	1/1	0.66	0.18	60,60,60,60	0
56	MG	AW	102	1/1	0.66	0.13	69,69,69,69	0
56	MG	DA	3524	1/1	0.67	0.14	53,53,53,53	0
56	MG	CA	3056	1/1	0.67	0.16	84,84,84,84	0
56	MG	BA	3750	1/1	0.68	0.15	54,54,54,54	0
56	MG	BA	3505	1/1	0.68	0.20	44,44,44,44	0
56	MG	BA	3361	1/1	0.68	0.21	41,41,41,41	0
56	MG	DA	3117	1/1	0.68	0.25	62,62,62,62	0
56	MG	BA	3484	1/1	0.69	0.22	42,42,42,42	0
56	MG	AA	3153	1/1	0.69	0.12	58,58,58,58	0
56	MG	BB	3021	1/1	0.69	0.26	73,73,73,73	0
56	MG	CX	3004	1/1	0.70	0.16	61,61,61,61	0
56	MG	BA	3021	1/1	0.70	0.22	53,53,53,53	0
56	MG	AA	3063	1/1	0.70	0.15	55,55,55,55	0
56	MG	BP	205	1/1	0.70	0.11	44,44,44,44	0
56	MG	DA	3276	1/1	0.70	0.19	60,60,60,60	0
56	MG	BA	3491	1/1	0.71	0.26	44,44,44,44	0
56	MG	AA	3197	1/1	0.71	0.18	65,65,65,65	0
56	MG	BA	3318	1/1	0.71	0.17	53,53,53,53	0
56	MG	AX	3013	1/1	0.71	0.14	61,61,61,61	0
56	MG	DA	3075	1/1	0.72	0.12	57,57,57,57	0
56	MG	BA	3381	1/1	0.72	0.12	56,56,56,56	0
56	MG	CA	3040	1/1	0.72	0.17	57,57,57,57	0
56	MG	AA	3008	1/1	0.72	0.19	71,71,71,71	0
56	MG	BA	3209	1/1	0.72	0.25	58,58,58,58	0
56	MG	BA	3630	1/1	0.72	0.22	29,29,29,29	0
56	MG	DA	3574	1/1	0.72	0.18	48,48,48,48	0
56	MG	BA	3448	1/1	0.72	0.14	48,48,48,48	0
56	MG	DA	3292	1/1	0.72	0.15	53,53,53,53	0
56	MG	DA	3505	1/1	0.72	0.10	61,61,61,61	0
56	MG	BA	3810	1/1	0.73	0.26	46,46,46,46	0
56	MG	DA	3658	1/1	0.73	0.36	60,60,60,60	0
56	MG	DA	3472	1/1	0.73	0.12	57,57,57,57	0
56	MG	BB	3020	1/1	0.73	0.15	64,64,64,64	0
56	MG	AA	3213	1/1	0.73	0.12	64,64,64,64	0
56	MG	DA	3521	1/1	0.73	0.14	56,56,56,56	0
56	MG	BA	3492	1/1	0.73	0.08	43,43,43,43	0
56	MG	BA	3673	1/1	0.73	0.22	62,62,62,62	0
56	MG	CA	3063	1/1	0.73	0.14	53,53,53,53	0
56	MG	CA	3125	1/1	0.73	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3638	1/1	0.74	0.11	58,58,58,58	0
56	MG	BA	3813	1/1	0.74	0.22	59,59,59,59	0
56	MG	BA	3731	1/1	0.74	0.09	64,64,64,64	0
56	MG	DA	3408	1/1	0.74	0.14	53,53,53,53	0
56	MG	CA	3077	1/1	0.74	0.16	54,54,54,54	0
56	MG	BA	3182	1/1	0.74	0.20	59,59,59,59	0
56	MG	BA	3757	1/1	0.74	0.17	49,49,49,49	0
56	MG	AN	502	1/1	0.74	0.12	45,45,45,45	0
56	MG	CA	3078	1/1	0.74	0.12	48,48,48,48	0
56	MG	DA	3181	1/1	0.74	0.18	52,52,52,52	0
56	MG	DA	3447	1/1	0.74	0.23	50,50,50,50	0
56	MG	AB	3001	1/1	0.74	0.22	73,73,73,73	0
56	MG	CA	3188	1/1	0.74	0.16	72,72,72,72	0
56	MG	BA	3466	1/1	0.75	0.21	46,46,46,46	0
56	MG	DA	3040	1/1	0.75	0.13	51,51,51,51	0
56	MG	BA	3095	1/1	0.75	0.17	43,43,43,43	0
56	MG	DA	3355	1/1	0.75	0.14	48,48,48,48	0
56	MG	AW	104	1/1	0.75	0.11	64,64,64,64	0
56	MG	CA	3190	1/1	0.75	0.10	67,67,67,67	0
56	MG	BA	3659	1/1	0.75	0.15	55,55,55,55	0
56	MG	AA	3005	1/1	0.76	0.15	66,66,66,66	0
56	MG	DA	3116	1/1	0.76	0.32	66,66,66,66	0
56	MG	BA	3671	1/1	0.76	0.18	50,50,50,50	0
56	MG	DA	3325	1/1	0.76	0.19	53,53,53,53	0
56	MG	DA	3311	1/1	0.76	0.18	55,55,55,55	0
56	MG	BA	3194	1/1	0.76	0.23	37,37,37,37	0
56	MG	BA	3508	1/1	0.76	0.17	48,48,48,48	0
56	MG	BA	3580	1/1	0.76	0.17	35,35,35,35	0
56	MG	CJ	5001	1/1	0.76	0.15	70,70,70,70	0
56	MG	BW	202	1/1	0.76	0.29	49,49,49,49	0
56	MG	CA	3009	1/1	0.76	0.15	46,46,46,46	0
56	MG	DA	3106	1/1	0.76	0.13	63,63,63,63	0
56	MG	BA	3665	1/1	0.76	0.16	49,49,49,49	0
56	MG	CA	3132	1/1	0.76	0.17	64,64,64,64	0
56	MG	BA	3212	1/1	0.76	0.13	49,49,49,49	0
56	MG	BB	3011	1/1	0.76	0.15	66,66,66,66	0
56	MG	DA	3360	1/1	0.76	0.09	47,47,47,47	0
56	MG	AA	3114	1/1	0.76	0.09	65,65,65,65	0
56	MG	CA	3175	1/1	0.77	0.13	62,62,62,62	0
56	MG	DA	3134	1/1	0.77	0.22	56,56,56,56	0
56	MG	DA	3076	1/1	0.77	0.22	44,44,44,44	0
56	MG	DA	3143	1/1	0.77	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3600	1/1	0.77	0.15	43,43,43,43	0
56	MG	DA	3504	1/1	0.77	0.10	58,58,58,58	0
56	MG	CA	3057	1/1	0.77	0.13	59,59,59,59	0
56	MG	AA	3003	1/1	0.77	0.10	62,62,62,62	0
56	MG	AA	3124	1/1	0.77	0.15	58,58,58,58	0
56	MG	DA	3035	1/1	0.77	0.13	36,36,36,36	0
56	MG	BA	3704	1/1	0.77	0.20	57,57,57,57	0
56	MG	BA	3447	1/1	0.78	0.15	46,46,46,46	0
56	MG	AA	3201	1/1	0.78	0.17	60,60,60,60	0
56	MG	DA	3079	1/1	0.78	0.19	49,49,49,49	0
56	MG	DA	3167	1/1	0.78	0.19	48,48,48,48	0
56	MG	AM	201	1/1	0.78	0.08	53,53,53,53	0
56	MG	BA	3614	1/1	0.78	0.15	53,53,53,53	0
56	MG	AX	3007	1/1	0.78	0.13	58,58,58,58	0
56	MG	BA	3541	1/1	0.78	0.15	59,59,59,59	0
56	MG	DR	5001	1/1	0.78	0.17	51,51,51,51	0
56	MG	DA	3114	1/1	0.78	0.24	55,55,55,55	0
56	MG	BA	3819	1/1	0.78	0.15	61,61,61,61	0
56	MG	DA	3542	1/1	0.78	0.11	45,45,45,45	0
56	MG	BA	3881	1/1	0.78	0.13	47,47,47,47	0
56	MG	DA	3461	1/1	0.78	0.08	48,48,48,48	0
56	MG	DA	3220	1/1	0.78	0.22	69,69,69,69	0
56	MG	AA	3147	1/1	0.78	0.17	65,65,65,65	0
56	MG	BA	3274	1/1	0.78	0.30	45,45,45,45	0
56	MG	AA	3099	1/1	0.79	0.11	64,64,64,64	0
56	MG	AA	3154	1/1	0.79	0.15	44,44,44,44	0
56	MG	DA	3100	1/1	0.79	0.16	46,46,46,46	0
56	MG	DA	3349	1/1	0.79	0.15	50,50,50,50	0
56	MG	DB	3016	1/1	0.79	0.23	61,61,61,61	0
56	MG	B6	101	1/1	0.79	0.24	47,47,47,47	0
56	MG	BB	3016	1/1	0.79	0.18	49,49,49,49	0
56	MG	BA	3474	1/1	0.79	0.15	53,53,53,53	0
56	MG	CA	3152	1/1	0.79	0.12	67,67,67,67	0
56	MG	B8	102	1/1	0.79	0.27	42,42,42,42	0
56	MG	AW	101	1/1	0.79	0.12	58,58,58,58	0
56	MG	AA	3192	1/1	0.79	0.12	50,50,50,50	0
56	MG	DA	3274	1/1	0.79	0.05	47,47,47,47	0
56	MG	DA	3673	1/1	0.79	0.12	61,61,61,61	0
56	MG	DA	3511	1/1	0.79	0.11	31,31,31,31	0
56	MG	BZ	3001	1/1	0.79	0.26	69,69,69,69	0
59	ZN	D4	501	1/1	0.79	0.09	95,95,95,95	0
56	MG	BA	3565	1/1	0.79	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3487	1/1	0.79	0.20	50,50,50,50	0
56	MG	BA	3147	1/1	0.79	0.23	39,39,39,39	0
56	MG	BA	3596	1/1	0.79	0.22	44,44,44,44	0
56	MG	AA	3137	1/1	0.79	0.10	64,64,64,64	0
56	MG	CA	3011	1/1	0.79	0.20	56,56,56,56	0
56	MG	DA	3453	1/1	0.79	0.24	51,51,51,51	0
56	MG	BA	3635	1/1	0.79	0.11	65,65,65,65	0
56	MG	BB	3026	1/1	0.79	0.24	66,66,66,66	0
56	MG	AR	101	1/1	0.79	0.27	56,56,56,56	0
56	MG	DA	3433	1/1	0.79	0.15	40,40,40,40	0
56	MG	AA	3131	1/1	0.80	0.12	56,56,56,56	0
56	MG	DA	3301	1/1	0.80	0.12	52,52,52,52	0
56	MG	BA	3628	1/1	0.80	0.13	51,51,51,51	0
56	MG	DA	3321	1/1	0.80	0.22	39,39,39,39	0
56	MG	BB	3013	1/1	0.80	0.14	52,52,52,52	0
56	MG	DA	3432	1/1	0.80	0.15	57,57,57,57	0
56	MG	BA	3611	1/1	0.80	0.12	61,61,61,61	0
56	MG	DA	3087	1/1	0.80	0.17	48,48,48,48	0
56	MG	BA	3456	1/1	0.80	0.20	41,41,41,41	0
56	MG	DA	3397	1/1	0.80	0.13	53,53,53,53	0
56	MG	DA	3160	1/1	0.80	0.43	38,38,38,38	0
56	MG	CA	3081	1/1	0.80	0.28	56,56,56,56	0
56	MG	DA	3228	1/1	0.80	0.16	38,38,38,38	0
56	MG	DA	3007	1/1	0.80	0.22	54,54,54,54	0
56	MG	DA	3370	1/1	0.80	0.19	49,49,49,49	0
56	MG	BA	3805	1/1	0.80	0.17	32,32,32,32	0
56	MG	DA	3529	1/1	0.80	0.09	48,48,48,48	0
56	MG	BA	3748	1/1	0.80	0.23	58,58,58,58	0
56	MG	DF	303	1/1	0.80	0.15	42,42,42,42	0
56	MG	CA	3041	1/1	0.80	0.11	49,49,49,49	0
56	MG	DB	3002	1/1	0.80	0.14	68,68,68,68	0
56	MG	BA	3409	1/1	0.80	0.10	65,65,65,65	0
56	MG	CG	5001	1/1	0.81	0.09	64,64,64,64	0
56	MG	DA	3023	1/1	0.81	0.14	48,48,48,48	0
56	MG	DA	3034	1/1	0.81	0.12	51,51,51,51	0
56	MG	AA	3214	1/1	0.81	0.14	60,60,60,60	0
56	MG	DA	3151	1/1	0.81	0.11	59,59,59,59	0
56	MG	AA	3210	1/1	0.81	0.14	76,76,76,76	0
56	MG	AA	3223	1/1	0.81	0.11	72,72,72,72	0
56	MG	BA	3203	1/1	0.81	0.24	41,41,41,41	0
56	MG	CA	3186	1/1	0.81	0.18	62,62,62,62	0
56	MG	BA	3161	1/1	0.81	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3133	1/1	0.81	0.17	45,45,45,45	0
56	MG	DA	3579	1/1	0.81	0.09	48,48,48,48	0
56	MG	CW	3002	1/1	0.81	0.15	60,60,60,60	0
56	MG	DA	3348	1/1	0.81	0.19	32,32,32,32	0
56	MG	BA	3719	1/1	0.81	0.17	61,61,61,61	0
56	MG	DW	3003	1/1	0.81	0.33	47,47,47,47	0
56	MG	BA	3005	1/1	0.81	0.15	49,49,49,49	0
56	MG	DA	3424	1/1	0.81	0.17	47,47,47,47	0
56	MG	AA	3047	1/1	0.81	0.15	56,56,56,56	0
56	MG	DA	3463	1/1	0.81	0.13	52,52,52,52	0
56	MG	BA	3501	1/1	0.81	0.30	50,50,50,50	0
56	MG	DA	3575	1/1	0.81	0.14	51,51,51,51	0
56	MG	DA	3668	1/1	0.81	0.16	61,61,61,61	0
56	MG	DA	3188	1/1	0.81	0.14	44,44,44,44	0
56	MG	BA	3727	1/1	0.81	0.31	64,64,64,64	0
56	MG	DA	3513	1/1	0.81	0.21	54,54,54,54	0
56	MG	AA	3120	1/1	0.81	0.10	67,67,67,67	0
56	MG	DA	3611	1/1	0.81	0.22	65,65,65,65	0
56	MG	BA	3285	1/1	0.81	0.29	48,48,48,48	0
56	MG	BA	3556	1/1	0.81	0.15	48,48,48,48	0
56	MG	AA	3023	1/1	0.81	0.15	56,56,56,56	0
56	MG	AA	3015	1/1	0.81	0.10	71,71,71,71	0
56	MG	DA	3018	1/1	0.81	0.12	45,45,45,45	0
56	MG	AA	3165	1/1	0.81	0.10	57,57,57,57	0
56	MG	BA	3566	1/1	0.81	0.16	25,25,25,25	0
56	MG	BA	3426	1/1	0.82	0.25	42,42,42,42	0
56	MG	AA	3222	1/1	0.82	0.15	55,55,55,55	0
56	MG	DA	3045	1/1	0.82	0.17	52,52,52,52	0
56	MG	CA	3158	1/1	0.82	0.11	76,76,76,76	0
56	MG	BA	3111	1/1	0.82	0.10	60,60,60,60	0
56	MG	BA	3094	1/1	0.82	0.20	33,33,33,33	0
56	MG	DA	3157	1/1	0.82	0.18	54,54,54,54	0
56	MG	BA	3058	1/1	0.82	0.15	48,48,48,48	0
56	MG	AE	3001	1/1	0.82	0.12	65,65,65,65	0
56	MG	DA	3223	1/1	0.82	0.18	51,51,51,51	0
56	MG	DA	3531	1/1	0.82	0.12	56,56,56,56	0
56	MG	BA	3083	1/1	0.82	0.17	54,54,54,54	0
56	MG	AA	3096	1/1	0.82	0.12	60,60,60,60	0
56	MG	DA	3216	1/1	0.82	0.10	48,48,48,48	0
56	MG	CA	3127	1/1	0.82	0.12	57,57,57,57	0
56	MG	DA	3591	1/1	0.82	0.08	55,55,55,55	0
56	MG	DB	3013	1/1	0.82	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BG	204	1/1	0.82	0.11	58,58,58,58	0
56	MG	DA	3506	1/1	0.82	0.18	55,55,55,55	0
56	MG	DW	3001	1/1	0.82	0.33	44,44,44,44	0
56	MG	DA	3261	1/1	0.82	0.14	47,47,47,47	0
56	MG	DA	3322	1/1	0.82	0.15	41,41,41,41	0
56	MG	CA	3088	1/1	0.82	0.32	62,62,62,62	0
56	MG	DA	3608	1/1	0.82	0.10	55,55,55,55	0
56	MG	DA	3395	1/1	0.82	0.14	45,45,45,45	0
56	MG	BA	3581	1/1	0.82	0.18	33,33,33,33	0
56	MG	B0	103	1/1	0.82	0.18	49,49,49,49	0
56	MG	DA	3125	1/1	0.82	0.24	44,44,44,44	0
56	MG	BA	3348	1/1	0.82	0.13	65,65,65,65	0
56	MG	CA	3116	1/1	0.82	0.23	54,54,54,54	0
56	MG	BA	3639	1/1	0.82	0.15	59,59,59,59	0
56	MG	DA	3328	1/1	0.82	0.23	64,64,64,64	0
56	MG	CA	3053	1/1	0.82	0.16	61,61,61,61	0
56	MG	CA	3114	1/1	0.82	0.26	60,60,60,60	0
56	MG	BA	3066	1/1	0.82	0.16	54,54,54,54	0
56	MG	BA	3314	1/1	0.82	0.19	60,60,60,60	0
56	MG	AA	3044	1/1	0.82	0.19	54,54,54,54	0
56	MG	CA	3061	1/1	0.82	0.21	58,58,58,58	0
56	MG	DA	3288	1/1	0.83	0.17	44,44,44,44	0
56	MG	AA	3117	1/1	0.83	0.15	68,68,68,68	0
56	MG	DA	3612	1/1	0.83	0.15	52,52,52,52	0
56	MG	AA	3028	1/1	0.83	0.24	50,50,50,50	0
56	MG	DA	3610	1/1	0.83	0.25	61,61,61,61	0
56	MG	AA	3060	1/1	0.83	0.21	62,62,62,62	0
56	MG	B0	101	1/1	0.83	0.22	44,44,44,44	0
56	MG	CA	3173	1/1	0.83	0.13	81,81,81,81	0
56	MG	B4	502	1/1	0.83	0.12	65,65,65,65	0
56	MG	BA	3699	1/1	0.83	0.13	45,45,45,45	0
56	MG	CA	3001	1/1	0.83	0.09	67,67,67,67	0
56	MG	AA	3071	1/1	0.83	0.26	61,61,61,61	0
56	MG	CA	3021	1/1	0.83	0.26	79,79,79,79	0
56	MG	BO	3001	1/1	0.83	0.30	62,62,62,62	0
56	MG	BA	3103	1/1	0.83	0.17	58,58,58,58	0
56	MG	CA	3193	1/1	0.83	0.09	66,66,66,66	0
56	MG	DA	3515	1/1	0.83	0.21	59,59,59,59	0
56	MG	BE	302	1/1	0.83	0.21	27,27,27,27	0
56	MG	BA	3298	1/1	0.83	0.27	51,51,51,51	0
56	MG	AA	3080	1/1	0.83	0.20	61,61,61,61	0
56	MG	BA	3351	1/1	0.83	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3219	1/1	0.83	0.21	63,63,63,63	0
56	MG	AA	3089	1/1	0.83	0.26	66,66,66,66	0
56	MG	BA	3486	1/1	0.83	0.19	29,29,29,29	0
56	MG	BA	3502	1/1	0.83	0.12	56,56,56,56	0
56	MG	BA	3795	1/1	0.83	0.22	22,22,22,22	0
56	MG	AA	3056	1/1	0.83	0.26	60,60,60,60	0
56	MG	DA	3129	1/1	0.83	0.22	37,37,37,37	0
56	MG	CA	3015	1/1	0.83	0.23	57,57,57,57	0
56	MG	BA	3493	1/1	0.83	0.14	41,41,41,41	0
56	MG	BA	3472	1/1	0.83	0.14	31,31,31,31	0
56	MG	BA	3855	1/1	0.83	0.11	53,53,53,53	0
56	MG	DA	3393	1/1	0.83	0.11	55,55,55,55	0
56	MG	CA	3090	1/1	0.83	0.11	74,74,74,74	0
56	MG	BA	3533	1/1	0.83	0.17	47,47,47,47	0
56	MG	BA	3557	1/1	0.83	0.14	41,41,41,41	0
56	MG	DA	3161	1/1	0.83	0.12	41,41,41,41	0
56	MG	DA	3429	1/1	0.83	0.14	35,35,35,35	0
56	MG	AA	3090	1/1	0.83	0.17	51,51,51,51	0
56	MG	DA	3329	1/1	0.83	0.15	51,51,51,51	0
56	MG	CA	3023	1/1	0.83	0.20	60,60,60,60	0
56	MG	BA	3573	1/1	0.83	0.18	34,34,34,34	0
56	MG	BA	3623	1/1	0.83	0.08	48,48,48,48	0
56	MG	CW	3004	1/1	0.83	0.19	64,64,64,64	0
56	MG	CA	3084	1/1	0.83	0.23	57,57,57,57	0
56	MG	BA	3906	1/1	0.83	0.23	48,48,48,48	0
56	MG	CX	3005	1/1	0.83	0.31	60,60,60,60	0
56	MG	DA	3363	1/1	0.83	0.13	42,42,42,42	0
56	MG	DA	3150	1/1	0.83	0.20	42,42,42,42	0
56	MG	BA	3445	1/1	0.83	0.15	48,48,48,48	0
56	MG	BA	3754	1/1	0.83	0.16	54,54,54,54	0
56	MG	CA	3184	1/1	0.83	0.14	68,68,68,68	0
56	MG	CA	3004	1/1	0.83	0.12	66,66,66,66	0
56	MG	CA	3138	1/1	0.84	0.14	59,59,59,59	0
56	MG	BA	3322	1/1	0.84	0.29	57,57,57,57	0
56	MG	AA	3031	1/1	0.84	0.15	43,43,43,43	0
56	MG	DA	3541	1/1	0.84	0.14	59,59,59,59	0
56	MG	DA	3238	1/1	0.84	0.20	48,48,48,48	0
56	MG	DA	3074	1/1	0.84	0.10	45,45,45,45	0
56	MG	CA	3020	1/1	0.84	0.17	57,57,57,57	0
56	MG	CA	3161	1/1	0.84	0.07	61,61,61,61	0
56	MG	BQ	3003	1/1	0.84	0.19	54,54,54,54	0
56	MG	BA	3417	1/1	0.84	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3844	1/1	0.84	0.13	49,49,49,49	0
56	MG	BA	3739	1/1	0.84	0.16	49,49,49,49	0
56	MG	DA	3446	1/1	0.84	0.14	68,68,68,68	0
56	MG	DA	3289	1/1	0.84	0.14	53,53,53,53	0
56	MG	DA	3002	1/1	0.84	0.12	60,60,60,60	0
56	MG	BN	3002	1/1	0.84	0.19	38,38,38,38	0
56	MG	DA	3362	1/1	0.84	0.14	61,61,61,61	0
57	UAM	CA	3202	30/30	0.84	0.38	45,72,83,85	0
56	MG	AD	502	1/1	0.84	0.25	55,55,55,55	0
56	MG	BA	3020	1/1	0.84	0.21	46,46,46,46	0
56	MG	BA	3204	1/1	0.84	0.14	34,34,34,34	0
56	MG	AA	3037	1/1	0.84	0.31	63,63,63,63	0
56	MG	CA	3073	1/1	0.84	0.10	64,64,64,64	0
56	MG	DB	3019	1/1	0.84	0.29	60,60,60,60	0
56	MG	AA	3009	1/1	0.84	0.11	49,49,49,49	0
56	MG	BA	3142	1/1	0.84	0.43	46,46,46,46	0
56	MG	D5	101	1/1	0.84	0.10	45,45,45,45	0
56	MG	DA	3633	1/1	0.84	0.17	50,50,50,50	0
56	MG	DA	3195	1/1	0.84	0.14	39,39,39,39	0
56	MG	BA	3356	1/1	0.84	0.10	52,52,52,52	0
56	MG	BA	3459	1/1	0.84	0.25	38,38,38,38	0
56	MG	DA	3062	1/1	0.84	0.14	49,49,49,49	0
56	MG	DA	3056	1/1	0.84	0.20	41,41,41,41	0
56	MG	BA	3552	1/1	0.84	0.17	38,38,38,38	0
56	MG	AA	3012	1/1	0.84	0.14	63,63,63,63	0
56	MG	BA	3432	1/1	0.84	0.10	55,55,55,55	0
56	MG	CA	3130	1/1	0.84	0.13	62,62,62,62	0
56	MG	DA	3445	1/1	0.84	0.14	45,45,45,45	0
56	MG	CA	3091	1/1	0.84	0.15	67,67,67,67	0
56	MG	DA	3107	1/1	0.84	0.21	48,48,48,48	0
56	MG	BA	3359	1/1	0.84	0.20	58,58,58,58	0
56	MG	DA	3372	1/1	0.84	0.09	51,51,51,51	0
56	MG	BA	3214	1/1	0.84	0.20	44,44,44,44	0
56	MG	BA	3269	1/1	0.84	0.17	45,45,45,45	0
56	MG	AA	3170	1/1	0.84	0.13	67,67,67,67	0
56	MG	BA	3482	1/1	0.84	0.22	39,39,39,39	0
56	MG	AA	3187	1/1	0.84	0.17	65,65,65,65	0
56	MG	BA	3849	1/1	0.84	0.21	29,29,29,29	0
56	MG	BA	3743	1/1	0.84	0.19	50,50,50,50	0
56	MG	BA	3901	1/1	0.84	0.16	39,39,39,39	0
56	MG	BA	3610	1/1	0.84	0.15	60,60,60,60	0
56	MG	AA	3073	1/1	0.84	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3585	1/1	0.84	0.17	36,36,36,36	0
56	MG	AA	3182	1/1	0.84	0.22	65,65,65,65	0
56	MG	DA	3588	1/1	0.84	0.15	64,64,64,64	0
56	MG	DA	3387	1/1	0.84	0.18	46,46,46,46	0
56	MG	AA	3218	1/1	0.84	0.07	75,75,75,75	0
56	MG	CA	3160	1/1	0.84	0.11	55,55,55,55	0
56	MG	BI	3001	1/1	0.84	0.08	60,60,60,60	0
56	MG	DE	301	1/1	0.84	0.17	47,47,47,47	0
56	MG	AA	3079	1/1	0.84	0.25	60,60,60,60	0
56	MG	CA	3013	1/1	0.84	0.19	62,62,62,62	0
56	MG	AA	3014	1/1	0.85	0.12	47,47,47,47	0
56	MG	BA	3512	1/1	0.85	0.16	57,57,57,57	0
56	MG	CA	3071	1/1	0.85	0.18	68,68,68,68	0
56	MG	DA	3519	1/1	0.85	0.14	46,46,46,46	0
56	MG	BA	3306	1/1	0.85	0.16	28,28,28,28	0
56	MG	BA	3168	1/1	0.85	0.17	35,35,35,35	0
56	MG	CA	3124	1/1	0.85	0.08	57,57,57,57	0
56	MG	BA	3818	1/1	0.85	0.19	58,58,58,58	0
56	MG	DA	3417	1/1	0.85	0.20	53,53,53,53	0
56	MG	BA	3261	1/1	0.85	0.26	38,38,38,38	0
56	MG	DA	3266	1/1	0.85	0.18	44,44,44,44	0
56	MG	BA	3365	1/1	0.85	0.08	44,44,44,44	0
56	MG	DA	3503	1/1	0.85	0.11	57,57,57,57	0
56	MG	BA	3471	1/1	0.85	0.12	57,57,57,57	0
56	MG	DF	302	1/1	0.85	0.10	55,55,55,55	0
56	MG	BA	3104	1/1	0.85	0.13	58,58,58,58	0
56	MG	DA	3415	1/1	0.85	0.19	39,39,39,39	0
56	MG	DA	3215	1/1	0.85	0.20	60,60,60,60	0
56	MG	CX	3002	1/1	0.85	0.18	63,63,63,63	0
56	MG	CA	3007	1/1	0.85	0.15	66,66,66,66	0
56	MG	AA	3200	1/1	0.85	0.20	61,61,61,61	0
56	MG	AA	3026	1/1	0.85	0.17	50,50,50,50	0
56	MG	DA	3380	1/1	0.85	0.13	49,49,49,49	0
56	MG	DA	3211	1/1	0.85	0.09	37,37,37,37	0
56	MG	D0	3001	1/1	0.85	0.12	51,51,51,51	0
56	MG	BA	3751	1/1	0.85	0.20	51,51,51,51	0
56	MG	CA	3192	1/1	0.85	0.20	69,69,69,69	0
56	MG	DA	3509	1/1	0.85	0.18	55,55,55,55	0
56	MG	AA	3231	1/1	0.85	0.25	61,61,61,61	0
56	MG	AX	3003	1/1	0.85	0.25	50,50,50,50	0
56	MG	BA	3801	1/1	0.85	0.13	27,27,27,27	0
56	MG	BA	3877	1/1	0.85	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3390	1/1	0.85	0.09	33,33,33,33	0
56	MG	CA	3135	1/1	0.85	0.22	57,57,57,57	0
56	MG	DA	3502	1/1	0.85	0.09	63,63,63,63	0
56	MG	DA	3402	1/1	0.85	0.17	56,56,56,56	0
56	MG	BA	3355	1/1	0.85	0.21	35,35,35,35	0
56	MG	CA	3019	1/1	0.85	0.11	44,44,44,44	0
56	MG	AA	3111	1/1	0.85	0.17	57,57,57,57	0
56	MG	CX	3006	1/1	0.85	0.11	50,50,50,50	0
56	MG	DA	3430	1/1	0.85	0.14	35,35,35,35	0
56	MG	AA	3101	1/1	0.85	0.12	45,45,45,45	0
56	MG	DA	3102	1/1	0.85	0.15	51,51,51,51	0
56	MG	DA	3566	1/1	0.85	0.08	67,67,67,67	0
56	MG	BA	3675	1/1	0.85	0.19	38,38,38,38	0
56	MG	BA	3165	1/1	0.85	0.24	32,32,32,32	0
56	MG	BA	3208	1/1	0.85	0.29	62,62,62,62	0
56	MG	BA	3782	1/1	0.85	0.21	46,46,46,46	0
56	MG	BA	3527	1/1	0.85	0.13	57,57,57,57	0
56	MG	DA	3296	1/1	0.85	0.10	56,56,56,56	0
56	MG	DA	3366	1/1	0.85	0.19	53,53,53,53	0
56	MG	CL	202	1/1	0.85	0.19	50,50,50,50	0
56	MG	DB	3007	1/1	0.85	0.17	64,64,64,64	0
56	MG	BF	307	1/1	0.85	0.17	31,31,31,31	0
56	MG	BA	3691	1/1	0.85	0.19	55,55,55,55	0
56	MG	DA	3270	1/1	0.85	0.17	33,33,33,33	0
56	MG	DA	3050	1/1	0.85	0.16	45,45,45,45	0
56	MG	CA	3039	1/1	0.85	0.14	55,55,55,55	0
56	MG	DU	3004	1/1	0.85	0.15	48,48,48,48	0
56	MG	AA	3084	1/1	0.85	0.16	53,53,53,53	0
56	MG	DA	3555	1/1	0.85	0.14	30,30,30,30	0
56	MG	DA	3225	1/1	0.86	0.16	38,38,38,38	0
56	MG	AA	3091	1/1	0.86	0.15	50,50,50,50	0
56	MG	DA	3092	1/1	0.86	0.14	50,50,50,50	0
56	MG	BA	3715	1/1	0.86	0.11	53,53,53,53	0
56	MG	BA	3097	1/1	0.86	0.17	48,48,48,48	0
56	MG	CA	3086	1/1	0.86	0.18	62,62,62,62	0
56	MG	DA	3490	1/1	0.86	0.09	51,51,51,51	0
56	MG	DA	3400	1/1	0.86	0.15	36,36,36,36	0
56	MG	AA	3158	1/1	0.86	0.24	54,54,54,54	0
56	MG	BB	3012	1/1	0.86	0.07	61,61,61,61	0
57	UAM	AA	3232	30/30	0.86	0.31	44,65,77,80	0
56	MG	DA	3303	1/1	0.86	0.10	30,30,30,30	0
56	MG	CA	3064	1/1	0.86	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3481	1/1	0.86	0.13	31,31,31,31	0
56	MG	AA	3149	1/1	0.86	0.11	51,51,51,51	0
56	MG	BA	3271	1/1	0.86	0.17	54,54,54,54	0
56	MG	BA	3567	1/1	0.86	0.14	46,46,46,46	0
56	MG	BA	3051	1/1	0.86	0.21	51,51,51,51	0
56	MG	BA	3470	1/1	0.86	0.17	46,46,46,46	0
56	MG	AA	3177	1/1	0.86	0.10	57,57,57,57	0
56	MG	BA	3399	1/1	0.86	0.12	57,57,57,57	0
56	MG	BA	3603	1/1	0.86	0.09	42,42,42,42	0
56	MG	BA	3518	1/1	0.86	0.09	57,57,57,57	0
56	MG	BA	3716	1/1	0.86	0.08	47,47,47,47	0
56	MG	BA	3729	1/1	0.86	0.23	56,56,56,56	0
56	MG	DA	3458	1/1	0.86	0.09	55,55,55,55	0
56	MG	BA	3540	1/1	0.86	0.10	50,50,50,50	0
56	MG	BA	3425	1/1	0.86	0.09	60,60,60,60	0
56	MG	DA	3414	1/1	0.86	0.20	56,56,56,56	0
56	MG	DB	3001	1/1	0.86	0.17	71,71,71,71	0
56	MG	DA	3438	1/1	0.86	0.16	42,42,42,42	0
56	MG	DA	3128	1/1	0.86	0.20	45,45,45,45	0
56	MG	AA	3027	1/1	0.86	0.26	60,60,60,60	0
56	MG	CA	3170	1/1	0.86	0.09	61,61,61,61	0
56	MG	BA	3579	1/1	0.86	0.21	42,42,42,42	0
56	MG	BA	3575	1/1	0.86	0.24	27,27,27,27	0
56	MG	CA	3049	1/1	0.86	0.45	67,67,67,67	0
56	MG	AA	3189	1/1	0.86	0.12	53,53,53,53	0
56	MG	BA	3446	1/1	0.86	0.17	63,63,63,63	0
56	MG	BA	3607	1/1	0.86	0.05	57,57,57,57	0
56	MG	DA	3252	1/1	0.86	0.08	57,57,57,57	0
56	MG	DG	3001	1/1	0.86	0.20	53,53,53,53	0
56	MG	BA	3571	1/1	0.86	0.21	23,23,23,23	0
56	MG	AA	3085	1/1	0.86	0.15	47,47,47,47	0
56	MG	CF	3002	1/1	0.86	0.17	59,59,59,59	0
56	MG	DA	3625	1/1	0.86	0.09	50,50,50,50	0
56	MG	DA	3244	1/1	0.86	0.09	47,47,47,47	0
56	MG	CA	3183	1/1	0.86	0.18	69,69,69,69	0
56	MG	BA	3262	1/1	0.86	0.29	48,48,48,48	0
56	MG	BB	3028	1/1	0.86	0.17	42,42,42,42	0
56	MG	CA	3169	1/1	0.86	0.11	60,60,60,60	0
56	MG	AA	3018	1/1	0.87	0.14	73,73,73,73	0
56	MG	AA	3050	1/1	0.87	0.25	67,67,67,67	0
56	MG	DA	3314	1/1	0.87	0.14	38,38,38,38	0
56	MG	DA	3607	1/1	0.87	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3385	1/1	0.87	0.17	47,47,47,47	0
56	MG	BG	203	1/1	0.87	0.20	51,51,51,51	0
56	MG	DA	3632	1/1	0.87	0.15	57,57,57,57	0
56	MG	BA	3763	1/1	0.87	0.14	58,58,58,58	0
56	MG	BA	3796	1/1	0.87	0.15	29,29,29,29	0
56	MG	BA	3102	1/1	0.87	0.24	44,44,44,44	0
56	MG	DA	3121	1/1	0.87	0.20	41,41,41,41	0
56	MG	AA	3025	1/1	0.87	0.12	50,50,50,50	0
56	MG	AA	3181	1/1	0.87	0.14	70,70,70,70	0
56	MG	BA	3320	1/1	0.87	0.22	50,50,50,50	0
56	MG	BA	3263	1/1	0.87	0.23	42,42,42,42	0
56	MG	DA	3618	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3207	1/1	0.87	0.12	53,53,53,53	0
56	MG	CA	3085	1/1	0.87	0.15	53,53,53,53	0
56	MG	BE	309	1/1	0.87	0.19	31,31,31,31	0
56	MG	CA	3050	1/1	0.87	0.09	72,72,72,72	0
56	MG	BA	3672	1/1	0.87	0.18	24,24,24,24	0
56	MG	CA	3103	1/1	0.87	0.12	63,63,63,63	0
56	MG	CA	3157	1/1	0.87	0.16	72,72,72,72	0
56	MG	BA	3831	1/1	0.87	0.18	53,53,53,53	0
56	MG	BA	3871	1/1	0.87	0.15	55,55,55,55	0
56	MG	CA	3140	1/1	0.87	0.13	56,56,56,56	0
56	MG	DA	3444	1/1	0.87	0.16	40,40,40,40	0
56	MG	BA	3100	1/1	0.87	0.28	33,33,33,33	0
56	MG	BA	3002	1/1	0.87	0.18	53,53,53,53	0
56	MG	DA	3570	1/1	0.87	0.11	28,28,28,28	0
56	MG	DA	3580	1/1	0.87	0.14	40,40,40,40	0
56	MG	AA	3082	1/1	0.87	0.21	34,34,34,34	0
56	MG	AA	3107	1/1	0.87	0.17	53,53,53,53	0
56	MG	BA	3836	1/1	0.87	0.23	59,59,59,59	0
56	MG	BE	306	1/1	0.87	0.19	34,34,34,34	0
56	MG	BA	3619	1/1	0.87	0.09	68,68,68,68	0
56	MG	CA	3089	1/1	0.87	0.24	65,65,65,65	0
56	MG	DA	3015	1/1	0.87	0.18	37,37,37,37	0
56	MG	DA	3077	1/1	0.87	0.12	44,44,44,44	0
56	MG	AA	3126	1/1	0.87	0.29	54,54,54,54	0
56	MG	CA	3195	1/1	0.87	0.12	69,69,69,69	0
56	MG	BA	3107	1/1	0.87	0.26	50,50,50,50	0
56	MG	AA	3019	1/1	0.87	0.18	54,54,54,54	0
56	MG	CA	3069	1/1	0.87	0.13	57,57,57,57	0
56	MG	AA	3109	1/1	0.87	0.14	60,60,60,60	0
56	MG	DA	3551	1/1	0.87	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3621	1/1	0.87	0.19	50,50,50,50	0
56	MG	BA	3842	1/1	0.87	0.18	43,43,43,43	0
56	MG	BA	3707	1/1	0.87	0.24	53,53,53,53	0
56	MG	DA	3617	1/1	0.87	0.09	49,49,49,49	0
56	MG	DA	3585	1/1	0.87	0.10	51,51,51,51	0
56	MG	BA	3415	1/1	0.87	0.17	33,33,33,33	0
56	MG	AX	3011	1/1	0.87	0.19	53,53,53,53	0
56	MG	BA	3663	1/1	0.87	0.13	39,39,39,39	0
56	MG	DA	3536	1/1	0.87	0.15	51,51,51,51	0
56	MG	CA	3002	1/1	0.87	0.13	55,55,55,55	0
56	MG	CP	101	1/1	0.87	0.19	57,57,57,57	0
56	MG	DA	3597	1/1	0.87	0.16	54,54,54,54	0
56	MG	DA	3054	1/1	0.87	0.26	52,52,52,52	0
56	MG	BA	3898	1/1	0.87	0.15	44,44,44,44	0
56	MG	CA	3172	1/1	0.87	0.14	54,54,54,54	0
56	MG	BG	202	1/1	0.87	0.17	36,36,36,36	0
56	MG	DA	3654	1/1	0.87	0.09	53,53,53,53	0
56	MG	DA	3664	1/1	0.87	0.13	71,71,71,71	0
56	MG	BA	3130	1/1	0.87	0.20	43,43,43,43	0
56	MG	DA	3191	1/1	0.87	0.09	52,52,52,52	0
56	MG	BA	3465	1/1	0.87	0.27	43,43,43,43	0
56	MG	CA	3102	1/1	0.88	0.17	52,52,52,52	0
56	MG	BA	3488	1/1	0.88	0.22	31,31,31,31	0
56	MG	BA	3882	1/1	0.88	0.25	53,53,53,53	0
56	MG	CA	3162	1/1	0.88	0.15	68,68,68,68	0
56	MG	BA	3840	1/1	0.88	0.17	50,50,50,50	0
56	MG	DA	3662	1/1	0.88	0.35	52,52,52,52	0
56	MG	BA	3424	1/1	0.88	0.11	50,50,50,50	0
56	MG	CA	3072	1/1	0.88	0.10	55,55,55,55	0
56	MG	BA	3389	1/1	0.88	0.20	21,21,21,21	0
56	MG	BA	3838	1/1	0.88	0.15	47,47,47,47	0
56	MG	BA	3833	1/1	0.88	0.20	57,57,57,57	0
56	MG	AA	3045	1/1	0.88	0.28	47,47,47,47	0
56	MG	DA	3653	1/1	0.88	0.15	46,46,46,46	0
56	MG	DA	3482	1/1	0.88	0.20	53,53,53,53	0
56	MG	DA	3265	1/1	0.88	0.16	39,39,39,39	0
56	MG	DA	3218	1/1	0.88	0.19	62,62,62,62	0
56	MG	BA	3589	1/1	0.88	0.27	42,42,42,42	0
56	MG	BA	3752	1/1	0.88	0.14	54,54,54,54	0
56	MG	AA	3040	1/1	0.88	0.18	68,68,68,68	0
56	MG	AA	3061	1/1	0.88	0.31	51,51,51,51	0
56	MG	BA	3173	1/1	0.88	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3028	1/1	0.88	0.10	45,45,45,45	0
56	MG	DA	3426	1/1	0.88	0.15	41,41,41,41	0
56	MG	BA	3048	1/1	0.88	0.24	36,36,36,36	0
56	MG	BA	3545	1/1	0.88	0.12	43,43,43,43	0
56	MG	AX	3006	1/1	0.88	0.15	46,46,46,46	0
56	MG	CA	3017	1/1	0.88	0.21	56,56,56,56	0
56	MG	AA	3194	1/1	0.88	0.14	58,58,58,58	0
56	MG	BA	3451	1/1	0.88	0.15	38,38,38,38	0
56	MG	BA	3476	1/1	0.88	0.22	54,54,54,54	0
56	MG	BA	3830	1/1	0.88	0.18	56,56,56,56	0
56	MG	DA	3550	1/1	0.88	0.09	63,63,63,63	0
56	MG	DA	3650	1/1	0.88	0.13	53,53,53,53	0
56	MG	DA	3624	1/1	0.88	0.12	32,32,32,32	0
56	MG	CA	3164	1/1	0.88	0.07	63,63,63,63	0
56	MG	BA	3865	1/1	0.88	0.18	36,36,36,36	0
56	MG	CA	3046	1/1	0.88	0.16	42,42,42,42	0
56	MG	BA	3730	1/1	0.88	0.27	45,45,45,45	0
56	MG	BA	3144	1/1	0.88	0.27	53,53,53,53	0
56	MG	DA	3338	1/1	0.88	0.10	43,43,43,43	0
56	MG	AA	3036	1/1	0.88	0.18	46,46,46,46	0
56	MG	BQ	3001	1/1	0.88	0.29	41,41,41,41	0
56	MG	DA	3577	1/1	0.88	0.10	54,54,54,54	0
56	MG	BA	3211	1/1	0.88	0.35	63,63,63,63	0
56	MG	BG	205	1/1	0.88	0.13	40,40,40,40	0
56	MG	CA	3191	1/1	0.88	0.14	71,71,71,71	0
56	MG	CA	3155	1/1	0.88	0.19	72,72,72,72	0
56	MG	DA	3176	1/1	0.88	0.21	36,36,36,36	0
56	MG	BA	3867	1/1	0.88	0.12	58,58,58,58	0
56	MG	AA	3221	1/1	0.88	0.13	55,55,55,55	0
56	MG	DA	3471	1/1	0.88	0.12	49,49,49,49	0
56	MG	BA	3294	1/1	0.88	0.22	38,38,38,38	0
56	MG	BA	3649	1/1	0.88	0.15	24,24,24,24	0
56	MG	DA	3158	1/1	0.88	0.09	49,49,49,49	0
56	MG	DA	3229	1/1	0.88	0.22	43,43,43,43	0
56	MG	DA	3622	1/1	0.88	0.18	51,51,51,51	0
56	MG	DA	3568	1/1	0.88	0.18	30,30,30,30	0
56	MG	BA	3515	1/1	0.88	0.18	64,64,64,64	0
56	MG	CA	3108	1/1	0.88	0.23	57,57,57,57	0
56	MG	DA	3237	1/1	0.88	0.18	47,47,47,47	0
56	MG	BX	3005	1/1	0.88	0.21	42,42,42,42	0
56	MG	DA	3409	1/1	0.88	0.08	36,36,36,36	0
56	MG	BA	3873	1/1	0.88	0.28	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3174	1/1	0.88	0.16	58,58,58,58	0
56	MG	DA	3368	1/1	0.88	0.10	47,47,47,47	0
56	MG	BA	3815	1/1	0.88	0.22	51,51,51,51	0
56	MG	BA	3450	1/1	0.88	0.17	35,35,35,35	0
56	MG	AA	3067	1/1	0.88	0.23	56,56,56,56	0
56	MG	BA	3420	1/1	0.88	0.19	47,47,47,47	0
56	MG	AA	3125	1/1	0.88	0.07	52,52,52,52	0
56	MG	DA	3306	1/1	0.88	0.16	33,33,33,33	0
56	MG	AA	3176	1/1	0.88	0.22	47,47,47,47	0
56	MG	BA	3019	1/1	0.88	0.18	34,34,34,34	0
56	MG	DA	3665	1/1	0.88	0.19	34,34,34,34	0
56	MG	DA	3227	1/1	0.88	0.23	39,39,39,39	0
56	MG	BA	3631	1/1	0.89	0.24	38,38,38,38	0
56	MG	BA	3695	1/1	0.89	0.19	56,56,56,56	0
56	MG	DA	3231	1/1	0.89	0.13	49,49,49,49	0
56	MG	BA	3655	1/1	0.89	0.14	44,44,44,44	0
56	MG	DA	3571	1/1	0.89	0.23	43,43,43,43	0
56	MG	CW	3003	1/1	0.89	0.09	58,58,58,58	0
56	MG	BA	3698	1/1	0.89	0.17	55,55,55,55	0
56	MG	DA	3088	1/1	0.89	0.18	47,47,47,47	0
56	MG	DA	3375	1/1	0.89	0.14	37,37,37,37	0
56	MG	BA	3468	1/1	0.89	0.23	36,36,36,36	0
56	MG	BA	3086	1/1	0.89	0.21	57,57,57,57	0
56	MG	AA	3035	1/1	0.89	0.13	41,41,41,41	0
56	MG	DA	3170	1/1	0.89	0.17	36,36,36,36	0
56	MG	BA	3427	1/1	0.89	0.16	57,57,57,57	0
56	MG	AA	3055	1/1	0.89	0.14	61,61,61,61	0
56	MG	BB	3024	1/1	0.89	0.10	60,60,60,60	0
56	MG	BA	3666	1/1	0.89	0.30	74,74,74,74	0
56	MG	DA	3171	1/1	0.89	0.16	45,45,45,45	0
56	MG	AA	3180	1/1	0.89	0.08	57,57,57,57	0
56	MG	BA	3436	1/1	0.89	0.18	54,54,54,54	0
56	MG	DA	3214	1/1	0.89	0.22	53,53,53,53	0
56	MG	BE	310	1/1	0.89	0.16	80,80,80,80	0
56	MG	CA	3065	1/1	0.89	0.24	58,58,58,58	0
56	MG	AA	3086	1/1	0.89	0.14	45,45,45,45	0
56	MG	BA	3313	1/1	0.89	0.09	60,60,60,60	0
56	MG	BA	3176	1/1	0.89	0.16	53,53,53,53	0
56	MG	BB	3004	1/1	0.89	0.26	59,59,59,59	0
56	MG	DA	3514	1/1	0.89	0.14	45,45,45,45	0
56	MG	BA	3498	1/1	0.89	0.23	26,26,26,26	0
56	MG	AA	3004	1/1	0.89	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3058	1/1	0.89	0.15	54,54,54,54	0
56	MG	BA	3017	1/1	0.89	0.15	52,52,52,52	0
56	MG	BA	3870	1/1	0.89	0.17	24,24,24,24	0
56	MG	DA	3560	1/1	0.89	0.14	50,50,50,50	0
56	MG	DA	3354	1/1	0.89	0.14	34,34,34,34	0
56	MG	DA	3031	1/1	0.89	0.19	44,44,44,44	0
56	MG	DB	3021	1/1	0.89	0.06	67,67,67,67	0
56	MG	DA	3401	1/1	0.89	0.14	37,37,37,37	0
56	MG	DA	3086	1/1	0.89	0.20	59,59,59,59	0
56	MG	AA	3188	1/1	0.89	0.18	67,67,67,67	0
56	MG	BA	3310	1/1	0.89	0.28	44,44,44,44	0
56	MG	DA	3396	1/1	0.89	0.12	41,41,41,41	0
56	MG	BA	3305	1/1	0.89	0.22	46,46,46,46	0
56	MG	DA	3573	1/1	0.89	0.13	46,46,46,46	0
56	MG	DA	3175	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3385	1/1	0.89	0.11	32,32,32,32	0
56	MG	AX	3004	1/1	0.89	0.19	53,53,53,53	0
56	MG	DA	3593	1/1	0.89	0.12	60,60,60,60	0
56	MG	BA	3861	1/1	0.89	0.26	34,34,34,34	0
56	MG	CA	3126	1/1	0.89	0.17	68,68,68,68	0
56	MG	DA	3263	1/1	0.89	0.16	40,40,40,40	0
56	MG	DA	3549	1/1	0.89	0.14	49,49,49,49	0
56	MG	BA	3781	1/1	0.89	0.19	47,47,47,47	0
56	MG	DA	3070	1/1	0.89	0.16	39,39,39,39	0
56	MG	DB	3014	1/1	0.89	0.17	61,61,61,61	0
56	MG	BA	3065	1/1	0.89	0.18	51,51,51,51	0
56	MG	BA	3170	1/1	0.89	0.12	40,40,40,40	0
56	MG	BB	3025	1/1	0.89	0.20	71,71,71,71	0
56	MG	BA	3522	1/1	0.89	0.14	50,50,50,50	0
56	MG	CA	3151	1/1	0.89	0.17	60,60,60,60	0
56	MG	BA	3654	1/1	0.89	0.14	54,54,54,54	0
56	MG	CA	3167	1/1	0.89	0.15	65,65,65,65	0
56	MG	CA	3182	1/1	0.89	0.23	58,58,58,58	0
56	MG	DB	3018	1/1	0.89	0.23	62,62,62,62	0
56	MG	DA	3267	1/1	0.89	0.07	53,53,53,53	0
56	MG	DA	3177	1/1	0.89	0.23	44,44,44,44	0
56	MG	DA	3264	1/1	0.89	0.12	48,48,48,48	0
56	MG	DA	3026	1/1	0.89	0.29	41,41,41,41	0
56	MG	CA	3008	1/1	0.89	0.15	49,49,49,49	0
56	MG	BA	3087	1/1	0.89	0.23	45,45,45,45	0
56	MG	AA	3208	1/1	0.89	0.11	48,48,48,48	0
56	MG	CA	3133	1/1	0.89	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3809	1/1	0.89	0.25	58,58,58,58	0
56	MG	DA	3657	1/1	0.89	0.12	44,44,44,44	0
56	MG	DA	3327	1/1	0.89	0.15	48,48,48,48	0
56	MG	DA	3073	1/1	0.89	0.12	45,45,45,45	0
56	MG	B5	105	1/1	0.89	0.07	52,52,52,52	0
56	MG	BA	3526	1/1	0.89	0.09	43,43,43,43	0
56	MG	DA	3183	1/1	0.89	0.27	44,44,44,44	0
56	MG	BF	312	1/1	0.89	0.27	49,49,49,49	0
56	MG	BA	3455	1/1	0.89	0.14	31,31,31,31	0
56	MG	BA	3116	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3808	1/1	0.89	0.24	40,40,40,40	0
56	MG	DA	3552	1/1	0.89	0.12	55,55,55,55	0
56	MG	BA	3059	1/1	0.89	0.23	36,36,36,36	0
56	MG	BA	3680	1/1	0.89	0.14	32,32,32,32	0
56	MG	BA	3485	1/1	0.89	0.18	29,29,29,29	0
56	MG	DA	3295	1/1	0.89	0.21	38,38,38,38	0
56	MG	CA	3179	1/1	0.89	0.13	49,49,49,49	0
56	MG	AA	3007	1/1	0.89	0.19	50,50,50,50	0
56	MG	DA	3341	1/1	0.89	0.25	43,43,43,43	0
56	MG	CA	3036	1/1	0.89	0.08	64,64,64,64	0
56	MG	DA	3532	1/1	0.89	0.13	61,61,61,61	0
56	MG	BA	3275	1/1	0.89	0.18	62,62,62,62	0
56	MG	BQ	3006	1/1	0.89	0.15	53,53,53,53	0
56	MG	DA	3061	1/1	0.90	0.18	43,43,43,43	0
56	MG	AA	3087	1/1	0.90	0.15	38,38,38,38	0
56	MG	BA	3706	1/1	0.90	0.14	54,54,54,54	0
56	MG	CA	3128	1/1	0.90	0.17	49,49,49,49	0
56	MG	AA	3038	1/1	0.90	0.27	55,55,55,55	0
56	MG	AA	3141	1/1	0.90	0.24	70,70,70,70	0
56	MG	DA	3659	1/1	0.90	0.27	53,53,53,53	0
56	MG	DA	3562	1/1	0.90	0.24	49,49,49,49	0
56	MG	BA	3561	1/1	0.90	0.21	54,54,54,54	0
56	MG	CA	3100	1/1	0.90	0.16	65,65,65,65	0
56	MG	AH	201	1/1	0.90	0.14	67,67,67,67	0
56	MG	DA	3072	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3133	1/1	0.90	0.21	50,50,50,50	0
56	MG	BA	3293	1/1	0.90	0.25	42,42,42,42	0
56	MG	DA	3122	1/1	0.90	0.17	51,51,51,51	0
56	MG	DA	3326	1/1	0.90	0.19	34,34,34,34	0
56	MG	BA	3490	1/1	0.90	0.26	31,31,31,31	0
56	MG	AA	3161	1/1	0.90	0.18	35,35,35,35	0
56	MG	DA	3309	1/1	0.90	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3374	1/1	0.90	0.15	54,54,54,54	0
56	MG	DA	3162	1/1	0.90	0.09	48,48,48,48	0
56	MG	DA	3379	1/1	0.90	0.18	46,46,46,46	0
56	MG	BA	3652	1/1	0.90	0.24	46,46,46,46	0
56	MG	BZ	3003	1/1	0.90	0.19	51,51,51,51	0
56	MG	BA	3398	1/1	0.90	0.14	58,58,58,58	0
56	MG	DU	3003	1/1	0.90	0.14	45,45,45,45	0
56	MG	AA	3166	1/1	0.90	0.16	81,81,81,81	0
56	MG	DA	3091	1/1	0.90	0.20	32,32,32,32	0
56	MG	DA	3278	1/1	0.90	0.16	49,49,49,49	0
56	MG	BA	3890	1/1	0.90	0.19	34,34,34,34	0
56	MG	BA	3112	1/1	0.90	0.27	49,49,49,49	0
56	MG	BA	3875	1/1	0.90	0.19	51,51,51,51	0
56	MG	BA	3769	1/1	0.90	0.15	46,46,46,46	0
56	MG	BA	3323	1/1	0.90	0.29	48,48,48,48	0
56	MG	BA	3578	1/1	0.90	0.20	23,23,23,23	0
56	MG	BA	3253	1/1	0.90	0.19	29,29,29,29	0
56	MG	DA	3488	1/1	0.90	0.10	55,55,55,55	0
56	MG	CA	3189	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3561	1/1	0.90	0.07	51,51,51,51	0
56	MG	D8	102	1/1	0.90	0.22	52,52,52,52	0
56	MG	AA	3144	1/1	0.90	0.12	47,47,47,47	0
56	MG	BA	3226	1/1	0.90	0.09	52,52,52,52	0
56	MG	DA	3285	1/1	0.90	0.23	42,42,42,42	0
56	MG	BA	3220	1/1	0.90	0.16	34,34,34,34	0
56	MG	BA	3814	1/1	0.90	0.10	43,43,43,43	0
56	MG	DA	3149	1/1	0.90	0.23	59,59,59,59	0
56	MG	BA	3570	1/1	0.90	0.28	51,51,51,51	0
56	MG	BA	3444	1/1	0.90	0.14	39,39,39,39	0
56	MG	AA	3102	1/1	0.90	0.18	44,44,44,44	0
56	MG	BA	3866	1/1	0.90	0.18	54,54,54,54	0
56	MG	AA	3010	1/1	0.90	0.16	52,52,52,52	0
56	MG	CA	3187	1/1	0.90	0.14	51,51,51,51	0
56	MG	DA	3016	1/1	0.90	0.14	59,59,59,59	0
56	MG	AA	3190	1/1	0.90	0.12	54,54,54,54	0
56	MG	DA	3620	1/1	0.90	0.16	49,49,49,49	0
56	MG	CA	3137	1/1	0.90	0.22	66,66,66,66	0
56	MG	BA	3696	1/1	0.90	0.15	46,46,46,46	0
56	MG	AA	3169	1/1	0.90	0.16	62,62,62,62	0
56	MG	AA	3104	1/1	0.90	0.15	64,64,64,64	0
56	MG	DA	3164	1/1	0.90	0.12	61,61,61,61	0
56	MG	BA	3108	1/1	0.90	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3544	1/1	0.90	0.13	44,44,44,44	0
56	MG	CA	3200	1/1	0.90	0.23	62,62,62,62	0
56	MG	DA	3130	1/1	0.90	0.14	49,49,49,49	0
56	MG	BA	3824	1/1	0.90	0.14	30,30,30,30	0
56	MG	BU	204	1/1	0.90	0.18	48,48,48,48	0
56	MG	BA	3852	1/1	0.90	0.14	33,33,33,33	0
56	MG	CA	3098	1/1	0.90	0.10	57,57,57,57	0
56	MG	DA	3553	1/1	0.90	0.04	58,58,58,58	0
56	MG	CA	3153	1/1	0.90	0.17	60,60,60,60	0
56	MG	DA	3606	1/1	0.90	0.07	61,61,61,61	0
56	MG	AL	5001	1/1	0.90	0.20	52,52,52,52	0
56	MG	DA	3399	1/1	0.90	0.10	47,47,47,47	0
56	MG	BA	3056	1/1	0.90	0.31	47,47,47,47	0
56	MG	BA	3302	1/1	0.90	0.22	43,43,43,43	0
56	MG	CA	3059	1/1	0.90	0.13	58,58,58,58	0
56	MG	DA	3193	1/1	0.90	0.14	59,59,59,59	0
56	MG	BA	3858	1/1	0.90	0.13	61,61,61,61	0
56	MG	CA	3177	1/1	0.90	0.15	64,64,64,64	0
56	MG	BA	3648	1/1	0.90	0.18	56,56,56,56	0
56	MG	BA	3588	1/1	0.90	0.19	30,30,30,30	0
56	MG	CA	3024	1/1	0.90	0.22	55,55,55,55	0
56	MG	CA	3131	1/1	0.90	0.10	76,76,76,76	0
56	MG	CA	3180	1/1	0.90	0.21	55,55,55,55	0
56	MG	BA	3897	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3776	1/1	0.90	0.16	27,27,27,27	0
56	MG	DA	3249	1/1	0.90	0.20	37,37,37,37	0
56	MG	DA	3639	1/1	0.90	0.26	57,57,57,57	0
56	MG	DA	3011	1/1	0.90	0.17	34,34,34,34	0
56	MG	BA	3006	1/1	0.90	0.15	43,43,43,43	0
56	MG	BB	3009	1/1	0.90	0.11	52,52,52,52	0
56	MG	AA	3030	1/1	0.90	0.22	49,49,49,49	0
56	MG	BA	3821	1/1	0.90	0.17	42,42,42,42	0
56	MG	DA	3572	1/1	0.90	0.11	45,45,45,45	0
56	MG	DA	3628	1/1	0.90	0.14	47,47,47,47	0
56	MG	CR	3001	1/1	0.90	0.13	64,64,64,64	0
56	MG	BA	3463	1/1	0.90	0.22	23,23,23,23	0
56	MG	DA	3394	1/1	0.90	0.16	55,55,55,55	0
56	MG	DA	3517	1/1	0.90	0.13	48,48,48,48	0
56	MG	BA	3067	1/1	0.90	0.20	62,62,62,62	0
56	MG	DA	3205	1/1	0.90	0.11	37,37,37,37	0
56	MG	BA	3645	1/1	0.90	0.15	57,57,57,57	0
56	MG	BA	3550	1/1	0.90	0.27	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3584	1/1	0.90	0.06	57,57,57,57	0
56	MG	DA	3619	1/1	0.90	0.09	65,65,65,65	0
56	MG	DA	3427	1/1	0.90	0.12	35,35,35,35	0
56	MG	BA	3740	1/1	0.90	0.08	41,41,41,41	0
56	MG	BA	3590	1/1	0.90	0.17	23,23,23,23	0
56	MG	DA	3320	1/1	0.90	0.16	48,48,48,48	0
56	MG	DA	3001	1/1	0.90	0.17	55,55,55,55	0
56	MG	AA	3106	1/1	0.90	0.18	54,54,54,54	0
56	MG	DA	3331	1/1	0.90	0.12	30,30,30,30	0
56	MG	BA	3770	1/1	0.90	0.31	54,54,54,54	0
56	MG	BA	3756	1/1	0.90	0.10	53,53,53,53	0
56	MG	DA	3146	1/1	0.90	0.09	40,40,40,40	0
56	MG	AA	3094	1/1	0.91	0.30	49,49,49,49	0
56	MG	CA	3006	1/1	0.91	0.09	62,62,62,62	0
56	MG	DA	3200	1/1	0.91	0.16	46,46,46,46	0
56	MG	BA	3295	1/1	0.91	0.22	37,37,37,37	0
56	MG	BA	3244	1/1	0.91	0.14	39,39,39,39	0
56	MG	DA	3279	1/1	0.91	0.13	56,56,56,56	0
56	MG	BA	3027	1/1	0.91	0.15	37,37,37,37	0
56	MG	AA	3150	1/1	0.91	0.18	66,66,66,66	0
56	MG	AA	3209	1/1	0.91	0.16	61,61,61,61	0
56	MG	DA	3576	1/1	0.91	0.08	49,49,49,49	0
56	MG	CD	503	1/1	0.91	0.27	53,53,53,53	0
56	MG	BA	3438	1/1	0.91	0.23	27,27,27,27	0
56	MG	BA	3721	1/1	0.91	0.32	52,52,52,52	0
56	MG	DA	3081	1/1	0.91	0.15	33,33,33,33	0
56	MG	BA	3442	1/1	0.91	0.16	37,37,37,37	0
56	MG	BA	3273	1/1	0.91	0.13	50,50,50,50	0
56	MG	DA	3557	1/1	0.91	0.10	54,54,54,54	0
56	MG	BA	3316	1/1	0.91	0.17	43,43,43,43	0
56	MG	DX	3001	1/1	0.91	0.21	44,44,44,44	0
56	MG	DA	3032	1/1	0.91	0.16	44,44,44,44	0
56	MG	BB	3014	1/1	0.91	0.20	43,43,43,43	0
56	MG	DP	201	1/1	0.91	0.13	57,57,57,57	0
56	MG	BA	3551	1/1	0.91	0.14	37,37,37,37	0
56	MG	BA	3449	1/1	0.91	0.23	39,39,39,39	0
56	MG	AA	3225	1/1	0.91	0.30	48,48,48,48	0
56	MG	CA	3082	1/1	0.91	0.06	58,58,58,58	0
56	MG	AA	3006	1/1	0.91	0.13	50,50,50,50	0
56	MG	BA	3101	1/1	0.91	0.29	42,42,42,42	0
56	MG	CT	3001	1/1	0.91	0.22	46,46,46,46	0
56	MG	AA	3171	1/1	0.91	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BW	203	1/1	0.91	0.26	47,47,47,47	0
56	MG	BB	3030	1/1	0.91	0.12	39,39,39,39	0
56	MG	DA	3596	1/1	0.91	0.13	62,62,62,62	0
56	MG	DA	3667	1/1	0.91	0.18	36,36,36,36	0
56	MG	DA	3545	1/1	0.91	0.07	52,52,52,52	0
56	MG	DA	3454	1/1	0.91	0.21	44,44,44,44	0
56	MG	BB	3007	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3612	1/1	0.91	0.19	53,53,53,53	0
56	MG	DA	3156	1/1	0.91	0.12	33,33,33,33	0
56	MG	DA	3422	1/1	0.91	0.12	52,52,52,52	0
56	MG	DA	3147	1/1	0.91	0.07	53,53,53,53	0
56	MG	BA	3668	1/1	0.91	0.21	48,48,48,48	0
56	MG	DA	3184	1/1	0.91	0.26	37,37,37,37	0
56	MG	DA	3067	1/1	0.91	0.17	54,54,54,54	0
56	MG	DA	3304	1/1	0.91	0.11	40,40,40,40	0
56	MG	BA	3210	1/1	0.91	0.19	53,53,53,53	0
56	MG	AA	3041	1/1	0.91	0.10	53,53,53,53	0
56	MG	B0	106	1/1	0.91	0.15	66,66,66,66	0
56	MG	DA	3496	1/1	0.91	0.15	53,53,53,53	0
56	MG	CA	3045	1/1	0.91	0.07	47,47,47,47	0
56	MG	BA	3400	1/1	0.91	0.23	32,32,32,32	0
56	MG	BA	3872	1/1	0.91	0.09	42,42,42,42	0
56	MG	BA	3510	1/1	0.91	0.28	49,49,49,49	0
56	MG	DA	3145	1/1	0.91	0.21	47,47,47,47	0
56	MG	DA	3043	1/1	0.91	0.12	39,39,39,39	0
56	MG	DA	3595	1/1	0.91	0.12	45,45,45,45	0
56	MG	DA	3487	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3269	1/1	0.91	0.13	54,54,54,54	0
56	MG	CA	3003	1/1	0.91	0.17	63,63,63,63	0
56	MG	DA	3307	1/1	0.91	0.13	41,41,41,41	0
56	MG	BA	3412	1/1	0.91	0.18	42,42,42,42	0
56	MG	DA	3365	1/1	0.91	0.10	38,38,38,38	0
56	MG	BA	3243	1/1	0.91	0.17	39,39,39,39	0
56	MG	BA	3479	1/1	0.91	0.15	41,41,41,41	0
56	MG	CA	3075	1/1	0.91	0.07	52,52,52,52	0
59	ZN	B4	501	1/1	0.91	0.15	75,75,75,75	0
56	MG	DA	3275	1/1	0.91	0.11	33,33,33,33	0
56	MG	BB	3023	1/1	0.91	0.13	71,71,71,71	0
56	MG	BA	3300	1/1	0.91	0.14	58,58,58,58	0
56	MG	DB	3004	1/1	0.91	0.22	57,57,57,57	0
56	MG	BA	3542	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3154	1/1	0.91	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3462	1/1	0.91	0.10	42,42,42,42	0
56	MG	AY	3002	1/1	0.91	0.10	66,66,66,66	0
56	MG	BA	3239	1/1	0.91	0.17	38,38,38,38	0
56	MG	DA	3323	1/1	0.91	0.15	34,34,34,34	0
56	MG	BA	3191	1/1	0.91	0.15	31,31,31,31	0
56	MG	BA	3800	1/1	0.91	0.23	29,29,29,29	0
56	MG	DA	3272	1/1	0.91	0.10	52,52,52,52	0
56	MG	DA	3337	1/1	0.91	0.13	44,44,44,44	0
56	MG	DA	3381	1/1	0.91	0.17	47,47,47,47	0
56	MG	DA	3670	1/1	0.91	0.11	51,51,51,51	0
56	MG	DA	3206	1/1	0.91	0.15	33,33,33,33	0
56	MG	DA	3153	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3113	1/1	0.91	0.16	66,66,66,66	0
56	MG	DA	3280	1/1	0.91	0.08	57,57,57,57	0
56	MG	DA	3212	1/1	0.91	0.14	52,52,52,52	0
56	MG	DA	3298	1/1	0.91	0.14	50,50,50,50	0
56	MG	BA	3396	1/1	0.91	0.15	42,42,42,42	0
56	MG	CA	3174	1/1	0.91	0.21	57,57,57,57	0
56	MG	BB	3018	1/1	0.91	0.25	32,32,32,32	0
56	MG	DA	3068	1/1	0.91	0.26	58,58,58,58	0
56	MG	DA	3594	1/1	0.91	0.12	56,56,56,56	0
56	MG	BE	303	1/1	0.91	0.20	35,35,35,35	0
56	MG	DE	307	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3495	1/1	0.91	0.22	40,40,40,40	0
56	MG	BA	3171	1/1	0.91	0.17	42,42,42,42	0
56	MG	AA	3220	1/1	0.91	0.16	57,57,57,57	0
56	MG	CA	3005	1/1	0.91	0.11	55,55,55,55	0
56	MG	BA	3423	1/1	0.91	0.09	34,34,34,34	0
56	MG	DB	3003	1/1	0.91	0.14	62,62,62,62	0
56	MG	CA	3035	1/1	0.91	0.17	49,49,49,49	0
56	MG	BA	3228	1/1	0.91	0.18	35,35,35,35	0
56	MG	BA	3546	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3264	1/1	0.91	0.15	38,38,38,38	0
56	MG	DA	3569	1/1	0.91	0.24	47,47,47,47	0
56	MG	CA	3028	1/1	0.91	0.19	58,58,58,58	0
56	MG	BA	3637	1/1	0.91	0.28	32,32,32,32	0
56	MG	DA	3132	1/1	0.91	0.22	50,50,50,50	0
56	MG	AA	3081	1/1	0.91	0.12	48,48,48,48	0
56	MG	CA	3048	1/1	0.91	0.18	53,53,53,53	0
56	MG	BA	3004	1/1	0.91	0.23	33,33,33,33	0
56	MG	CA	3067	1/1	0.91	0.21	55,55,55,55	0
56	MG	BZ	3002	1/1	0.91	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3124	1/1	0.91	0.20	26,26,26,26	0
56	MG	BA	3880	1/1	0.91	0.09	35,35,35,35	0
56	MG	DA	3405	1/1	0.91	0.12	44,44,44,44	0
56	MG	CW	3001	1/1	0.91	0.47	57,57,57,57	0
56	MG	BA	3791	1/1	0.91	0.09	47,47,47,47	0
56	MG	CA	3099	1/1	0.91	0.21	72,72,72,72	0
56	MG	DA	3174	1/1	0.91	0.27	49,49,49,49	0
56	MG	BA	3562	1/1	0.91	0.20	41,41,41,41	0
56	MG	DA	3005	1/1	0.91	0.22	52,52,52,52	0
56	MG	DA	3099	1/1	0.91	0.18	44,44,44,44	0
56	MG	DA	3049	1/1	0.91	0.19	43,43,43,43	0
56	MG	CA	3097	1/1	0.91	0.10	43,43,43,43	0
56	MG	DA	3661	1/1	0.91	0.10	39,39,39,39	0
56	MG	DA	3587	1/1	0.91	0.09	64,64,64,64	0
56	MG	AA	3024	1/1	0.91	0.18	39,39,39,39	0
56	MG	BA	3418	1/1	0.91	0.14	60,60,60,60	0
56	MG	CA	3147	1/1	0.91	0.13	64,64,64,64	0
56	MG	CA	3112	1/1	0.91	0.17	65,65,65,65	0
56	MG	CA	3156	1/1	0.91	0.15	59,59,59,59	0
56	MG	CA	3070	1/1	0.91	0.09	59,59,59,59	0
56	MG	DA	3538	1/1	0.91	0.17	57,57,57,57	0
56	MG	BB	3006	1/1	0.91	0.23	40,40,40,40	0
56	MG	BA	3718	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3079	1/1	0.91	0.28	40,40,40,40	0
56	MG	DA	3127	1/1	0.91	0.18	47,47,47,47	0
56	MG	BB	3017	1/1	0.91	0.26	37,37,37,37	0
56	MG	BA	3308	1/1	0.91	0.21	40,40,40,40	0
56	MG	DA	3374	1/1	0.91	0.08	36,36,36,36	0
56	MG	BA	3787	1/1	0.91	0.18	24,24,24,24	0
56	MG	BQ	3005	1/1	0.91	0.13	37,37,37,37	0
56	MG	BD	305	1/1	0.91	0.16	35,35,35,35	0
56	MG	BA	3267	1/1	0.92	0.14	51,51,51,51	0
56	MG	AA	3098	1/1	0.92	0.12	60,60,60,60	0
56	MG	CA	3038	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3291	1/1	0.92	0.28	49,49,49,49	0
56	MG	BA	3015	1/1	0.92	0.14	33,33,33,33	0
56	MG	DA	3642	1/1	0.92	0.13	40,40,40,40	0
56	MG	BF	301	1/1	0.92	0.28	41,41,41,41	0
56	MG	CA	3196	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3864	1/1	0.92	0.17	26,26,26,26	0
56	MG	BA	3854	1/1	0.92	0.13	51,51,51,51	0
56	MG	DA	3510	1/1	0.92	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3894	1/1	0.92	0.27	44,44,44,44	0
56	MG	BA	3352	1/1	0.92	0.17	42,42,42,42	0
56	MG	BA	3126	1/1	0.92	0.13	38,38,38,38	0
56	MG	BA	3335	1/1	0.92	0.22	33,33,33,33	0
56	MG	DA	3131	1/1	0.92	0.26	48,48,48,48	0
56	MG	BD	304	1/1	0.92	0.53	49,49,49,49	0
56	MG	BA	3473	1/1	0.92	0.21	59,59,59,59	0
56	MG	BA	3188	1/1	0.92	0.29	55,55,55,55	0
56	MG	BA	3159	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3095	1/1	0.92	0.14	46,46,46,46	0
56	MG	DA	3004	1/1	0.92	0.21	36,36,36,36	0
56	MG	DA	3382	1/1	0.92	0.23	40,40,40,40	0
56	MG	BH	3001	1/1	0.92	0.33	40,40,40,40	0
56	MG	DA	3460	1/1	0.92	0.23	51,51,51,51	0
56	MG	BA	3700	1/1	0.92	0.16	51,51,51,51	0
56	MG	BA	3548	1/1	0.92	0.10	49,49,49,49	0
56	MG	BA	3156	1/1	0.92	0.15	46,46,46,46	0
56	MG	DA	3421	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3847	1/1	0.92	0.11	52,52,52,52	0
56	MG	DV	201	1/1	0.92	0.38	51,51,51,51	0
56	MG	BA	3384	1/1	0.92	0.14	48,48,48,48	0
56	MG	DA	3305	1/1	0.92	0.12	42,42,42,42	0
56	MG	DA	3232	1/1	0.92	0.11	44,44,44,44	0
56	MG	BA	3679	1/1	0.92	0.18	33,33,33,33	0
56	MG	BA	3062	1/1	0.92	0.21	41,41,41,41	0
56	MG	BA	3084	1/1	0.92	0.25	42,42,42,42	0
56	MG	AA	3172	1/1	0.92	0.07	43,43,43,43	0
56	MG	BA	3070	1/1	0.92	0.34	47,47,47,47	0
56	MG	DA	3448	1/1	0.92	0.19	36,36,36,36	0
56	MG	CA	3120	1/1	0.92	0.14	62,62,62,62	0
56	MG	DA	3403	1/1	0.92	0.14	46,46,46,46	0
56	MG	BA	3633	1/1	0.92	0.10	42,42,42,42	0
56	MG	BX	3002	1/1	0.92	0.18	37,37,37,37	0
56	MG	BA	3461	1/1	0.92	0.22	23,23,23,23	0
56	MG	BE	304	1/1	0.92	0.30	56,56,56,56	0
56	MG	BU	206	1/1	0.92	0.20	38,38,38,38	0
56	MG	BA	3554	1/1	0.92	0.20	48,48,48,48	0
56	MG	DA	3636	1/1	0.92	0.18	55,55,55,55	0
56	MG	DA	3085	1/1	0.92	0.10	39,39,39,39	0
56	MG	BA	3169	1/1	0.92	0.30	40,40,40,40	0
56	MG	BA	3032	1/1	0.92	0.16	29,29,29,29	0
56	MG	DA	3246	1/1	0.92	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DF	301	1/1	0.92	0.15	36,36,36,36	0
56	MG	DA	3630	1/1	0.92	0.17	45,45,45,45	0
56	MG	BA	3016	1/1	0.92	0.27	51,51,51,51	0
56	MG	BE	307	1/1	0.92	0.18	37,37,37,37	0
56	MG	BA	3163	1/1	0.92	0.24	46,46,46,46	0
56	MG	AA	3074	1/1	0.92	0.13	57,57,57,57	0
56	MG	BA	3798	1/1	0.92	0.27	55,55,55,55	0
56	MG	DA	3605	1/1	0.92	0.22	51,51,51,51	0
56	MG	CA	3129	1/1	0.92	0.13	69,69,69,69	0
56	MG	DA	3342	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3145	1/1	0.92	0.19	41,41,41,41	0
56	MG	BA	3734	1/1	0.92	0.25	32,32,32,32	0
56	MG	CA	3029	1/1	0.92	0.13	60,60,60,60	0
56	MG	BA	3009	1/1	0.92	0.17	23,23,23,23	0
56	MG	DA	3535	1/1	0.92	0.13	41,41,41,41	0
56	MG	BA	3789	1/1	0.92	0.23	23,23,23,23	0
56	MG	BA	3594	1/1	0.92	0.14	22,22,22,22	0
56	MG	DA	3353	1/1	0.92	0.15	34,34,34,34	0
56	MG	BA	3001	1/1	0.92	0.19	45,45,45,45	0
56	MG	DA	3313	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3112	1/1	0.92	0.13	42,42,42,42	0
56	MG	BA	3783	1/1	0.92	0.18	33,33,33,33	0
56	MG	BA	3022	1/1	0.92	0.12	40,40,40,40	0
56	MG	AA	3020	1/1	0.92	0.19	45,45,45,45	0
56	MG	BA	3179	1/1	0.92	0.16	37,37,37,37	0
56	MG	DA	3512	1/1	0.92	0.19	54,54,54,54	0
56	MG	BA	3693	1/1	0.92	0.23	39,39,39,39	0
56	MG	BX	3001	1/1	0.92	0.33	37,37,37,37	0
56	MG	AA	3016	1/1	0.92	0.18	57,57,57,57	0
56	MG	BR	202	1/1	0.92	0.28	38,38,38,38	0
56	MG	BA	3279	1/1	0.92	0.18	32,32,32,32	0
56	MG	DA	3060	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3205	1/1	0.92	0.15	50,50,50,50	0
56	MG	DD	302	1/1	0.92	0.11	42,42,42,42	0
56	MG	DA	3371	1/1	0.92	0.10	42,42,42,42	0
56	MG	BA	3137	1/1	0.92	0.16	35,35,35,35	0
56	MG	B0	105	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3347	1/1	0.92	0.11	41,41,41,41	0
56	MG	BA	3434	1/1	0.92	0.22	41,41,41,41	0
56	MG	DA	3644	1/1	0.92	0.10	60,60,60,60	0
56	MG	AW	103	1/1	0.92	0.22	45,45,45,45	0
56	MG	BA	3676	1/1	0.92	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3602	1/1	0.92	0.15	20,20,20,20	0
56	MG	BA	3139	1/1	0.92	0.22	45,45,45,45	0
56	MG	BA	3710	1/1	0.92	0.22	49,49,49,49	0
56	MG	DA	3547	1/1	0.92	0.17	52,52,52,52	0
56	MG	DA	3110	1/1	0.92	0.32	38,38,38,38	0
56	MG	BA	3152	1/1	0.92	0.15	48,48,48,48	0
56	MG	DB	3005	1/1	0.92	0.17	61,61,61,61	0
56	MG	BA	3193	1/1	0.92	0.17	50,50,50,50	0
56	MG	BA	3345	1/1	0.92	0.19	47,47,47,47	0
56	MG	BA	3206	1/1	0.92	0.15	59,59,59,59	0
56	MG	DA	3197	1/1	0.92	0.15	32,32,32,32	0
56	MG	BA	3071	1/1	0.92	0.23	32,32,32,32	0
56	MG	DA	3217	1/1	0.92	0.15	63,63,63,63	0
56	MG	BU	202	1/1	0.92	0.12	31,31,31,31	0
56	MG	BA	3141	1/1	0.92	0.20	32,32,32,32	0
56	MG	AA	3134	1/1	0.92	0.18	47,47,47,47	0
59	ZN	CN	501	1/1	0.92	0.06	83,83,83,83	0
56	MG	DA	3631	1/1	0.92	0.11	52,52,52,52	0
56	MG	AA	3198	1/1	0.92	0.18	58,58,58,58	0
56	MG	BA	3764	1/1	0.92	0.27	32,32,32,32	0
56	MG	BA	3703	1/1	0.92	0.16	55,55,55,55	0
56	MG	B7	101	1/1	0.92	0.17	41,41,41,41	0
56	MG	BA	3073	1/1	0.92	0.18	49,49,49,49	0
56	MG	CA	3026	1/1	0.92	0.26	56,56,56,56	0
56	MG	AA	3065	1/1	0.92	0.26	45,45,45,45	0
56	MG	DA	3248	1/1	0.92	0.19	50,50,50,50	0
56	MG	DF	306	1/1	0.92	0.36	46,46,46,46	0
56	MG	DA	3343	1/1	0.92	0.08	39,39,39,39	0
56	MG	BA	3146	1/1	0.92	0.11	62,62,62,62	0
56	MG	AE	3002	1/1	0.92	0.21	57,57,57,57	0
56	MG	DQ	3003	1/1	0.92	0.23	57,57,57,57	0
56	MG	BA	3096	1/1	0.92	0.28	42,42,42,42	0
56	MG	BA	3669	1/1	0.92	0.26	44,44,44,44	0
56	MG	CQ	3002	1/1	0.92	0.18	65,65,65,65	0
56	MG	BA	3288	1/1	0.92	0.30	51,51,51,51	0
56	MG	BA	3689	1/1	0.92	0.21	44,44,44,44	0
56	MG	BA	3896	1/1	0.92	0.17	41,41,41,41	0
56	MG	BA	3530	1/1	0.92	0.18	43,43,43,43	0
56	MG	AX	3009	1/1	0.92	0.15	32,32,32,32	0
56	MG	CA	3111	1/1	0.92	0.24	53,53,53,53	0
56	MG	BA	3622	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3390	1/1	0.92	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3016	1/1	0.92	0.11	45,45,45,45	0
56	MG	DA	3467	1/1	0.92	0.13	40,40,40,40	0
56	MG	B9	502	1/1	0.92	0.28	47,47,47,47	0
56	MG	BA	3199	1/1	0.92	0.13	31,31,31,31	0
56	MG	BA	3807	1/1	0.92	0.21	46,46,46,46	0
56	MG	DZ	5001	1/1	0.92	0.11	73,73,73,73	0
56	MG	BA	3746	1/1	0.92	0.18	57,57,57,57	0
56	MG	AY	3001	1/1	0.92	0.34	76,76,76,76	0
56	MG	BA	3118	1/1	0.92	0.16	38,38,38,38	0
56	MG	BA	3895	1/1	0.92	0.17	30,30,30,30	0
56	MG	DA	3233	1/1	0.92	0.13	36,36,36,36	0
56	MG	BA	3117	1/1	0.92	0.15	29,29,29,29	0
56	MG	BA	3902	1/1	0.92	0.28	55,55,55,55	0
56	MG	CA	3079	1/1	0.92	0.16	58,58,58,58	0
56	MG	AA	3059	1/1	0.92	0.18	60,60,60,60	0
56	MG	BA	3061	1/1	0.93	0.25	19,19,19,19	0
56	MG	CA	3143	1/1	0.93	0.23	65,65,65,65	0
56	MG	AA	3046	1/1	0.93	0.15	43,43,43,43	0
56	MG	BA	3804	1/1	0.93	0.14	37,37,37,37	0
56	MG	DA	3310	1/1	0.93	0.16	54,54,54,54	0
56	MG	CA	3185	1/1	0.93	0.18	59,59,59,59	0
56	MG	DA	3104	1/1	0.93	0.11	45,45,45,45	0
56	MG	DA	3089	1/1	0.93	0.27	46,46,46,46	0
56	MG	BA	3286	1/1	0.93	0.22	52,52,52,52	0
56	MG	DA	3556	1/1	0.93	0.09	57,57,57,57	0
56	MG	AA	3083	1/1	0.93	0.14	34,34,34,34	0
56	MG	DA	3111	1/1	0.93	0.16	40,40,40,40	0
56	MG	BA	3832	1/1	0.93	0.15	38,38,38,38	0
56	MG	AA	3052	1/1	0.93	0.20	58,58,58,58	0
56	MG	AA	3110	1/1	0.93	0.24	51,51,51,51	0
56	MG	CA	3030	1/1	0.93	0.19	61,61,61,61	0
56	MG	CA	3163	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3722	1/1	0.93	0.14	52,52,52,52	0
56	MG	AA	3216	1/1	0.93	0.12	68,68,68,68	0
56	MG	CA	3165	1/1	0.93	0.08	36,36,36,36	0
56	MG	AA	3206	1/1	0.93	0.11	53,53,53,53	0
56	MG	DA	3235	1/1	0.93	0.08	52,52,52,52	0
56	MG	DA	3581	1/1	0.93	0.15	55,55,55,55	0
56	MG	BA	3616	1/1	0.93	0.28	43,43,43,43	0
56	MG	B7	103	1/1	0.93	0.13	44,44,44,44	0
56	MG	BA	3601	1/1	0.93	0.13	33,33,33,33	0
56	MG	BA	3303	1/1	0.93	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3256	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3388	1/1	0.93	0.08	32,32,32,32	0
56	MG	DA	3559	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3501	1/1	0.93	0.20	33,33,33,33	0
56	MG	BU	201	1/1	0.93	0.18	39,39,39,39	0
56	MG	BA	3827	1/1	0.93	0.14	41,41,41,41	0
56	MG	DB	3017	1/1	0.93	0.13	58,58,58,58	0
56	MG	DA	3373	1/1	0.93	0.11	60,60,60,60	0
56	MG	BB	3005	1/1	0.93	0.10	52,52,52,52	0
56	MG	DA	3221	1/1	0.93	0.22	46,46,46,46	0
56	MG	DB	3011	1/1	0.93	0.19	60,60,60,60	0
56	MG	AA	3116	1/1	0.93	0.20	58,58,58,58	0
56	MG	AX	3002	1/1	0.93	0.23	49,49,49,49	0
56	MG	CA	3052	1/1	0.93	0.30	53,53,53,53	0
56	MG	DD	303	1/1	0.93	0.38	46,46,46,46	0
56	MG	BA	3593	1/1	0.93	0.10	44,44,44,44	0
56	MG	BV	204	1/1	0.93	0.22	44,44,44,44	0
56	MG	BA	3595	1/1	0.93	0.18	36,36,36,36	0
56	MG	DA	3344	1/1	0.93	0.07	54,54,54,54	0
56	MG	BA	3428	1/1	0.93	0.21	40,40,40,40	0
56	MG	DA	3240	1/1	0.93	0.15	45,45,45,45	0
56	MG	AA	3160	1/1	0.93	0.11	38,38,38,38	0
56	MG	BA	3047	1/1	0.93	0.23	31,31,31,31	0
56	MG	DA	3109	1/1	0.93	0.24	34,34,34,34	0
56	MG	DA	3126	1/1	0.93	0.14	33,33,33,33	0
56	MG	BA	3029	1/1	0.93	0.19	48,48,48,48	0
56	MG	DA	3613	1/1	0.93	0.16	44,44,44,44	0
56	MG	AA	3032	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3845	1/1	0.93	0.19	28,28,28,28	0
56	MG	DA	3014	1/1	0.93	0.12	33,33,33,33	0
56	MG	DA	3523	1/1	0.93	0.10	46,46,46,46	0
56	MG	BA	3324	1/1	0.93	0.17	36,36,36,36	0
56	MG	BA	3702	1/1	0.93	0.09	39,39,39,39	0
56	MG	BA	3331	1/1	0.93	0.20	32,32,32,32	0
56	MG	AA	3162	1/1	0.93	0.22	67,67,67,67	0
56	MG	DA	3308	1/1	0.93	0.14	45,45,45,45	0
56	MG	BD	303	1/1	0.93	0.19	40,40,40,40	0
56	MG	AX	3014	1/1	0.93	0.11	51,51,51,51	0
56	MG	CA	3117	1/1	0.93	0.10	58,58,58,58	0
56	MG	AA	3132	1/1	0.93	0.08	42,42,42,42	0
56	MG	DA	3230	1/1	0.93	0.27	54,54,54,54	0
56	MG	BA	3537	1/1	0.93	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3230	1/1	0.93	0.22	56,56,56,56	0
56	MG	BA	3069	1/1	0.93	0.24	32,32,32,32	0
56	MG	AA	3178	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3843	1/1	0.93	0.17	34,34,34,34	0
56	MG	BA	3232	1/1	0.93	0.17	33,33,33,33	0
56	MG	CA	3171	1/1	0.93	0.10	52,52,52,52	0
56	MG	BA	3464	1/1	0.93	0.21	25,25,25,25	0
56	MG	BA	3268	1/1	0.93	0.15	46,46,46,46	0
56	MG	DA	3251	1/1	0.93	0.10	43,43,43,43	0
56	MG	CA	3198	1/1	0.93	0.14	39,39,39,39	0
56	MG	DA	3634	1/1	0.93	0.12	62,62,62,62	0
56	MG	DA	3507	1/1	0.93	0.06	63,63,63,63	0
56	MG	CA	3027	1/1	0.93	0.16	49,49,49,49	0
56	MG	DA	3312	1/1	0.93	0.15	36,36,36,36	0
56	MG	DA	3477	1/1	0.93	0.18	51,51,51,51	0
56	MG	CA	3148	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3219	1/1	0.93	0.15	28,28,28,28	0
56	MG	BA	3629	1/1	0.93	0.13	25,25,25,25	0
56	MG	AA	3088	1/1	0.93	0.20	46,46,46,46	0
56	MG	DA	3359	1/1	0.93	0.29	47,47,47,47	0
56	MG	AA	3064	1/1	0.93	0.33	54,54,54,54	0
56	MG	AA	3156	1/1	0.93	0.23	62,62,62,62	0
56	MG	BA	3686	1/1	0.93	0.09	52,52,52,52	0
56	MG	DA	3209	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3080	1/1	0.93	0.20	41,41,41,41	0
56	MG	BA	3863	1/1	0.93	0.20	44,44,44,44	0
56	MG	BA	3549	1/1	0.93	0.15	38,38,38,38	0
56	MG	AA	3127	1/1	0.93	0.12	33,33,33,33	0
56	MG	BA	3592	1/1	0.93	0.26	27,27,27,27	0
56	MG	DA	3097	1/1	0.93	0.20	44,44,44,44	0
56	MG	BA	3829	1/1	0.93	0.15	51,51,51,51	0
56	MG	DA	3627	1/1	0.93	0.11	42,42,42,42	0
56	MG	BA	3606	1/1	0.93	0.20	29,29,29,29	0
56	MG	DA	3044	1/1	0.93	0.17	48,48,48,48	0
56	MG	DB	3006	1/1	0.93	0.14	40,40,40,40	0
56	MG	DA	3589	1/1	0.93	0.08	50,50,50,50	0
56	MG	CA	3014	1/1	0.93	0.18	51,51,51,51	0
56	MG	DA	3663	1/1	0.93	0.16	46,46,46,46	0
56	MG	DA	3065	1/1	0.93	0.12	50,50,50,50	0
56	MG	CA	3066	1/1	0.93	0.21	44,44,44,44	0
56	MG	BA	3247	1/1	0.93	0.14	35,35,35,35	0
56	MG	BA	3745	1/1	0.93	0.22	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3260	1/1	0.93	0.12	39,39,39,39	0
56	MG	BA	3555	1/1	0.93	0.19	64,64,64,64	0
56	MG	DA	3437	1/1	0.93	0.09	53,53,53,53	0
56	MG	BA	3658	1/1	0.93	0.24	44,44,44,44	0
56	MG	DA	3412	1/1	0.93	0.20	50,50,50,50	0
56	MG	AT	3001	1/1	0.93	0.12	54,54,54,54	0
56	MG	BA	3569	1/1	0.93	0.24	48,48,48,48	0
56	MG	BB	3015	1/1	0.93	0.16	51,51,51,51	0
56	MG	BA	3350	1/1	0.93	0.15	29,29,29,29	0
56	MG	BA	3089	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3713	1/1	0.93	0.15	59,59,59,59	0
56	MG	BA	3382	1/1	0.93	0.25	26,26,26,26	0
56	MG	AA	3184	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3516	1/1	0.93	0.09	49,49,49,49	0
56	MG	DA	3564	1/1	0.93	0.17	43,43,43,43	0
56	MG	BA	3129	1/1	0.93	0.18	37,37,37,37	0
56	MG	BA	3098	1/1	0.93	0.20	43,43,43,43	0
56	MG	CA	3018	1/1	0.93	0.21	46,46,46,46	0
56	MG	DA	3476	1/1	0.93	0.13	42,42,42,42	0
56	MG	CA	3096	1/1	0.93	0.13	39,39,39,39	0
56	MG	BA	3319	1/1	0.93	0.12	36,36,36,36	0
56	MG	DA	3450	1/1	0.93	0.15	35,35,35,35	0
56	MG	BA	3167	1/1	0.93	0.18	33,33,33,33	0
56	MG	CA	3104	1/1	0.93	0.05	53,53,53,53	0
56	MG	BA	3825	1/1	0.93	0.12	39,39,39,39	0
56	MG	AA	3202	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3626	1/1	0.93	0.39	41,41,41,41	0
56	MG	BF	306	1/1	0.93	0.16	34,34,34,34	0
56	MG	BA	3509	1/1	0.93	0.10	48,48,48,48	0
56	MG	CJ	5002	1/1	0.93	0.07	65,65,65,65	0
56	MG	BA	3181	1/1	0.93	0.22	38,38,38,38	0
56	MG	BA	3114	1/1	0.93	0.39	55,55,55,55	0
56	MG	BA	3099	1/1	0.93	0.14	49,49,49,49	0
56	MG	AA	3062	1/1	0.93	0.19	61,61,61,61	0
56	MG	DA	3407	1/1	0.93	0.16	67,67,67,67	0
56	MG	CA	3093	1/1	0.93	0.08	65,65,65,65	0
56	MG	CA	3094	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3142	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3217	1/1	0.93	0.28	49,49,49,49	0
56	MG	CA	3194	1/1	0.93	0.21	66,66,66,66	0
56	MG	BA	3670	1/1	0.93	0.24	57,57,57,57	0
56	MG	BA	3806	1/1	0.93	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3234	1/1	0.93	0.20	43,43,43,43	0
56	MG	DA	3066	1/1	0.93	0.20	49,49,49,49	0
56	MG	BA	3543	1/1	0.93	0.15	48,48,48,48	0
56	MG	DA	3459	1/1	0.93	0.25	50,50,50,50	0
56	MG	AA	3076	1/1	0.93	0.30	58,58,58,58	0
56	MG	BA	3312	1/1	0.93	0.24	54,54,54,54	0
56	MG	BA	3136	1/1	0.93	0.42	49,49,49,49	0
56	MG	DA	3115	1/1	0.93	0.20	44,44,44,44	0
56	MG	AA	3097	1/1	0.93	0.14	54,54,54,54	0
56	MG	AA	3212	1/1	0.93	0.22	59,59,59,59	0
56	MG	BA	3717	1/1	0.93	0.11	57,57,57,57	0
56	MG	DA	3135	1/1	0.93	0.25	47,47,47,47	0
56	MG	CA	3149	1/1	0.93	0.20	71,71,71,71	0
56	MG	BA	3839	1/1	0.93	0.10	47,47,47,47	0
56	MG	BA	3192	1/1	0.93	0.18	41,41,41,41	0
56	MG	DA	3024	1/1	0.93	0.12	46,46,46,46	0
56	MG	BA	3251	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3187	1/1	0.93	0.18	41,41,41,41	0
56	MG	CA	3025	1/1	0.93	0.17	51,51,51,51	0
56	MG	DA	3443	1/1	0.93	0.11	50,50,50,50	0
56	MG	BA	3309	1/1	0.93	0.31	50,50,50,50	0
56	MG	AA	3133	1/1	0.93	0.13	32,32,32,32	0
56	MG	DA	3210	1/1	0.93	0.22	30,30,30,30	0
56	MG	AA	3042	1/1	0.93	0.29	47,47,47,47	0
56	MG	BA	3627	1/1	0.93	0.16	34,34,34,34	0
56	MG	BT	5002	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3646	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3862	1/1	0.94	0.12	29,29,29,29	0
56	MG	DA	3033	1/1	0.94	0.14	40,40,40,40	0
56	MG	AA	3043	1/1	0.94	0.11	56,56,56,56	0
56	MG	AA	3103	1/1	0.94	0.17	50,50,50,50	0
56	MG	DT	3001	1/1	0.94	0.29	54,54,54,54	0
56	MG	BA	3011	1/1	0.94	0.17	37,37,37,37	0
56	MG	DA	3498	1/1	0.94	0.09	42,42,42,42	0
56	MG	BA	3311	1/1	0.94	0.18	43,43,43,43	0
56	MG	DA	3010	1/1	0.94	0.19	36,36,36,36	0
56	MG	CA	3095	1/1	0.94	0.24	46,46,46,46	0
56	MG	DA	3196	1/1	0.94	0.18	46,46,46,46	0
56	MG	DA	3290	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3273	1/1	0.94	0.14	30,30,30,30	0
56	MG	BA	3414	1/1	0.94	0.15	32,32,32,32	0
56	MG	DA	3219	1/1	0.94	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3859	1/1	0.94	0.18	34,34,34,34	0
56	MG	DA	3119	1/1	0.94	0.22	36,36,36,36	0
56	MG	BA	3364	1/1	0.94	0.22	57,57,57,57	0
56	MG	AA	3092	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3526	1/1	0.94	0.20	42,42,42,42	0
56	MG	AA	3152	1/1	0.94	0.15	54,54,54,54	0
56	MG	AA	3033	1/1	0.94	0.13	55,55,55,55	0
56	MG	AA	3093	1/1	0.94	0.20	53,53,53,53	0
56	MG	BA	3307	1/1	0.94	0.17	36,36,36,36	0
56	MG	BA	3705	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3249	1/1	0.94	0.26	41,41,41,41	0
56	MG	DA	3609	1/1	0.94	0.05	53,53,53,53	0
56	MG	BA	3519	1/1	0.94	0.20	46,46,46,46	0
56	MG	BA	3507	1/1	0.94	0.16	33,33,33,33	0
56	MG	DA	3052	1/1	0.94	0.13	38,38,38,38	0
56	MG	BA	3088	1/1	0.94	0.18	28,28,28,28	0
56	MG	DB	3008	1/1	0.94	0.16	55,55,55,55	0
59	ZN	D9	501	1/1	0.94	0.11	63,63,63,63	0
56	MG	BA	3332	1/1	0.94	0.16	43,43,43,43	0
56	MG	BO	3003	1/1	0.94	0.17	42,42,42,42	0
56	MG	BA	3405	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3724	1/1	0.94	0.13	37,37,37,37	0
56	MG	BA	3230	1/1	0.94	0.17	35,35,35,35	0
56	MG	DA	3546	1/1	0.94	0.13	53,53,53,53	0
56	MG	BW	201	1/1	0.94	0.08	45,45,45,45	0
56	MG	DA	3182	1/1	0.94	0.18	33,33,33,33	0
56	MG	CA	3166	1/1	0.94	0.20	53,53,53,53	0
56	MG	AA	3068	1/1	0.94	0.32	55,55,55,55	0
56	MG	DW	3002	1/1	0.94	0.16	44,44,44,44	0
56	MG	BA	3195	1/1	0.94	0.16	37,37,37,37	0
56	MG	AA	3142	1/1	0.94	0.13	44,44,44,44	0
56	MG	CA	3068	1/1	0.94	0.27	53,53,53,53	0
56	MG	BA	3539	1/1	0.94	0.24	38,38,38,38	0
56	MG	BA	3583	1/1	0.94	0.29	35,35,35,35	0
56	MG	CA	3010	1/1	0.94	0.26	52,52,52,52	0
59	ZN	D6	501	1/1	0.94	0.17	58,58,58,58	0
56	MG	DA	3428	1/1	0.94	0.18	42,42,42,42	0
56	MG	BA	3252	1/1	0.94	0.14	38,38,38,38	0
56	MG	AA	3049	1/1	0.94	0.25	62,62,62,62	0
56	MG	CA	3092	1/1	0.94	0.21	63,63,63,63	0
56	MG	CA	3054	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3779	1/1	0.94	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3197	1/1	0.94	0.11	27,27,27,27	0
56	MG	CA	3106	1/1	0.94	0.12	67,67,67,67	0
56	MG	AA	3130	1/1	0.94	0.11	62,62,62,62	0
56	MG	CA	3060	1/1	0.94	0.25	55,55,55,55	0
56	MG	CA	3119	1/1	0.94	0.22	48,48,48,48	0
56	MG	DA	3163	1/1	0.94	0.21	52,52,52,52	0
56	MG	AA	3233	1/1	0.94	0.27	52,52,52,52	0
56	MG	DF	304	1/1	0.94	0.21	38,38,38,38	0
56	MG	CA	3136	1/1	0.94	0.05	59,59,59,59	0
56	MG	DB	3009	1/1	0.94	0.17	59,59,59,59	0
56	MG	DA	3241	1/1	0.94	0.10	60,60,60,60	0
56	MG	BA	3524	1/1	0.94	0.16	24,24,24,24	0
56	MG	BA	3768	1/1	0.94	0.21	29,29,29,29	0
56	MG	DA	3069	1/1	0.94	0.21	58,58,58,58	0
56	MG	BA	3082	1/1	0.94	0.19	23,23,23,23	0
56	MG	AA	3002	1/1	0.94	0.12	55,55,55,55	0
56	MG	BA	3202	1/1	0.94	0.19	30,30,30,30	0
56	MG	DA	3528	1/1	0.94	0.11	67,67,67,67	0
56	MG	BA	3140	1/1	0.94	0.23	49,49,49,49	0
56	MG	DA	3224	1/1	0.94	0.20	32,32,32,32	0
56	MG	BA	3856	1/1	0.94	0.11	40,40,40,40	0
56	MG	AA	3145	1/1	0.94	0.09	35,35,35,35	0
56	MG	DE	304	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3480	1/1	0.94	0.15	54,54,54,54	0
56	MG	DA	3645	1/1	0.94	0.18	49,49,49,49	0
56	MG	BA	3884	1/1	0.94	0.17	27,27,27,27	0
56	MG	BA	3026	1/1	0.94	0.15	42,42,42,42	0
56	MG	DA	3441	1/1	0.94	0.08	44,44,44,44	0
56	MG	DA	3598	1/1	0.94	0.14	63,63,63,63	0
56	MG	BA	3281	1/1	0.94	0.23	38,38,38,38	0
56	MG	BA	3517	1/1	0.94	0.10	31,31,31,31	0
56	MG	CX	3007	1/1	0.94	0.15	57,57,57,57	0
56	MG	CA	3115	1/1	0.94	0.14	60,60,60,60	0
56	MG	BA	3780	1/1	0.94	0.15	45,45,45,45	0
56	MG	BA	3166	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3742	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3620	1/1	0.94	0.20	39,39,39,39	0
56	MG	BA	3853	1/1	0.94	0.16	41,41,41,41	0
56	MG	DA	3615	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3096	1/1	0.94	0.12	44,44,44,44	0
56	MG	BA	3375	1/1	0.94	0.18	30,30,30,30	0
56	MG	BA	3876	1/1	0.94	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3651	1/1	0.94	0.17	52,52,52,52	0
56	MG	DA	3420	1/1	0.94	0.09	45,45,45,45	0
56	MG	B0	104	1/1	0.94	0.13	35,35,35,35	0
56	MG	B1	102	1/1	0.94	0.09	59,59,59,59	0
56	MG	BA	3503	1/1	0.94	0.19	44,44,44,44	0
56	MG	DA	3053	1/1	0.94	0.22	43,43,43,43	0
56	MG	BA	3007	1/1	0.94	0.12	43,43,43,43	0
56	MG	DA	3466	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3222	1/1	0.94	0.28	42,42,42,42	0
56	MG	BA	3260	1/1	0.94	0.17	40,40,40,40	0
56	MG	BA	3349	1/1	0.94	0.19	42,42,42,42	0
56	MG	BX	3006	1/1	0.94	0.20	35,35,35,35	0
56	MG	DA	3318	1/1	0.94	0.11	59,59,59,59	0
56	MG	DA	3319	1/1	0.94	0.09	43,43,43,43	0
56	MG	BA	3528	1/1	0.94	0.09	58,58,58,58	0
56	MG	BA	3582	1/1	0.94	0.22	34,34,34,34	0
56	MG	BA	3266	1/1	0.94	0.14	28,28,28,28	0
56	MG	CA	3139	1/1	0.94	0.18	61,61,61,61	0
56	MG	AF	3001	1/1	0.94	0.21	31,31,31,31	0
56	MG	BA	3437	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3560	1/1	0.94	0.20	28,28,28,28	0
56	MG	BA	3301	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3484	1/1	0.94	0.08	39,39,39,39	0
56	MG	BA	3826	1/1	0.94	0.19	42,42,42,42	0
56	MG	BA	3778	1/1	0.94	0.30	40,40,40,40	0
56	MG	DA	3660	1/1	0.94	0.11	34,34,34,34	0
56	MG	BA	3883	1/1	0.94	0.26	45,45,45,45	0
56	MG	BF	311	1/1	0.94	0.20	40,40,40,40	0
56	MG	BA	3105	1/1	0.94	0.23	44,44,44,44	0
56	MG	BA	3797	1/1	0.94	0.22	52,52,52,52	0
56	MG	BA	3333	1/1	0.94	0.28	55,55,55,55	0
56	MG	DA	3592	1/1	0.94	0.13	54,54,54,54	0
56	MG	BX	3003	1/1	0.94	0.15	36,36,36,36	0
56	MG	BA	3367	1/1	0.94	0.17	49,49,49,49	0
56	MG	BB	3027	1/1	0.94	0.17	58,58,58,58	0
56	MG	BA	3238	1/1	0.94	0.23	42,42,42,42	0
56	MG	DA	3136	1/1	0.94	0.16	41,41,41,41	0
56	MG	BA	3357	1/1	0.94	0.20	40,40,40,40	0
56	MG	CA	3144	1/1	0.94	0.21	69,69,69,69	0
56	MG	BA	3732	1/1	0.94	0.18	24,24,24,24	0
56	MG	DA	3324	1/1	0.94	0.21	47,47,47,47	0
56	MG	CA	3076	1/1	0.94	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3257	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3609	1/1	0.94	0.17	30,30,30,30	0
56	MG	BA	3259	1/1	0.94	0.21	33,33,33,33	0
56	MG	BF	314	1/1	0.94	0.11	46,46,46,46	0
56	MG	AA	3175	1/1	0.94	0.13	62,62,62,62	0
56	MG	DA	3199	1/1	0.94	0.20	51,51,51,51	0
56	MG	BA	3586	1/1	0.94	0.21	40,40,40,40	0
59	ZN	DY	501	1/1	0.94	0.11	81,81,81,81	0
56	MG	BA	3240	1/1	0.94	0.18	39,39,39,39	0
56	MG	AA	3070	1/1	0.94	0.21	51,51,51,51	0
56	MG	BA	3299	1/1	0.94	0.32	51,51,51,51	0
56	MG	BA	3499	1/1	0.94	0.16	35,35,35,35	0
56	MG	BA	3885	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3155	1/1	0.94	0.13	41,41,41,41	0
56	MG	CA	3141	1/1	0.94	0.13	65,65,65,65	0
56	MG	BA	3457	1/1	0.94	0.16	25,25,25,25	0
56	MG	DA	3623	1/1	0.94	0.17	54,54,54,54	0
56	MG	DA	3452	1/1	0.94	0.18	49,49,49,49	0
56	MG	BA	3591	1/1	0.94	0.22	31,31,31,31	0
56	MG	DA	3039	1/1	0.94	0.10	29,29,29,29	0
56	MG	B8	101	1/1	0.94	0.30	47,47,47,47	0
56	MG	BA	3598	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3023	1/1	0.94	0.19	20,20,20,20	0
56	MG	AA	3048	1/1	0.94	0.26	46,46,46,46	0
56	MG	DA	3604	1/1	0.94	0.14	50,50,50,50	0
56	MG	AA	3204	1/1	0.94	0.18	53,53,53,53	0
56	MG	B2	3002	1/1	0.94	0.21	43,43,43,43	0
56	MG	AA	3164	1/1	0.94	0.17	62,62,62,62	0
56	MG	DA	3242	1/1	0.94	0.15	40,40,40,40	0
56	MG	DA	3548	1/1	0.94	0.10	55,55,55,55	0
56	MG	CA	3043	1/1	0.94	0.27	57,57,57,57	0
56	MG	BA	3828	1/1	0.94	0.11	46,46,46,46	0
56	MG	DA	3058	1/1	0.94	0.14	56,56,56,56	0
56	MG	BA	3326	1/1	0.94	0.17	38,38,38,38	0
56	MG	AA	3183	1/1	0.94	0.12	59,59,59,59	0
56	MG	CA	3062	1/1	0.94	0.25	64,64,64,64	0
56	MG	DA	3616	1/1	0.94	0.15	54,54,54,54	0
56	MG	BA	3119	1/1	0.94	0.21	40,40,40,40	0
56	MG	AA	3112	1/1	0.94	0.17	40,40,40,40	0
56	MG	BO	3002	1/1	0.94	0.16	50,50,50,50	0
56	MG	BA	3564	1/1	0.94	0.09	39,39,39,39	0
56	MG	DA	3025	1/1	0.94	0.43	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BE	311	1/1	0.94	0.10	37,37,37,37	0
56	MG	BA	3216	1/1	0.94	0.27	35,35,35,35	0
56	MG	BA	3584	1/1	0.94	0.23	40,40,40,40	0
56	MG	BA	3376	1/1	0.94	0.20	32,32,32,32	0
56	MG	BA	3330	1/1	0.94	0.25	41,41,41,41	0
56	MG	BA	3613	1/1	0.94	0.15	54,54,54,54	0
56	MG	BA	3068	1/1	0.94	0.23	44,44,44,44	0
56	MG	DA	3599	1/1	0.94	0.10	51,51,51,51	0
56	MG	BA	3287	1/1	0.94	0.23	48,48,48,48	0
56	MG	BA	3031	1/1	0.94	0.17	40,40,40,40	0
56	MG	CA	3146	1/1	0.94	0.17	43,43,43,43	0
56	MG	DA	3469	1/1	0.94	0.07	45,45,45,45	0
56	MG	DA	3451	1/1	0.94	0.10	34,34,34,34	0
56	MG	DA	3483	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3567	1/1	0.94	0.09	44,44,44,44	0
56	MG	DA	3120	1/1	0.94	0.18	47,47,47,47	0
56	MG	CA	3118	1/1	0.94	0.11	63,63,63,63	0
56	MG	DA	3351	1/1	0.94	0.13	36,36,36,36	0
56	MG	DA	3340	1/1	0.94	0.13	45,45,45,45	0
56	MG	AA	3205	1/1	0.94	0.21	56,56,56,56	0
56	MG	DA	3180	1/1	0.94	0.25	57,57,57,57	0
56	MG	BA	3128	1/1	0.94	0.26	35,35,35,35	0
56	MG	DA	3317	1/1	0.94	0.12	56,56,56,56	0
56	MG	BN	3001	1/1	0.94	0.19	41,41,41,41	0
56	MG	DA	3243	1/1	0.94	0.13	39,39,39,39	0
56	MG	AA	3179	1/1	0.94	0.21	66,66,66,66	0
56	MG	CA	3142	1/1	0.94	0.07	61,61,61,61	0
56	MG	BA	3758	1/1	0.94	0.20	48,48,48,48	0
56	MG	BA	3774	1/1	0.94	0.25	47,47,47,47	0
56	MG	AA	3017	1/1	0.94	0.21	48,48,48,48	0
56	MG	AA	3119	1/1	0.94	0.12	60,60,60,60	0
56	MG	CA	3047	1/1	0.94	0.24	53,53,53,53	0
56	MG	BA	3289	1/1	0.94	0.18	30,30,30,30	0
56	MG	DE	302	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3082	1/1	0.94	0.14	48,48,48,48	0
56	MG	DA	3666	1/1	0.94	0.12	55,55,55,55	0
56	MG	DA	3330	1/1	0.94	0.21	47,47,47,47	0
56	MG	BA	3525	1/1	0.94	0.06	59,59,59,59	0
56	MG	B2	3001	1/1	0.94	0.14	44,44,44,44	0
56	MG	BA	3738	1/1	0.95	0.21	46,46,46,46	0
56	MG	DA	3391	1/1	0.95	0.18	50,50,50,50	0
56	MG	BA	3074	1/1	0.95	0.26	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3135	1/1	0.95	0.15	54,54,54,54	0
56	MG	BA	3799	1/1	0.95	0.20	22,22,22,22	0
56	MG	AA	3163	1/1	0.95	0.23	53,53,53,53	0
56	MG	CA	3034	1/1	0.95	0.15	52,52,52,52	0
56	MG	DQ	3002	1/1	0.95	0.18	35,35,35,35	0
56	MG	BA	3236	1/1	0.95	0.17	30,30,30,30	0
56	MG	AA	3039	1/1	0.95	0.29	51,51,51,51	0
56	MG	BA	3536	1/1	0.95	0.21	34,34,34,34	0
56	MG	DA	3537	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3760	1/1	0.95	0.16	36,36,36,36	0
56	MG	BA	3803	1/1	0.95	0.14	67,67,67,67	0
56	MG	BA	3605	1/1	0.95	0.15	49,49,49,49	0
56	MG	CQ	3001	1/1	0.95	0.11	56,56,56,56	0
56	MG	DV	202	1/1	0.95	0.21	49,49,49,49	0
56	MG	BA	3221	1/1	0.95	0.19	49,49,49,49	0
56	MG	BA	3343	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3392	1/1	0.95	0.12	39,39,39,39	0
56	MG	BA	3431	1/1	0.95	0.17	54,54,54,54	0
56	MG	DA	3416	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3653	1/1	0.95	0.15	45,45,45,45	0
56	MG	AA	3167	1/1	0.95	0.17	53,53,53,53	0
56	MG	DA	3046	1/1	0.95	0.15	40,40,40,40	0
56	MG	BB	3029	1/1	0.95	0.15	21,21,21,21	0
56	MG	BA	3060	1/1	0.95	0.18	39,39,39,39	0
56	MG	BA	3256	1/1	0.95	0.21	39,39,39,39	0
56	MG	BA	3837	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3006	1/1	0.95	0.19	41,41,41,41	0
56	MG	BA	3395	1/1	0.95	0.21	44,44,44,44	0
56	MG	DA	3234	1/1	0.95	0.15	47,47,47,47	0
56	MG	DA	3413	1/1	0.95	0.21	42,42,42,42	0
56	MG	CA	3074	1/1	0.95	0.43	73,73,73,73	0
56	MG	BA	3851	1/1	0.95	0.16	33,33,33,33	0
56	MG	AA	3211	1/1	0.95	0.17	56,56,56,56	0
56	MG	BA	3063	1/1	0.95	0.31	41,41,41,41	0
56	MG	BA	3338	1/1	0.95	0.20	44,44,44,44	0
56	MG	DA	3516	1/1	0.95	0.12	56,56,56,56	0
56	MG	CX	3003	1/1	0.95	0.20	59,59,59,59	0
56	MG	BA	3122	1/1	0.95	0.20	22,22,22,22	0
56	MG	BA	3538	1/1	0.95	0.17	25,25,25,25	0
56	MG	AA	3227	1/1	0.95	0.13	25,25,25,25	0
56	MG	BA	3677	1/1	0.95	0.14	29,29,29,29	0
56	MG	AA	3095	1/1	0.95	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3334	1/1	0.95	0.21	35,35,35,35	0
56	MG	DA	3141	1/1	0.95	0.14	42,42,42,42	0
56	MG	BA	3175	1/1	0.95	0.15	39,39,39,39	0
56	MG	DA	3213	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3572	1/1	0.95	0.18	48,48,48,48	0
56	MG	BA	3200	1/1	0.95	0.22	35,35,35,35	0
56	MG	BA	3811	1/1	0.95	0.14	40,40,40,40	0
56	MG	DA	3457	1/1	0.95	0.16	30,30,30,30	0
60	K	AX	3001	1/1	0.95	0.16	45,45,45,45	0
56	MG	BA	3386	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3110	1/1	0.95	0.26	17,17,17,17	0
56	MG	BA	3762	1/1	0.95	0.12	60,60,60,60	0
56	MG	BA	3368	1/1	0.95	0.19	37,37,37,37	0
56	MG	BA	3014	1/1	0.95	0.20	21,21,21,21	0
56	MG	BP	203	1/1	0.95	0.21	28,28,28,28	0
56	MG	DA	3435	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3317	1/1	0.95	0.17	47,47,47,47	0
56	MG	DA	3071	1/1	0.95	0.12	41,41,41,41	0
56	MG	BA	3383	1/1	0.95	0.12	42,42,42,42	0
56	MG	BA	3053	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3453	1/1	0.95	0.18	17,17,17,17	0
56	MG	DA	3291	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3480	1/1	0.95	0.12	43,43,43,43	0
56	MG	DA	3629	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3297	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3282	1/1	0.95	0.24	32,32,32,32	0
56	MG	BA	3360	1/1	0.95	0.12	49,49,49,49	0
56	MG	BQ	3002	1/1	0.95	0.27	24,24,24,24	0
56	MG	CA	3044	1/1	0.95	0.23	52,52,52,52	0
56	MG	DA	3475	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3456	1/1	0.95	0.26	55,55,55,55	0
56	MG	DA	3442	1/1	0.95	0.10	46,46,46,46	0
56	MG	CA	3145	1/1	0.95	0.30	46,46,46,46	0
56	MG	DA	3036	1/1	0.95	0.12	34,34,34,34	0
56	MG	BA	3711	1/1	0.95	0.26	53,53,53,53	0
56	MG	AA	3069	1/1	0.95	0.16	44,44,44,44	0
56	MG	BP	206	1/1	0.95	0.18	31,31,31,31	0
56	MG	BE	301	1/1	0.95	0.17	36,36,36,36	0
56	MG	AA	3191	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3406	1/1	0.95	0.18	28,28,28,28	0
56	MG	CA	3154	1/1	0.95	0.24	56,56,56,56	0
56	MG	DA	3525	1/1	0.95	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3342	1/1	0.95	0.20	41,41,41,41	0
56	MG	BA	3667	1/1	0.95	0.14	43,43,43,43	0
56	MG	BA	3577	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3160	1/1	0.95	0.18	44,44,44,44	0
56	MG	BA	3404	1/1	0.95	0.19	38,38,38,38	0
56	MG	BA	3177	1/1	0.95	0.22	40,40,40,40	0
56	MG	BA	3246	1/1	0.95	0.15	30,30,30,30	0
56	MG	DA	3138	1/1	0.95	0.13	55,55,55,55	0
56	MG	DB	3020	1/1	0.95	0.17	52,52,52,52	0
56	MG	AA	3029	1/1	0.95	0.34	56,56,56,56	0
56	MG	DA	3101	1/1	0.95	0.11	46,46,46,46	0
56	MG	DA	3583	1/1	0.95	0.13	54,54,54,54	0
56	MG	BA	3520	1/1	0.95	0.12	42,42,42,42	0
56	MG	BF	313	1/1	0.95	0.18	49,49,49,49	0
56	MG	BA	3773	1/1	0.95	0.21	29,29,29,29	0
56	MG	CA	3199	1/1	0.95	0.27	51,51,51,51	0
56	MG	CA	3087	1/1	0.95	0.24	60,60,60,60	0
56	MG	BA	3358	1/1	0.95	0.21	28,28,28,28	0
56	MG	DA	3059	1/1	0.95	0.13	39,39,39,39	0
56	MG	BA	3370	1/1	0.95	0.20	34,34,34,34	0
56	MG	DB	3015	1/1	0.95	0.24	44,44,44,44	0
56	MG	DA	3017	1/1	0.95	0.21	42,42,42,42	0
56	MG	BA	3081	1/1	0.95	0.18	21,21,21,21	0
56	MG	DA	3486	1/1	0.95	0.25	38,38,38,38	0
56	MG	AA	3129	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3903	1/1	0.95	0.19	42,42,42,42	0
56	MG	DA	3671	1/1	0.95	0.22	36,36,36,36	0
56	MG	DA	3367	1/1	0.95	0.10	57,57,57,57	0
56	MG	BA	3802	1/1	0.95	0.16	27,27,27,27	0
56	MG	B3	3002	1/1	0.95	0.29	39,39,39,39	0
56	MG	BA	3272	1/1	0.95	0.20	40,40,40,40	0
56	MG	BA	3513	1/1	0.95	0.20	51,51,51,51	0
56	MG	DA	3190	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3539	1/1	0.95	0.10	56,56,56,56	0
56	MG	CL	201	1/1	0.95	0.12	55,55,55,55	0
56	MG	D3	3001	1/1	0.95	0.12	62,62,62,62	0
56	MG	BA	3632	1/1	0.95	0.18	41,41,41,41	0
56	MG	BA	3377	1/1	0.95	0.22	35,35,35,35	0
56	MG	BA	3131	1/1	0.95	0.19	37,37,37,37	0
56	MG	BA	3248	1/1	0.95	0.12	47,47,47,47	0
56	MG	BA	3625	1/1	0.95	0.20	20,20,20,20	0
56	MG	BF	302	1/1	0.95	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3558	1/1	0.95	0.20	46,46,46,46	0
56	MG	BA	3547	1/1	0.95	0.11	48,48,48,48	0
60	K	CX	3001	1/1	0.95	0.08	62,62,62,62	0
56	MG	AA	3100	1/1	0.95	0.17	41,41,41,41	0
56	MG	BA	3344	1/1	0.95	0.25	33,33,33,33	0
56	MG	BF	305	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3741	1/1	0.95	0.19	63,63,63,63	0
56	MG	DA	3201	1/1	0.95	0.11	52,52,52,52	0
56	MG	DA	3189	1/1	0.95	0.14	39,39,39,39	0
56	MG	DA	3578	1/1	0.95	0.07	46,46,46,46	0
56	MG	DA	3186	1/1	0.95	0.22	54,54,54,54	0
56	MG	DA	3603	1/1	0.95	0.15	52,52,52,52	0
56	MG	DA	3108	1/1	0.95	0.16	38,38,38,38	0
56	MG	BA	3336	1/1	0.95	0.21	43,43,43,43	0
56	MG	AA	3066	1/1	0.95	0.16	30,30,30,30	0
56	MG	BA	3057	1/1	0.95	0.14	39,39,39,39	0
56	MG	BA	3599	1/1	0.95	0.06	60,60,60,60	0
56	MG	BA	3904	1/1	0.95	0.15	46,46,46,46	0
56	MG	BA	3237	1/1	0.95	0.20	57,57,57,57	0
56	MG	CA	3037	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3184	1/1	0.95	0.22	41,41,41,41	0
56	MG	BA	3419	1/1	0.95	0.14	38,38,38,38	0
56	MG	AA	3199	1/1	0.95	0.21	54,54,54,54	0
56	MG	BA	3363	1/1	0.95	0.17	45,45,45,45	0
56	MG	CA	3122	1/1	0.95	0.20	66,66,66,66	0
56	MG	DA	3222	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3043	1/1	0.95	0.18	43,43,43,43	0
56	MG	DA	3464	1/1	0.95	0.21	31,31,31,31	0
56	MG	BA	3393	1/1	0.95	0.17	23,23,23,23	0
56	MG	BA	3475	1/1	0.95	0.20	28,28,28,28	0
56	MG	AA	3001	1/1	0.95	0.19	35,35,35,35	0
56	MG	BA	3692	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3529	1/1	0.95	0.14	53,53,53,53	0
56	MG	BA	3725	1/1	0.95	0.22	42,42,42,42	0
56	MG	BA	3189	1/1	0.95	0.21	30,30,30,30	0
56	MG	BA	3411	1/1	0.95	0.19	44,44,44,44	0
56	MG	BA	3723	1/1	0.95	0.22	27,27,27,27	0
56	MG	DA	3083	1/1	0.95	0.17	31,31,31,31	0
56	MG	DA	3334	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3401	1/1	0.95	0.24	10,10,10,10	0
56	MG	BO	3004	1/1	0.95	0.19	53,53,53,53	0
56	MG	BA	3155	1/1	0.95	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3737	1/1	0.95	0.23	29,29,29,29	0
56	MG	BA	3280	1/1	0.95	0.18	23,23,23,23	0
56	MG	BB	3002	1/1	0.95	0.28	43,43,43,43	0
56	MG	DA	3179	1/1	0.95	0.25	42,42,42,42	0
56	MG	DA	3098	1/1	0.95	0.18	36,36,36,36	0
56	MG	BA	3785	1/1	0.95	0.17	39,39,39,39	0
56	MG	DA	3470	1/1	0.95	0.13	46,46,46,46	0
56	MG	AA	3118	1/1	0.95	0.21	45,45,45,45	0
56	MG	DA	3406	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3366	1/1	0.95	0.18	25,25,25,25	0
56	MG	DD	306	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3683	1/1	0.95	0.22	37,37,37,37	0
56	MG	BG	206	1/1	0.95	0.11	59,59,59,59	0
56	MG	DA	3051	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3020	1/1	0.95	0.16	48,48,48,48	0
56	MG	BA	3186	1/1	0.96	0.23	37,37,37,37	0
56	MG	DD	301	1/1	0.96	0.23	38,38,38,38	0
56	MG	DA	3169	1/1	0.96	0.10	44,44,44,44	0
56	MG	DA	3376	1/1	0.96	0.10	27,27,27,27	0
56	MG	DA	3640	1/1	0.96	0.07	56,56,56,56	0
56	MG	BA	3392	1/1	0.96	0.23	48,48,48,48	0
56	MG	DA	3302	1/1	0.96	0.13	57,57,57,57	0
56	MG	DA	3643	1/1	0.96	0.12	51,51,51,51	0
56	MG	CA	3033	1/1	0.96	0.07	65,65,65,65	0
56	MG	BA	3439	1/1	0.96	0.22	53,53,53,53	0
56	MG	AA	3078	1/1	0.96	0.24	47,47,47,47	0
56	MG	CA	3051	1/1	0.96	0.21	32,32,32,32	0
56	MG	AA	3228	1/1	0.96	0.33	58,58,58,58	0
56	MG	BD	310	1/1	0.96	0.15	46,46,46,46	0
56	MG	BY	502	1/1	0.96	0.22	45,45,45,45	0
56	MG	DA	3669	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3325	1/1	0.96	0.13	33,33,33,33	0
56	MG	BA	3321	1/1	0.96	0.13	43,43,43,43	0
56	MG	DA	3254	1/1	0.96	0.17	37,37,37,37	0
56	MG	AA	3053	1/1	0.96	0.20	42,42,42,42	0
56	MG	AA	3011	1/1	0.96	0.28	46,46,46,46	0
56	MG	BA	3850	1/1	0.96	0.20	47,47,47,47	0
56	MG	BA	3429	1/1	0.96	0.17	51,51,51,51	0
56	MG	DA	3271	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3276	1/1	0.96	0.24	42,42,42,42	0
56	MG	BA	3792	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3297	1/1	0.96	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3077	1/1	0.96	0.22	27,27,27,27	0
56	MG	DA	3064	1/1	0.96	0.12	44,44,44,44	0
56	MG	DA	3185	1/1	0.96	0.17	39,39,39,39	0
56	MG	DA	3078	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3823	1/1	0.96	0.13	57,57,57,57	0
56	MG	BW	204	1/1	0.96	0.20	23,23,23,23	0
56	MG	AA	3138	1/1	0.96	0.17	57,57,57,57	0
56	MG	BA	3777	1/1	0.96	0.26	52,52,52,52	0
56	MG	DA	3207	1/1	0.96	0.22	52,52,52,52	0
56	MG	BA	3353	1/1	0.96	0.29	49,49,49,49	0
56	MG	DA	3520	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3233	1/1	0.96	0.18	26,26,26,26	0
56	MG	BA	3132	1/1	0.96	0.21	57,57,57,57	0
56	MG	AA	3136	1/1	0.96	0.15	52,52,52,52	0
56	MG	DA	3590	1/1	0.96	0.07	37,37,37,37	0
56	MG	DA	3333	1/1	0.96	0.18	31,31,31,31	0
56	MG	BA	3893	1/1	0.96	0.12	26,26,26,26	0
56	MG	BU	208	1/1	0.96	0.16	34,34,34,34	0
56	MG	BA	3008	1/1	0.96	0.26	24,24,24,24	0
56	MG	DA	3478	1/1	0.96	0.12	50,50,50,50	0
56	MG	DA	3499	1/1	0.96	0.20	44,44,44,44	0
56	MG	BA	3042	1/1	0.96	0.26	43,43,43,43	0
56	MG	BA	3012	1/1	0.96	0.15	31,31,31,31	0
56	MG	DA	3137	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3649	1/1	0.96	0.20	55,55,55,55	0
56	MG	BA	3115	1/1	0.96	0.09	44,44,44,44	0
56	MG	DA	3600	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3614	1/1	0.96	0.06	47,47,47,47	0
56	MG	BB	3022	1/1	0.96	0.24	46,46,46,46	0
56	MG	BA	3391	1/1	0.96	0.17	24,24,24,24	0
56	MG	BA	3416	1/1	0.96	0.20	29,29,29,29	0
56	MG	CA	3197	1/1	0.96	0.19	43,43,43,43	0
56	MG	DA	3236	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3440	1/1	0.96	0.14	34,34,34,34	0
56	MG	BA	3422	1/1	0.96	0.20	24,24,24,24	0
56	MG	BA	3076	1/1	0.96	0.28	17,17,17,17	0
56	MG	CA	3201	1/1	0.96	0.06	51,51,51,51	0
56	MG	BF	303	1/1	0.96	0.20	31,31,31,31	0
56	MG	DA	3389	1/1	0.96	0.13	54,54,54,54	0
56	MG	CA	3123	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3495	1/1	0.96	0.12	48,48,48,48	0
56	MG	BB	3019	1/1	0.96	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3094	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3377	1/1	0.96	0.15	43,43,43,43	0
56	MG	BA	3378	1/1	0.96	0.18	43,43,43,43	0
56	MG	AA	3193	1/1	0.96	0.21	51,51,51,51	0
56	MG	DA	3431	1/1	0.96	0.14	34,34,34,34	0
56	MG	BY	503	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3121	1/1	0.96	0.21	33,33,33,33	0
56	MG	BA	3380	1/1	0.96	0.23	45,45,45,45	0
56	MG	BU	207	1/1	0.96	0.15	37,37,37,37	0
56	MG	DA	3345	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3559	1/1	0.96	0.13	37,37,37,37	0
56	MG	DA	3652	1/1	0.96	0.15	53,53,53,53	0
56	MG	DA	3534	1/1	0.96	0.11	39,39,39,39	0
56	MG	DA	3335	1/1	0.96	0.17	28,28,28,28	0
56	MG	BA	3568	1/1	0.96	0.23	56,56,56,56	0
56	MG	BA	3874	1/1	0.96	0.20	31,31,31,31	0
56	MG	BA	3687	1/1	0.96	0.23	49,49,49,49	0
56	MG	CA	3031	1/1	0.96	0.09	51,51,51,51	0
56	MG	AA	3057	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3157	1/1	0.96	0.24	41,41,41,41	0
56	MG	BA	3494	1/1	0.96	0.18	32,32,32,32	0
56	MG	AA	3185	1/1	0.96	0.24	52,52,52,52	0
56	MG	DA	3009	1/1	0.96	0.22	39,39,39,39	0
56	MG	BA	3134	1/1	0.96	0.28	29,29,29,29	0
56	MG	DA	3300	1/1	0.96	0.14	29,29,29,29	0
56	MG	DA	3586	1/1	0.96	0.20	31,31,31,31	0
56	MG	D1	101	1/1	0.96	0.14	44,44,44,44	0
56	MG	AA	3146	1/1	0.96	0.14	42,42,42,42	0
56	MG	BN	3004	1/1	0.96	0.13	37,37,37,37	0
56	MG	DA	3105	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3346	1/1	0.96	0.10	31,31,31,31	0
56	MG	BA	3534	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3618	1/1	0.96	0.20	19,19,19,19	0
56	MG	BA	3817	1/1	0.96	0.18	50,50,50,50	0
56	MG	BA	3647	1/1	0.96	0.23	47,47,47,47	0
56	MG	BQ	3007	1/1	0.96	0.16	44,44,44,44	0
56	MG	BA	3604	1/1	0.96	0.21	52,52,52,52	0
56	MG	BA	3489	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3886	1/1	0.96	0.10	37,37,37,37	0
56	MG	BA	3218	1/1	0.96	0.29	33,33,33,33	0
56	MG	AX	3012	1/1	0.96	0.06	60,60,60,60	0
56	MG	DA	3084	1/1	0.96	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3259	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3033	1/1	0.96	0.23	37,37,37,37	0
56	MG	BA	3339	1/1	0.96	0.20	30,30,30,30	0
56	MG	AA	3143	1/1	0.96	0.10	38,38,38,38	0
56	MG	BA	3151	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3194	1/1	0.96	0.15	40,40,40,40	0
56	MG	BA	3497	1/1	0.96	0.22	49,49,49,49	0
56	MG	DF	307	1/1	0.96	0.07	48,48,48,48	0
56	MG	B1	101	1/1	0.96	0.33	40,40,40,40	0
56	MG	DA	3063	1/1	0.96	0.12	34,34,34,34	0
56	MG	BA	3223	1/1	0.96	0.40	36,36,36,36	0
56	MG	AA	3151	1/1	0.96	0.12	48,48,48,48	0
56	MG	AX	3005	1/1	0.96	0.12	60,60,60,60	0
56	MG	DA	3113	1/1	0.96	0.06	39,39,39,39	0
56	MG	CA	3134	1/1	0.96	0.20	53,53,53,53	0
56	MG	BA	3397	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3050	1/1	0.96	0.16	15,15,15,15	0
56	MG	BA	3045	1/1	0.96	0.15	35,35,35,35	0
56	MG	DA	3152	1/1	0.96	0.27	39,39,39,39	0
56	MG	BA	3346	1/1	0.96	0.14	38,38,38,38	0
56	MG	DA	3638	1/1	0.96	0.13	50,50,50,50	0
56	MG	BA	3553	1/1	0.96	0.19	19,19,19,19	0
56	MG	BA	3090	1/1	0.96	0.21	28,28,28,28	0
56	MG	BA	3511	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3452	1/1	0.96	0.18	25,25,25,25	0
56	MG	DA	3204	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3369	1/1	0.96	0.19	58,58,58,58	0
56	MG	DA	3019	1/1	0.96	0.28	30,30,30,30	0
56	MG	DE	303	1/1	0.96	0.10	38,38,38,38	0
56	MG	BB	3003	1/1	0.96	0.19	31,31,31,31	0
56	MG	DA	3436	1/1	0.96	0.11	38,38,38,38	0
56	MG	DA	3386	1/1	0.96	0.24	46,46,46,46	0
56	MG	CA	3107	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3283	1/1	0.96	0.11	43,43,43,43	0
56	MG	CA	3032	1/1	0.96	0.17	56,56,56,56	0
56	MG	B8	103	1/1	0.96	0.17	31,31,31,31	0
56	MG	BA	3443	1/1	0.96	0.18	22,22,22,22	0
56	MG	DA	3479	1/1	0.96	0.13	43,43,43,43	0
56	MG	AA	3203	1/1	0.96	0.21	59,59,59,59	0
56	MG	D8	101	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3215	1/1	0.96	0.24	38,38,38,38	0
56	MG	BA	3841	1/1	0.96	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BX	3004	1/1	0.96	0.67	48,48,48,48	0
56	MG	DA	3672	1/1	0.96	0.17	43,43,43,43	0
56	MG	BA	3149	1/1	0.96	0.11	35,35,35,35	0
56	MG	BA	3435	1/1	0.96	0.15	60,60,60,60	0
56	MG	BA	3018	1/1	0.96	0.20	32,32,32,32	0
56	MG	AA	3224	1/1	0.96	0.24	51,51,51,51	0
56	MG	DA	3563	1/1	0.96	0.14	60,60,60,60	0
56	MG	BU	209	1/1	0.96	0.13	24,24,24,24	0
56	MG	AA	3108	1/1	0.96	0.09	65,65,65,65	0
56	MG	BA	3458	1/1	0.96	0.17	25,25,25,25	0
56	MG	BA	3661	1/1	0.96	0.08	47,47,47,47	0
56	MG	BV	203	1/1	0.96	0.12	23,23,23,23	0
56	MG	BS	3002	1/1	0.96	0.11	39,39,39,39	0
56	MG	AA	3051	1/1	0.96	0.25	22,22,22,22	0
56	MG	BR	201	1/1	0.96	0.13	35,35,35,35	0
56	MG	BU	203	1/1	0.96	0.29	44,44,44,44	0
56	MG	DA	3635	1/1	0.96	0.18	44,44,44,44	0
56	MG	DA	3540	1/1	0.96	0.09	51,51,51,51	0
56	MG	BA	3678	1/1	0.96	0.15	25,25,25,25	0
56	MG	BA	3093	1/1	0.96	0.41	41,41,41,41	0
56	MG	DA	3352	1/1	0.96	0.20	35,35,35,35	0
56	MG	DF	305	1/1	0.96	0.16	39,39,39,39	0
56	MG	BA	3701	1/1	0.96	0.22	44,44,44,44	0
56	MG	BA	3013	1/1	0.96	0.14	25,25,25,25	0
56	MG	DA	3202	1/1	0.96	0.33	42,42,42,42	0
56	MG	BA	3657	1/1	0.96	0.16	65,65,65,65	0
56	MG	DA	3192	1/1	0.96	0.21	38,38,38,38	0
56	MG	BA	3761	1/1	0.96	0.16	52,52,52,52	0
56	MG	BA	3587	1/1	0.96	0.21	32,32,32,32	0
56	MG	BA	3402	1/1	0.96	0.12	39,39,39,39	0
56	MG	DA	3173	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3085	1/1	0.96	0.26	27,27,27,27	0
56	MG	CA	3121	1/1	0.96	0.21	52,52,52,52	0
56	MG	CA	3176	1/1	0.96	0.17	62,62,62,62	0
56	MG	AA	3021	1/1	0.96	0.14	41,41,41,41	0
56	MG	DA	3294	1/1	0.96	0.11	39,39,39,39	0
56	MG	DA	3647	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3165	1/1	0.96	0.12	27,27,27,27	0
56	MG	BA	3052	1/1	0.96	0.22	15,15,15,15	0
56	MG	BA	3148	1/1	0.96	0.17	36,36,36,36	0
56	MG	DA	3008	1/1	0.96	0.12	33,33,33,33	0
56	MG	DA	3037	1/1	0.96	0.23	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BP	201	1/1	0.96	0.16	29,29,29,29	0
56	MG	BA	3158	1/1	0.96	0.23	12,12,12,12	0
56	MG	DA	3090	1/1	0.96	0.22	53,53,53,53	0
56	MG	DA	3648	1/1	0.96	0.14	39,39,39,39	0
56	MG	AA	3121	1/1	0.96	0.18	49,49,49,49	0
56	MG	DA	3250	1/1	0.96	0.11	50,50,50,50	0
56	MG	BA	3626	1/1	0.96	0.20	22,22,22,22	0
56	MG	BA	3328	1/1	0.96	0.18	36,36,36,36	0
56	MG	DA	3410	1/1	0.96	0.20	55,55,55,55	0
56	MG	DA	3641	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3284	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3270	1/1	0.96	0.19	28,28,28,28	0
56	MG	DA	3047	1/1	0.96	0.27	38,38,38,38	0
56	MG	BA	3708	1/1	0.96	0.16	40,40,40,40	0
56	MG	AA	3157	1/1	0.96	0.26	39,39,39,39	0
56	MG	BA	3767	1/1	0.96	0.17	34,34,34,34	0
56	MG	B5	104	1/1	0.96	0.11	27,27,27,27	0
56	MG	BW	205	1/1	0.96	0.15	34,34,34,34	0
56	MG	DA	3315	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3139	1/1	0.96	0.15	35,35,35,35	0
56	MG	BA	3857	1/1	0.96	0.20	46,46,46,46	0
56	MG	BA	3736	1/1	0.96	0.22	45,45,45,45	0
56	MG	BA	3681	1/1	0.97	0.16	39,39,39,39	0
56	MG	BA	3185	1/1	0.97	0.23	23,23,23,23	0
56	MG	BA	3597	1/1	0.97	0.17	18,18,18,18	0
56	MG	BA	3371	1/1	0.97	0.29	34,34,34,34	0
56	MG	BA	3624	1/1	0.97	0.19	40,40,40,40	0
56	MG	DA	3347	1/1	0.97	0.09	38,38,38,38	0
56	MG	DE	306	1/1	0.97	0.13	43,43,43,43	0
56	MG	BA	3812	1/1	0.97	0.21	22,22,22,22	0
56	MG	AA	3113	1/1	0.97	0.30	55,55,55,55	0
56	MG	CA	3159	1/1	0.97	0.13	61,61,61,61	0
56	MG	DA	3527	1/1	0.97	0.14	22,22,22,22	0
56	MG	DA	3187	1/1	0.97	0.27	44,44,44,44	0
56	MG	DA	3281	1/1	0.97	0.22	42,42,42,42	0
56	MG	BA	3153	1/1	0.97	0.18	31,31,31,31	0
56	MG	CA	3080	1/1	0.97	0.34	55,55,55,55	0
56	MG	AA	3234	1/1	0.97	0.13	40,40,40,40	0
56	MG	BA	3304	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3337	1/1	0.97	0.12	24,24,24,24	0
56	MG	DA	3533	1/1	0.97	0.14	59,59,59,59	0
56	MG	BG	201	1/1	0.97	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3650	1/1	0.97	0.19	33,33,33,33	0
56	MG	AX	3008	1/1	0.97	0.13	54,54,54,54	0
56	MG	BA	3135	1/1	0.97	0.21	37,37,37,37	0
56	MG	BA	3120	1/1	0.97	0.15	50,50,50,50	0
56	MG	BA	3660	1/1	0.97	0.29	46,46,46,46	0
56	MG	BA	3615	1/1	0.97	0.10	28,28,28,28	0
56	MG	BA	3642	1/1	0.97	0.19	27,27,27,27	0
56	MG	BA	3728	1/1	0.97	0.18	36,36,36,36	0
56	MG	DA	3178	1/1	0.97	0.16	31,31,31,31	0
56	MG	BA	3241	1/1	0.97	0.20	48,48,48,48	0
56	MG	BA	3477	1/1	0.97	0.32	41,41,41,41	0
56	MG	BA	3753	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3282	1/1	0.97	0.21	32,32,32,32	0
56	MG	BA	3662	1/1	0.97	0.16	23,23,23,23	0
56	MG	BA	3467	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3054	1/1	0.97	0.20	20,20,20,20	0
56	MG	DA	3497	1/1	0.97	0.11	50,50,50,50	0
56	MG	DA	3277	1/1	0.97	0.17	41,41,41,41	0
56	MG	DA	3030	1/1	0.97	0.40	43,43,43,43	0
56	MG	DA	3055	1/1	0.97	0.12	33,33,33,33	0
56	MG	BB	3001	1/1	0.97	0.21	41,41,41,41	0
56	MG	BA	3196	1/1	0.97	0.12	26,26,26,26	0
56	MG	DA	3543	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3041	1/1	0.97	0.16	30,30,30,30	0
56	MG	DA	3093	1/1	0.97	0.20	26,26,26,26	0
56	MG	AA	3173	1/1	0.97	0.11	43,43,43,43	0
56	MG	BA	3072	1/1	0.97	0.24	27,27,27,27	0
56	MG	DA	3637	1/1	0.97	0.09	48,48,48,48	0
56	MG	DA	3655	1/1	0.97	0.28	57,57,57,57	0
56	MG	DA	3293	1/1	0.97	0.10	34,34,34,34	0
56	MG	BA	3786	1/1	0.97	0.16	20,20,20,20	0
56	MG	BA	3277	1/1	0.97	0.15	21,21,21,21	0
56	MG	BA	3403	1/1	0.97	0.27	52,52,52,52	0
56	MG	BA	3744	1/1	0.97	0.12	41,41,41,41	0
56	MG	DA	3168	1/1	0.97	0.14	28,28,28,28	0
56	MG	BB	3008	1/1	0.97	0.29	50,50,50,50	0
56	MG	DQ	3001	1/1	0.97	0.16	42,42,42,42	0
56	MG	DA	3103	1/1	0.97	0.16	45,45,45,45	0
56	MG	AA	3115	1/1	0.97	0.18	54,54,54,54	0
56	MG	BA	3387	1/1	0.97	0.12	60,60,60,60	0
56	MG	AA	3022	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3684	1/1	0.97	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3656	1/1	0.97	0.19	32,32,32,32	0
56	MG	DD	305	1/1	0.97	0.38	38,38,38,38	0
56	MG	BA	3462	1/1	0.97	0.13	30,30,30,30	0
56	MG	BA	3075	1/1	0.97	0.28	22,22,22,22	0
56	MG	B5	101	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3339	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3373	1/1	0.97	0.24	28,28,28,28	0
56	MG	DA	3048	1/1	0.97	0.13	46,46,46,46	0
56	MG	DB	3012	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	3356	1/1	0.97	0.22	44,44,44,44	0
56	MG	BA	3788	1/1	0.97	0.17	25,25,25,25	0
56	MG	BA	3726	1/1	0.97	0.22	39,39,39,39	0
56	MG	DA	3284	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3245	1/1	0.97	0.24	26,26,26,26	0
56	MG	DA	3226	1/1	0.97	0.27	54,54,54,54	0
56	MG	CF	3001	1/1	0.97	0.19	31,31,31,31	0
56	MG	BA	3574	1/1	0.97	0.28	42,42,42,42	0
56	MG	DA	3159	1/1	0.97	0.14	45,45,45,45	0
56	MG	DA	3518	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3532	1/1	0.97	0.14	50,50,50,50	0
56	MG	AA	3140	1/1	0.97	0.12	45,45,45,45	0
56	MG	CA	3113	1/1	0.97	0.15	37,37,37,37	0
56	MG	AA	3077	1/1	0.97	0.29	60,60,60,60	0
56	MG	AA	3105	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3602	1/1	0.97	0.14	44,44,44,44	0
56	MG	AA	3128	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3460	1/1	0.97	0.15	20,20,20,20	0
56	MG	BA	3440	1/1	0.97	0.22	32,32,32,32	0
56	MG	BA	3329	1/1	0.97	0.15	32,32,32,32	0
56	MG	BA	3905	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3049	1/1	0.97	0.19	32,32,32,32	0
59	ZN	BY	501	1/1	0.97	0.17	63,63,63,63	0
56	MG	BA	3634	1/1	0.97	0.24	23,23,23,23	0
56	MG	AA	3155	1/1	0.97	0.14	42,42,42,42	0
56	MG	DU	3001	1/1	0.97	0.18	43,43,43,43	0
56	MG	BF	309	1/1	0.97	0.17	30,30,30,30	0
56	MG	AA	3186	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3690	1/1	0.97	0.20	53,53,53,53	0
56	MG	CA	3042	1/1	0.97	0.17	48,48,48,48	0
56	MG	BA	3037	1/1	0.97	0.13	35,35,35,35	0
56	MG	AA	3072	1/1	0.97	0.19	40,40,40,40	0
56	MG	B6	103	1/1	0.97	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3735	1/1	0.97	0.23	30,30,30,30	0
56	MG	DA	3258	1/1	0.97	0.19	39,39,39,39	0
56	MG	B5	102	1/1	0.97	0.20	36,36,36,36	0
56	MG	DA	3208	1/1	0.97	0.25	46,46,46,46	0
56	MG	DA	3493	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3041	1/1	0.97	0.21	31,31,31,31	0
56	MG	DA	3350	1/1	0.97	0.20	29,29,29,29	0
56	MG	AA	3229	1/1	0.97	0.17	50,50,50,50	0
56	MG	AA	3075	1/1	0.97	0.22	44,44,44,44	0
56	MG	DA	3118	1/1	0.97	0.16	47,47,47,47	0
56	MG	BA	3878	1/1	0.97	0.20	15,15,15,15	0
56	MG	AB	3002	1/1	0.97	0.15	70,70,70,70	0
56	MG	DU	3002	1/1	0.97	0.28	52,52,52,52	0
56	MG	BA	3064	1/1	0.97	0.15	40,40,40,40	0
56	MG	BF	315	1/1	0.97	0.20	47,47,47,47	0
56	MG	BA	3154	1/1	0.97	0.24	31,31,31,31	0
56	MG	BA	3820	1/1	0.97	0.12	30,30,30,30	0
56	MG	BA	3733	1/1	0.97	0.19	42,42,42,42	0
56	MG	BD	311	1/1	0.97	0.21	40,40,40,40	0
56	MG	DA	3286	1/1	0.97	0.18	29,29,29,29	0
56	MG	DA	3481	1/1	0.97	0.11	41,41,41,41	0
56	MG	BA	3408	1/1	0.97	0.19	41,41,41,41	0
56	MG	DA	3418	1/1	0.97	0.26	44,44,44,44	0
56	MG	AA	3226	1/1	0.97	0.20	34,34,34,34	0
56	MG	BA	3044	1/1	0.97	0.18	32,32,32,32	0
56	MG	AA	3195	1/1	0.97	0.20	38,38,38,38	0
56	MG	BA	3608	1/1	0.97	0.23	58,58,58,58	0
56	MG	CA	3105	1/1	0.97	0.11	53,53,53,53	0
56	MG	AA	3196	1/1	0.97	0.16	42,42,42,42	0
56	MG	BA	3544	1/1	0.97	0.13	40,40,40,40	0
56	MG	DA	3491	1/1	0.97	0.22	53,53,53,53	0
56	MG	BA	3092	1/1	0.97	0.31	31,31,31,31	0
56	MG	DA	3489	1/1	0.97	0.08	40,40,40,40	0
56	MG	CA	3181	1/1	0.97	0.07	55,55,55,55	0
56	MG	BA	3258	1/1	0.97	0.24	38,38,38,38	0
56	MG	DA	3003	1/1	0.97	0.20	24,24,24,24	0
56	MG	AA	3215	1/1	0.97	0.17	47,47,47,47	0
56	MG	DA	3554	1/1	0.97	0.18	48,48,48,48	0
56	MG	DA	3384	1/1	0.97	0.12	55,55,55,55	0
56	MG	BF	304	1/1	0.97	0.17	34,34,34,34	0
56	MG	BA	3198	1/1	0.97	0.19	34,34,34,34	0
56	MG	DA	3198	1/1	0.97	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3846	1/1	0.97	0.17	30,30,30,30	0
56	MG	BA	3535	1/1	0.97	0.12	46,46,46,46	0
56	MG	BA	3010	1/1	0.97	0.28	26,26,26,26	0
56	MG	DA	3299	1/1	0.97	0.15	37,37,37,37	0
56	MG	BA	3172	1/1	0.97	0.27	32,32,32,32	0
56	MG	DA	3123	1/1	0.97	0.16	38,38,38,38	0
56	MG	BA	3003	1/1	0.97	0.22	24,24,24,24	0
56	MG	BA	3765	1/1	0.97	0.16	33,33,33,33	0
56	MG	DD	304	1/1	0.97	0.19	26,26,26,26	0
56	MG	CA	3168	1/1	0.97	0.10	65,65,65,65	0
56	MG	B0	102	1/1	0.97	0.14	47,47,47,47	0
56	MG	DA	3332	1/1	0.97	0.20	53,53,53,53	0
56	MG	DA	3148	1/1	0.97	0.18	50,50,50,50	0
56	MG	DA	3262	1/1	0.97	0.12	36,36,36,36	0
56	MG	B0	107	1/1	0.97	0.11	46,46,46,46	0
56	MG	DA	3022	1/1	0.97	0.26	34,34,34,34	0
56	MG	DA	3492	1/1	0.97	0.19	51,51,51,51	0
56	MG	DA	3425	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3433	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3887	1/1	0.97	0.13	35,35,35,35	0
56	MG	BA	3224	1/1	0.97	0.16	30,30,30,30	0
56	MG	BA	3747	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3174	1/1	0.97	0.20	34,34,34,34	0
56	MG	DA	3203	1/1	0.97	0.20	46,46,46,46	0
56	MG	BA	3421	1/1	0.97	0.17	24,24,24,24	0
56	MG	DA	3140	1/1	0.97	0.19	43,43,43,43	0
56	MG	DA	3423	1/1	0.97	0.11	56,56,56,56	0
56	MG	BA	3362	1/1	0.97	0.17	37,37,37,37	0
56	MG	DA	3455	1/1	0.97	0.13	35,35,35,35	0
56	MG	B7	102	1/1	0.97	0.15	27,27,27,27	0
56	MG	BA	3231	1/1	0.97	0.21	21,21,21,21	0
56	MG	D5	102	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3183	1/1	0.97	0.16	35,35,35,35	0
56	MG	BD	312	1/1	0.97	0.20	27,27,27,27	0
56	MG	DA	3027	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3245	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3822	1/1	0.97	0.26	18,18,18,18	0
56	MG	BA	3869	1/1	0.97	0.27	20,20,20,20	0
56	MG	BA	3207	1/1	0.97	0.23	52,52,52,52	0
56	MG	BA	3478	1/1	0.97	0.17	27,27,27,27	0
56	MG	BA	3254	1/1	0.97	0.16	41,41,41,41	0
56	MG	DA	3013	1/1	0.97	0.23	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3900	1/1	0.97	0.29	40,40,40,40	0
58	SF4	CD	501	8/8	0.97	0.09	50,59,70,75	0
56	MG	BA	3688	1/1	0.97	0.14	41,41,41,41	0
56	MG	DA	3411	1/1	0.97	0.14	44,44,44,44	0
56	MG	AA	3123	1/1	0.97	0.25	46,46,46,46	0
56	MG	BA	3315	1/1	0.97	0.17	39,39,39,39	0
56	MG	DA	3124	1/1	0.97	0.21	35,35,35,35	0
56	MG	BN	3003	1/1	0.97	0.22	41,41,41,41	0
56	MG	BA	3899	1/1	0.97	0.17	40,40,40,40	0
56	MG	DA	3378	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3506	1/1	0.97	0.23	34,34,34,34	0
56	MG	BA	3709	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3834	1/1	0.97	0.15	35,35,35,35	0
56	MG	AA	3034	1/1	0.98	0.12	52,52,52,52	0
56	MG	BP	204	1/1	0.98	0.18	19,19,19,19	0
56	MG	BA	3039	1/1	0.98	0.22	17,17,17,17	0
56	MG	BA	3213	1/1	0.98	0.35	48,48,48,48	0
58	SF4	AD	501	8/8	0.98	0.11	50,60,65,68	0
56	MG	DA	3166	1/1	0.98	0.16	39,39,39,39	0
56	MG	B3	3001	1/1	0.98	0.19	23,23,23,23	0
56	MG	BA	3242	1/1	0.98	0.18	60,60,60,60	0
56	MG	DA	3530	1/1	0.98	0.15	30,30,30,30	0
56	MG	DA	3057	1/1	0.98	0.15	20,20,20,20	0
56	MG	BA	3106	1/1	0.98	0.17	27,27,27,27	0
56	MG	BA	3091	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3035	1/1	0.98	0.22	27,27,27,27	0
56	MG	DA	3255	1/1	0.98	0.20	23,23,23,23	0
56	MG	BV	201	1/1	0.98	0.20	32,32,32,32	0
56	MG	DA	3419	1/1	0.98	0.17	42,42,42,42	0
56	MG	DA	3361	1/1	0.98	0.14	44,44,44,44	0
56	MG	DA	3253	1/1	0.98	0.13	41,41,41,41	0
56	MG	BA	3296	1/1	0.98	0.25	40,40,40,40	0
56	MG	DA	3508	1/1	0.98	0.23	39,39,39,39	0
56	MG	CD	502	1/1	0.98	0.12	51,51,51,51	0
56	MG	AA	3159	1/1	0.98	0.15	32,32,32,32	0
56	MG	DA	3468	1/1	0.98	0.12	49,49,49,49	0
56	MG	BA	3523	1/1	0.98	0.14	49,49,49,49	0
56	MG	BS	3001	1/1	0.98	0.18	39,39,39,39	0
56	MG	DA	3080	1/1	0.98	0.21	33,33,33,33	0
56	MG	BA	3664	1/1	0.98	0.24	46,46,46,46	0
56	MG	BA	3636	1/1	0.98	0.21	28,28,28,28	0
56	MG	CA	3012	1/1	0.98	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3794	1/1	0.98	0.07	48,48,48,48	0
56	MG	AA	3148	1/1	0.98	0.17	43,43,43,43	0
56	MG	BA	3891	1/1	0.98	0.21	33,33,33,33	0
56	MG	BA	3190	1/1	0.98	0.23	38,38,38,38	0
56	MG	DA	3268	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3441	1/1	0.98	0.20	26,26,26,26	0
56	MG	BQ	3004	1/1	0.98	0.31	46,46,46,46	0
56	MG	BA	3040	1/1	0.98	0.18	25,25,25,25	0
56	MG	BA	3034	1/1	0.98	0.20	20,20,20,20	0
56	MG	DA	3439	1/1	0.98	0.19	50,50,50,50	0
56	MG	BD	306	1/1	0.98	0.20	25,25,25,25	0
56	MG	CV	101	1/1	0.98	0.20	51,51,51,51	0
56	MG	BA	3109	1/1	0.98	0.22	20,20,20,20	0
56	MG	DA	3364	1/1	0.98	0.17	58,58,58,58	0
56	MG	DA	3601	1/1	0.98	0.08	38,38,38,38	0
56	MG	BD	302	1/1	0.98	0.34	39,39,39,39	0
56	MG	BA	3038	1/1	0.98	0.17	42,42,42,42	0
56	MG	BA	3327	1/1	0.98	0.20	20,20,20,20	0
56	MG	BA	3046	1/1	0.98	0.16	30,30,30,30	0
56	MG	BA	3055	1/1	0.98	0.28	25,25,25,25	0
56	MG	BA	3162	1/1	0.98	0.18	26,26,26,26	0
56	MG	AA	3168	1/1	0.98	0.14	53,53,53,53	0
56	MG	DA	3651	1/1	0.98	0.13	50,50,50,50	0
56	MG	DA	3144	1/1	0.98	0.22	49,49,49,49	0
56	MG	DA	3336	1/1	0.98	0.15	27,27,27,27	0
56	MG	DA	3239	1/1	0.98	0.13	44,44,44,44	0
56	MG	DA	3012	1/1	0.98	0.21	42,42,42,42	0
56	MG	DA	3465	1/1	0.98	0.14	38,38,38,38	0
56	MG	DA	3474	1/1	0.98	0.21	35,35,35,35	0
56	MG	DA	3565	1/1	0.98	0.12	27,27,27,27	0
56	MG	BA	3514	1/1	0.98	0.19	9,9,9,9	0
56	MG	BA	3341	1/1	0.98	0.17	28,28,28,28	0
56	MG	BT	5001	1/1	0.98	0.14	56,56,56,56	0
56	MG	DA	3316	1/1	0.98	0.16	29,29,29,29	0
56	MG	BA	3407	1/1	0.98	0.17	13,13,13,13	0
56	MG	DA	3358	1/1	0.98	0.14	45,45,45,45	0
56	MG	DA	3485	1/1	0.98	0.13	31,31,31,31	0
56	MG	BS	3003	1/1	0.98	0.08	48,48,48,48	0
56	MG	BA	3848	1/1	0.98	0.23	45,45,45,45	0
56	MG	BA	3500	1/1	0.98	0.17	15,15,15,15	0
56	MG	DA	3434	1/1	0.98	0.18	47,47,47,47	0
56	MG	BA	3229	1/1	0.98	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3028	1/1	0.98	0.18	40,40,40,40	0
56	MG	DA	3398	1/1	0.98	0.21	42,42,42,42	0
56	MG	BE	308	1/1	0.98	0.19	25,25,25,25	0
56	MG	DB	3010	1/1	0.98	0.28	45,45,45,45	0
56	MG	BO	3005	1/1	0.98	0.17	61,61,61,61	0
56	MG	DY	502	1/1	0.98	0.18	44,44,44,44	0
56	MG	BA	3292	1/1	0.98	0.25	42,42,42,42	0
56	MG	CA	3110	1/1	0.98	0.10	51,51,51,51	0
56	MG	BA	3430	1/1	0.98	0.18	44,44,44,44	0
56	MG	BR	203	1/1	0.98	0.21	29,29,29,29	0
56	MG	BE	312	1/1	0.98	0.25	56,56,56,56	0
56	MG	CK	3001	1/1	0.98	0.12	46,46,46,46	0
56	MG	BD	309	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3250	1/1	0.98	0.19	38,38,38,38	0
56	MG	BA	3278	1/1	0.98	0.14	42,42,42,42	0
56	MG	BA	3712	1/1	0.98	0.28	32,32,32,32	0
56	MG	DA	3029	1/1	0.98	0.17	36,36,36,36	0
56	MG	DA	3038	1/1	0.98	0.18	34,34,34,34	0
56	MG	BA	3125	1/1	0.98	0.21	29,29,29,29	0
56	MG	DA	3042	1/1	0.98	0.19	27,27,27,27	0
56	MG	BA	3255	1/1	0.98	0.16	42,42,42,42	0
56	MG	BA	3749	1/1	0.98	0.23	24,24,24,24	0
56	MG	BA	3413	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3036	1/1	0.98	0.31	34,34,34,34	0
56	MG	BA	3388	1/1	0.98	0.13	44,44,44,44	0
56	MG	CA	3101	1/1	0.98	0.15	60,60,60,60	0
56	MG	BB	3010	1/1	0.98	0.17	38,38,38,38	0
56	MG	CA	3083	1/1	0.98	0.21	52,52,52,52	0
56	MG	DA	3283	1/1	0.98	0.04	44,44,44,44	0
56	MG	BA	3290	1/1	0.98	0.32	54,54,54,54	0
56	MG	BA	3201	1/1	0.98	0.25	17,17,17,17	0
56	MG	DA	3357	1/1	0.98	0.16	24,24,24,24	0
56	MG	BA	3644	1/1	0.98	0.20	18,18,18,18	0
56	MG	DA	3473	1/1	0.98	0.13	43,43,43,43	0
56	MG	BA	3641	1/1	0.98	0.19	22,22,22,22	0
56	MG	BA	3576	1/1	0.98	0.28	39,39,39,39	0
56	MG	BA	3682	1/1	0.98	0.18	39,39,39,39	0
56	MG	AK	3001	1/1	0.98	0.17	41,41,41,41	0
56	MG	BA	3889	1/1	0.98	0.11	29,29,29,29	0
56	MG	CA	3109	1/1	0.98	0.16	45,45,45,45	0
56	MG	DO	5001	1/1	0.98	0.18	51,51,51,51	0
56	MG	AA	3217	1/1	0.98	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3755	1/1	0.98	0.18	45,45,45,45	0
56	MG	BD	308	1/1	0.98	0.23	41,41,41,41	0
56	MG	BA	3354	1/1	0.98	0.22	53,53,53,53	0
56	MG	BA	3674	1/1	0.98	0.19	31,31,31,31	0
56	MG	CA	3150	1/1	0.98	0.23	58,58,58,58	0
56	MG	AA	3013	1/1	0.98	0.23	21,21,21,21	0
56	MG	DA	3558	1/1	0.98	0.19	47,47,47,47	0
56	MG	BA	3521	1/1	0.98	0.22	38,38,38,38	0
56	MG	CA	3055	1/1	0.98	0.14	57,57,57,57	0
56	MG	BE	305	1/1	0.98	0.16	21,21,21,21	0
56	MG	BA	3265	1/1	0.98	0.12	23,23,23,23	0
56	MG	BA	3227	1/1	0.98	0.18	33,33,33,33	0
56	MG	BA	3816	1/1	0.98	0.22	35,35,35,35	0
56	MG	BA	3685	1/1	0.98	0.17	29,29,29,29	0
56	MG	DA	3646	1/1	0.98	0.16	27,27,27,27	0
56	MG	BA	3178	1/1	0.98	0.18	29,29,29,29	0
56	MG	BA	3775	1/1	0.98	0.19	35,35,35,35	0
56	MG	DA	3494	1/1	0.98	0.10	39,39,39,39	0
56	MG	BD	313	1/1	0.98	0.20	39,39,39,39	0
56	MG	BF	310	1/1	0.98	0.32	37,37,37,37	0
56	MG	BA	3892	1/1	0.98	0.20	28,28,28,28	0
56	MG	BA	3138	1/1	0.98	0.24	40,40,40,40	0
56	MG	BA	3772	1/1	0.98	0.21	26,26,26,26	0
56	MG	BA	3860	1/1	0.98	0.22	37,37,37,37	0
56	MG	BA	3379	1/1	0.98	0.17	52,52,52,52	0
56	MG	BU	205	1/1	0.98	0.23	42,42,42,42	0
56	MG	DA	3021	1/1	0.98	0.21	29,29,29,29	0
56	MG	BA	3879	1/1	0.98	0.27	28,28,28,28	0
56	MG	BD	301	1/1	0.98	0.20	31,31,31,31	0
56	MG	BA	3697	1/1	0.98	0.09	35,35,35,35	0
56	MG	CA	3178	1/1	0.99	0.06	52,52,52,52	0
59	ZN	B5	103	1/1	0.99	0.18	40,40,40,40	0
56	MG	BD	307	1/1	0.99	0.22	30,30,30,30	0
56	MG	BA	3868	1/1	0.99	0.22	8,8,8,8	0
56	MG	BF	308	1/1	0.99	0.15	33,33,33,33	0
56	MG	AX	3010	1/1	0.99	0.10	53,53,53,53	0
56	MG	BA	3123	1/1	0.99	0.24	28,28,28,28	0
56	MG	BA	3024	1/1	0.99	0.18	40,40,40,40	0
56	MG	BA	3143	1/1	0.99	0.24	37,37,37,37	0
56	MG	BA	3504	1/1	0.99	0.19	31,31,31,31	0
56	MG	BA	3340	1/1	0.99	0.24	34,34,34,34	0
56	MG	DA	3287	1/1	0.99	0.22	33,33,33,33	0

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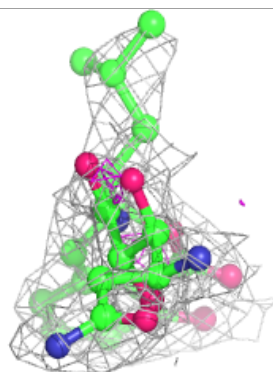
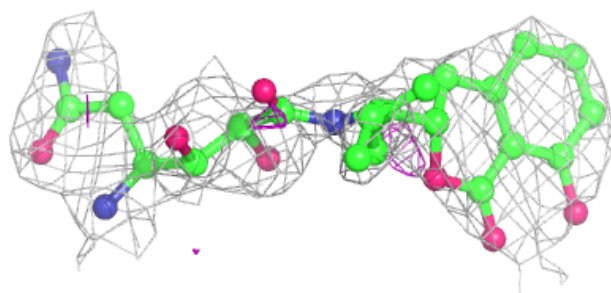
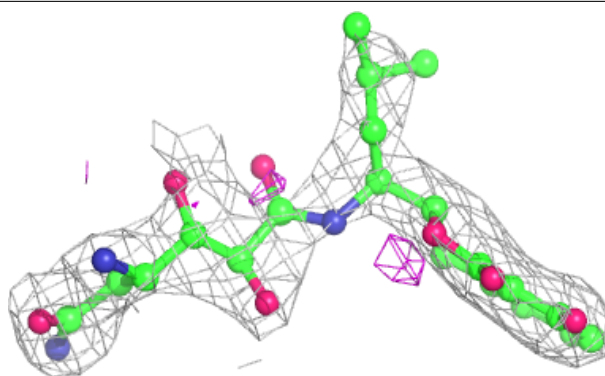
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3022	1/1	0.99	0.14	33,33,33,33	0
56	MG	BA	3164	1/1	0.99	0.29	33,33,33,33	0
56	MG	BA	3127	1/1	0.99	0.14	33,33,33,33	0
56	MG	BA	3483	1/1	0.99	0.13	30,30,30,30	0
56	MG	DA	3257	1/1	0.99	0.17	53,53,53,53	0
56	MG	BA	3496	1/1	0.99	0.25	22,22,22,22	0
59	ZN	AN	501	1/1	0.99	0.16	62,62,62,62	0
56	MG	DA	3172	1/1	0.99	0.25	38,38,38,38	0
56	MG	BA	3235	1/1	0.99	0.23	17,17,17,17	0
56	MG	BA	3835	1/1	0.99	0.19	34,34,34,34	0
56	MG	BA	3531	1/1	0.99	0.21	46,46,46,46	0
56	MG	BV	202	1/1	0.99	0.23	23,23,23,23	0
56	MG	BA	3563	1/1	0.99	0.17	43,43,43,43	0
56	MG	BP	202	1/1	0.99	0.16	27,27,27,27	0
56	MG	BA	3790	1/1	0.99	0.15	21,21,21,21	0
56	MG	BA	3369	1/1	0.99	0.23	12,12,12,12	0
56	MG	BA	3180	1/1	0.99	0.22	31,31,31,31	0
59	ZN	D5	103	1/1	0.99	0.19	51,51,51,51	0
56	MG	BA	3771	1/1	0.99	0.22	29,29,29,29	0
56	MG	BY	504	1/1	0.99	0.24	39,39,39,39	0
56	MG	CE	3001	1/1	0.99	0.06	67,67,67,67	0
56	MG	BA	3150	1/1	0.99	0.17	42,42,42,42	0
56	MG	DA	3656	1/1	0.99	0.14	56,56,56,56	0
56	MG	BU	210	1/1	0.99	0.22	28,28,28,28	0
56	MG	BA	3225	1/1	0.99	0.23	32,32,32,32	0
56	MG	BA	3078	1/1	0.99	0.21	11,11,11,11	0
56	MG	DA	3522	1/1	0.99	0.18	35,35,35,35	0
56	MG	BV	205	1/1	0.99	0.17	46,46,46,46	0
56	MG	BA	3394	1/1	0.99	0.20	20,20,20,20	0
56	MG	BA	3030	1/1	0.99	0.18	28,28,28,28	0
56	MG	BA	3410	1/1	0.99	0.23	19,19,19,19	0
56	MG	BA	3888	1/1	0.99	0.13	26,26,26,26	0
56	MG	BA	3025	1/1	0.99	0.20	23,23,23,23	0
59	ZN	B9	501	1/1	1.00	0.20	38,38,38,38	0
59	ZN	B6	102	1/1	1.00	0.23	39,39,39,39	0

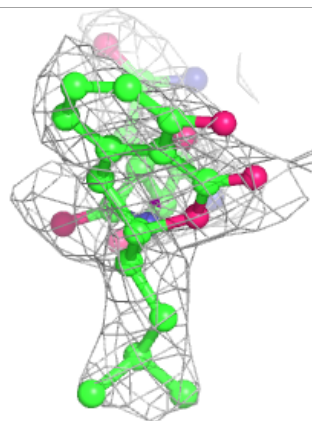
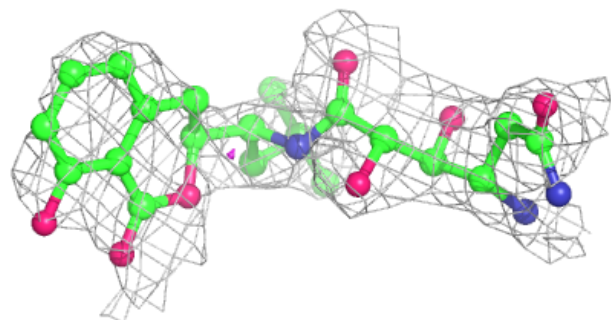
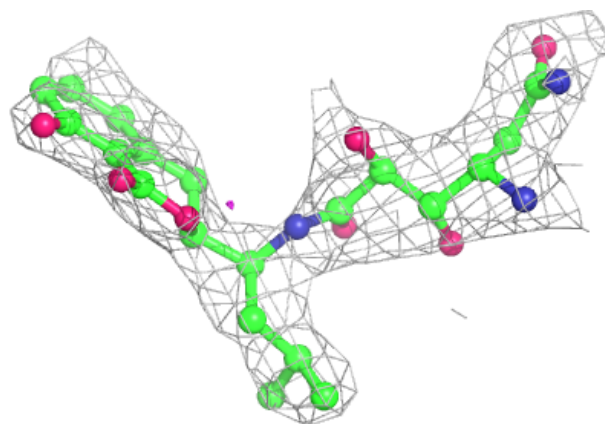
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UAM CA 3202:

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

**Electron density around UAM AA 3232:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.