



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:42 AM UTC

PDB ID : 1VY7 / pdb_00001vy7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

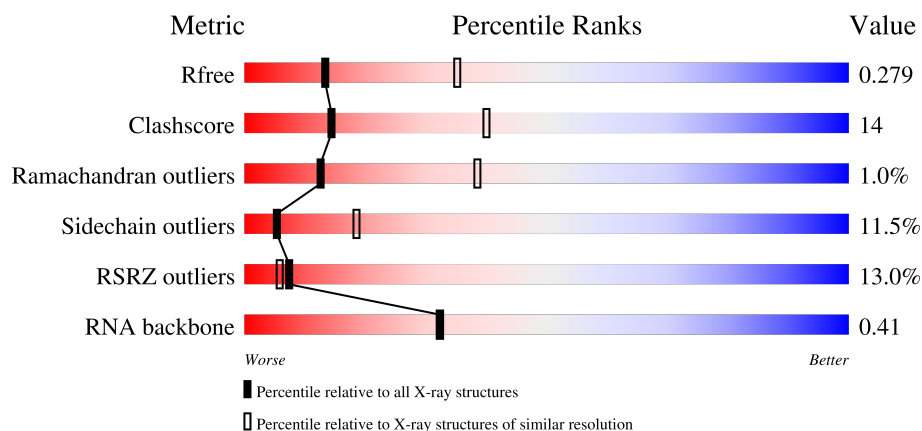
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	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	3	
23	CW	3	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	

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

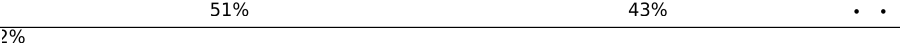
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Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	3145	-	-	-	X
57	MG	CA	3062	-	-	-	X
57	MG	DR	3001	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	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 type Z.

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	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
23	CW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1633	730	296	529	76	2			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			
25	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	207	Total	Mg	0	0
			207	207		
57	AD	2	Total	Mg	0	0
			2	2		
57	AE	2	Total	Mg	0	0
			2	2		
57	AF	1	Total	Mg	0	0
			1	1		
57	AJ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AK	1	Total 1	Mg 1	0	0
57	AM	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	AS	1	Total 1	Mg 1	0	0
57	AV	1	Total 1	Mg 1	0	0
57	AW	1	Total 1	Mg 1	0	0
57	AX	11	Total 11	Mg 11	0	0
57	BA	720	Total 720	Mg 720	0	0
57	BB	20	Total 20	Mg 20	0	0
57	BD	11	Total 11	Mg 11	0	0
57	BE	7	Total 7	Mg 7	0	0
57	BF	10	Total 10	Mg 10	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BN	6	Total 6	Mg 6	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BP	4	Total 4	Mg 4	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	BR	3	Total 3	Mg 3	0	0
57	BU	8	Total 8	Mg 8	0	0
57	BV	4	Total 4	Mg 4	0	0
57	BW	5	Total 5	Mg 5	0	0

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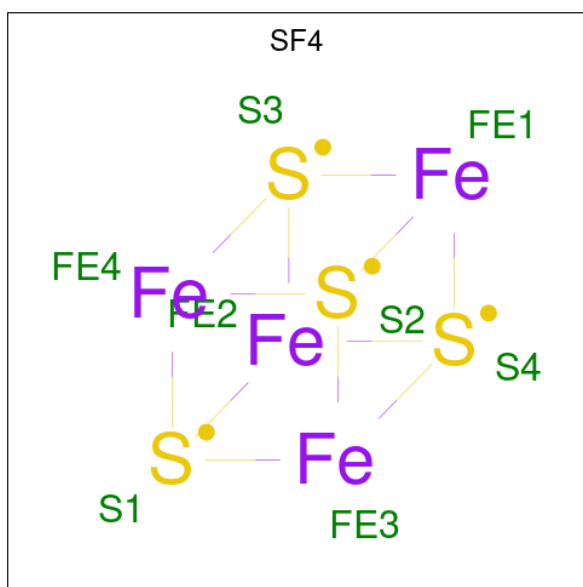
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BX	1	Total 1	Mg 1	0	0
57	BY	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	B0	4	Total 4	Mg 4	0	0
57	B1	1	Total 1	Mg 1	0	0
57	B2	1	Total 1	Mg 1	0	0
57	B3	2	Total 2	Mg 2	0	0
57	B5	2	Total 2	Mg 2	0	0
57	B7	3	Total 3	Mg 3	0	0
57	B8	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	CA	160	Total 160	Mg 160	0	0
57	CE	1	Total 1	Mg 1	0	0
57	CF	1	Total 1	Mg 1	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	CK	1	Total 1	Mg 1	0	0
57	CT	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DA	629	Total 629	Mg 629	0	0
57	DB	10	Total 10	Mg 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	7	Total 7	Mg 7	0	0
57	DE	4	Total 4	Mg 4	0	0
57	DF	4	Total 4	Mg 4	0	0
57	DG	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DO	1	Total 1	Mg 1	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DQ	3	Total 3	Mg 3	0	0
57	DR	2	Total 2	Mg 2	0	0
57	DU	4	Total 4	Mg 4	0	0
57	DV	2	Total 2	Mg 2	0	0
57	DW	2	Total 2	Mg 2	0	0
57	DY	1	Total 1	Mg 1	0	0
57	D3	1	Total 1	Mg 1	0	0
57	D5	1	Total 1	Mg 1	0	0
57	D8	2	Total 2	Mg 2	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	170	Total 170	O 170	0	0
61	AL	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	3	Total 3	O 3	0	0
61	BA	1102	Total 1102	O 1102	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	8	Total 8	O 8	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	4	Total 4	O 4	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BS	1	Total 1	O 1	0	0
61	BT	3	Total 3	O 3	0	0
61	BU	1	Total 1	O 1	0	0
61	BV	4	Total 4	O 4	0	0
61	BW	2	Total 2	O 2	0	0
61	BX	2	Total 2	O 2	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	5	Total 5	O 5	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	130	Total 130	O 130	0	0
61	CE	1	Total 1	O 1	0	0
61	CJ	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0

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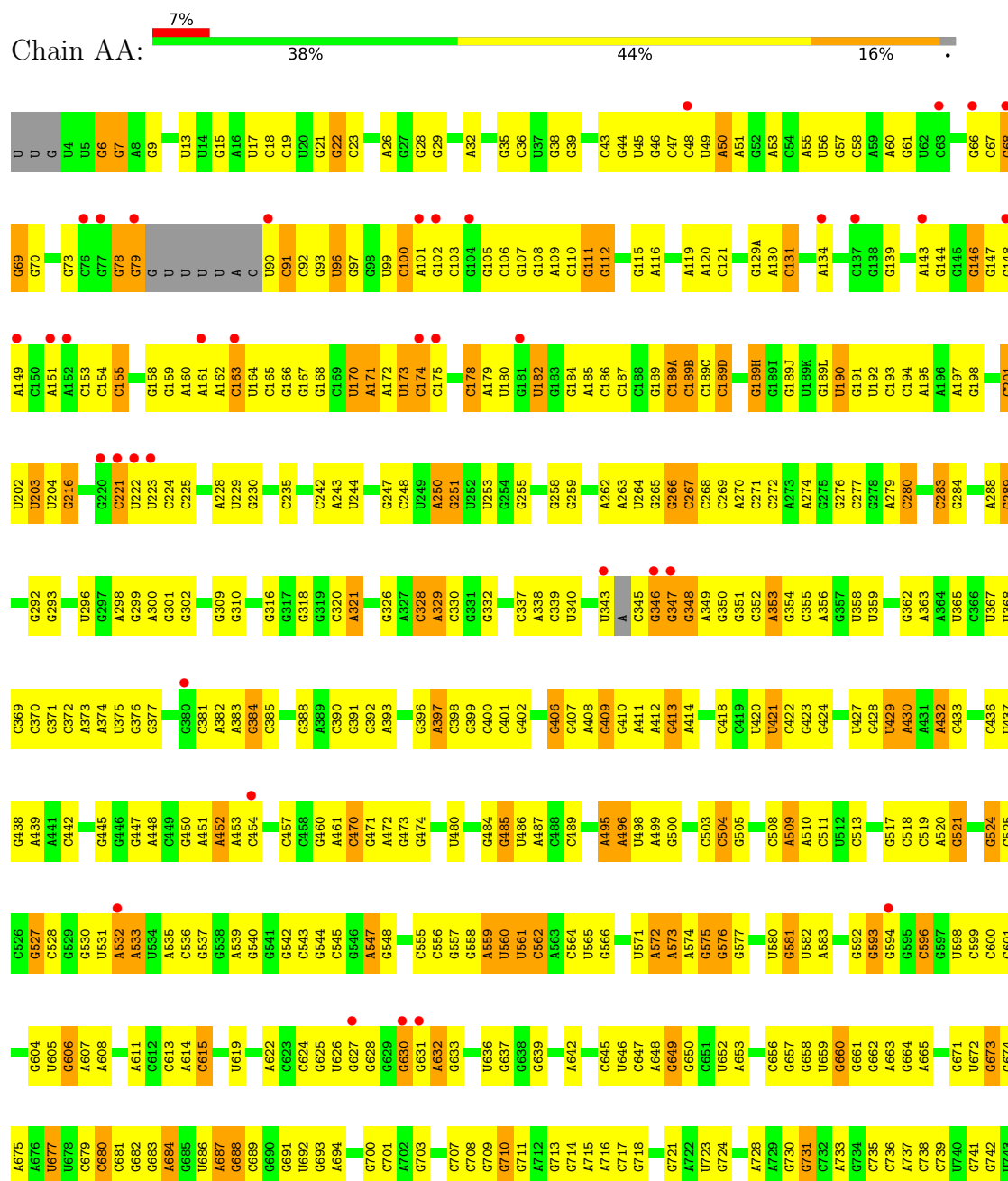
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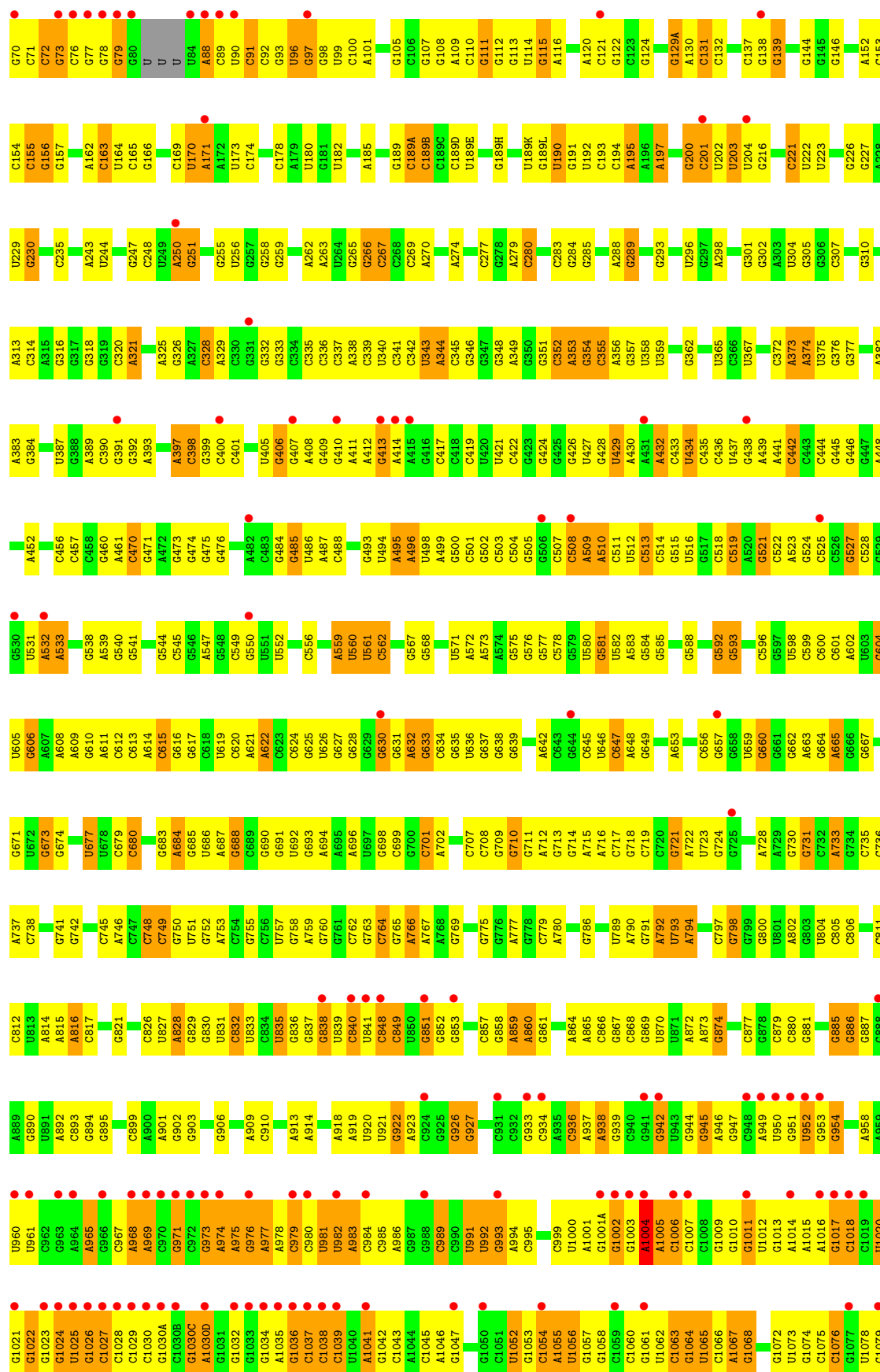
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	1	Total	O	0	0
			1	1		
61	CX	1	Total	O	0	0
			1	1		
61	DA	767	Total	O	0	0
			767	767		
61	DB	9	Total	O	0	0
			9	9		
61	DD	9	Total	O	0	0
			9	9		
61	DE	5	Total	O	0	0
			5	5		
61	DF	6	Total	O	0	0
			6	6		
61	DN	2	Total	O	0	0
			2	2		
61	DP	12	Total	O	0	0
			12	12		
61	DR	2	Total	O	0	0
			2	2		
61	DT	1	Total	O	0	0
			1	1		
61	DU	2	Total	O	0	0
			2	2		
61	DV	1	Total	O	0	0
			1	1		
61	DX	2	Total	O	0	0
			2	2		
61	DY	1	Total	O	0	0
			1	1		
61	D0	5	Total	O	0	0
			5	5		
61	D1	1	Total	O	0	0
			1	1		
61	D3	2	Total	O	0	0
			2	2		
61	D7	1	Total	O	0	0
			1	1		
61	D8	4	Total	O	0	0
			4	4		

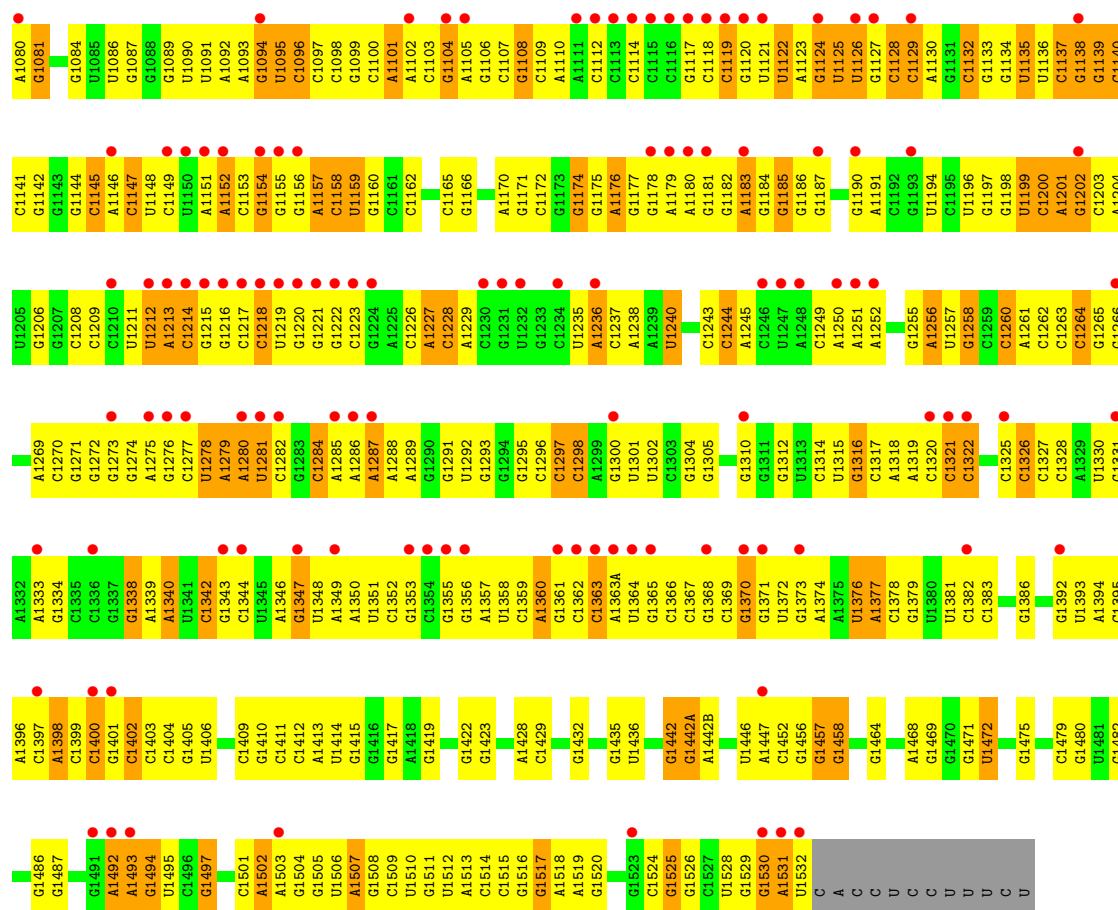
3 Residue-property plots

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

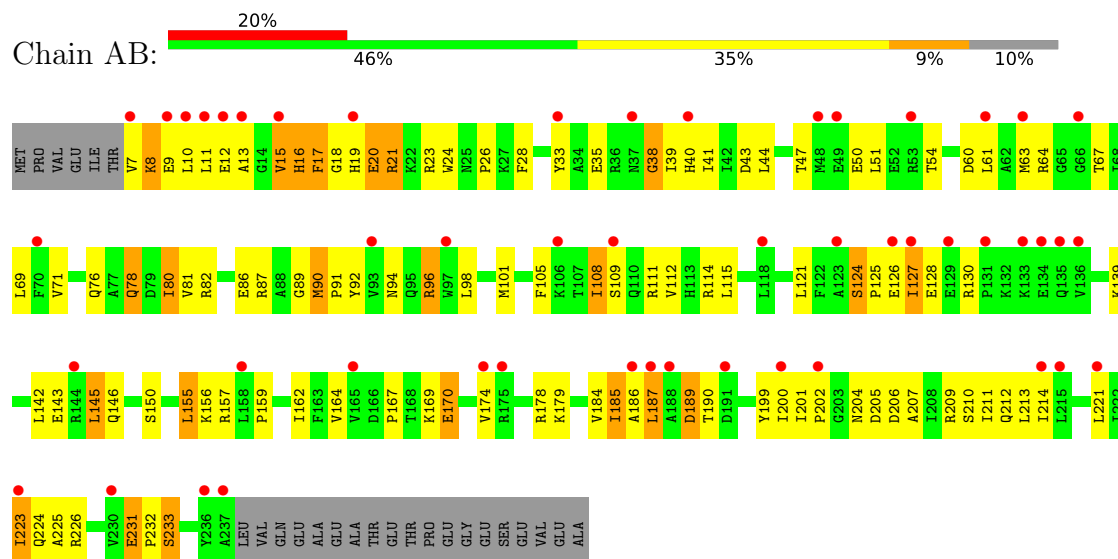
• Molecule 1: 16S Ribosomal RNA



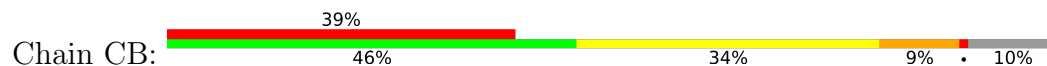


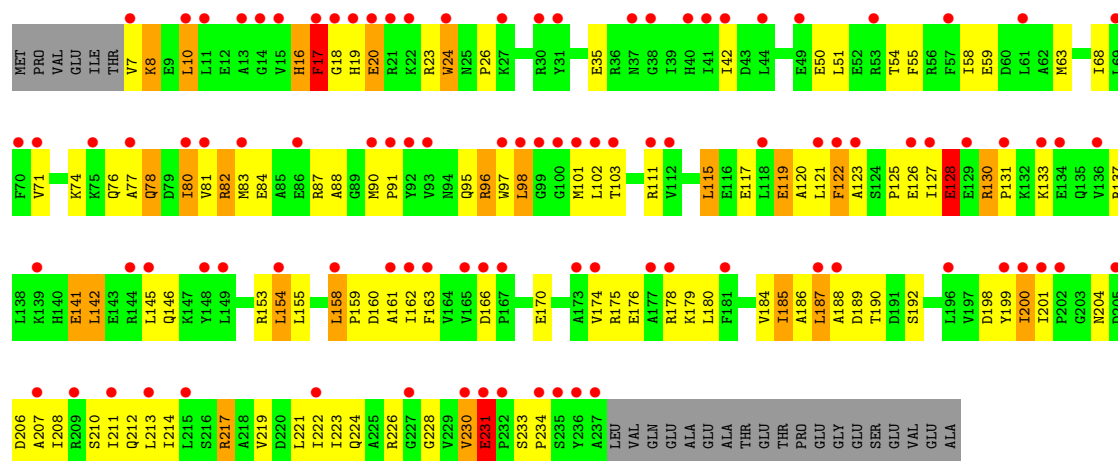


• Molecule 2: 30S ribosomal protein S2

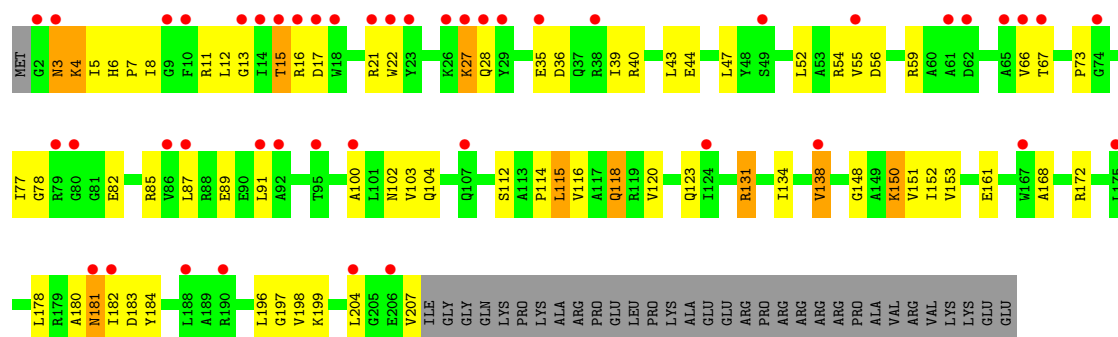


• Molecule 2: 30S ribosomal protein S2

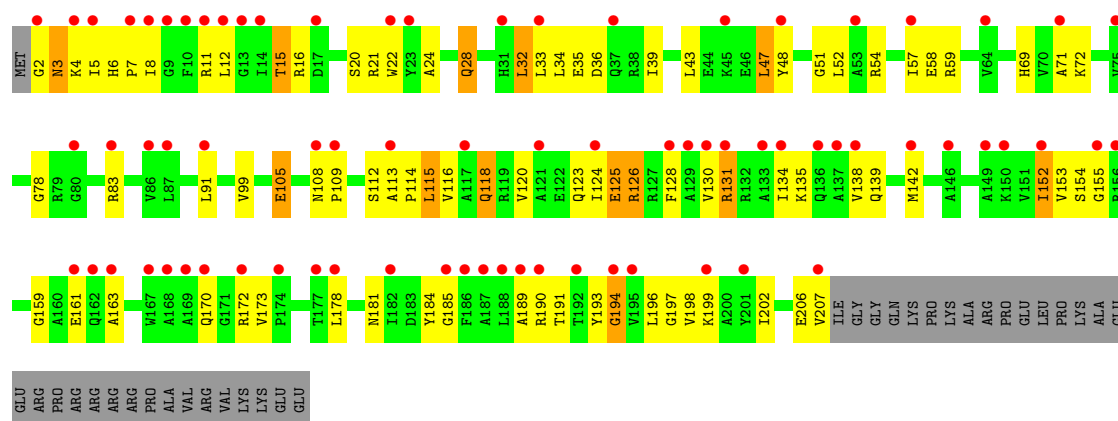




• Molecule 3: 30S ribosomal protein S3

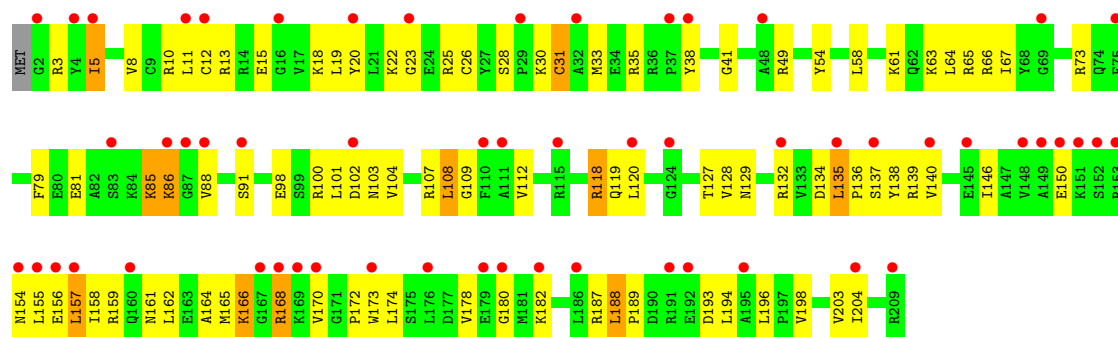


• Molecule 3: 30S ribosomal protein S3

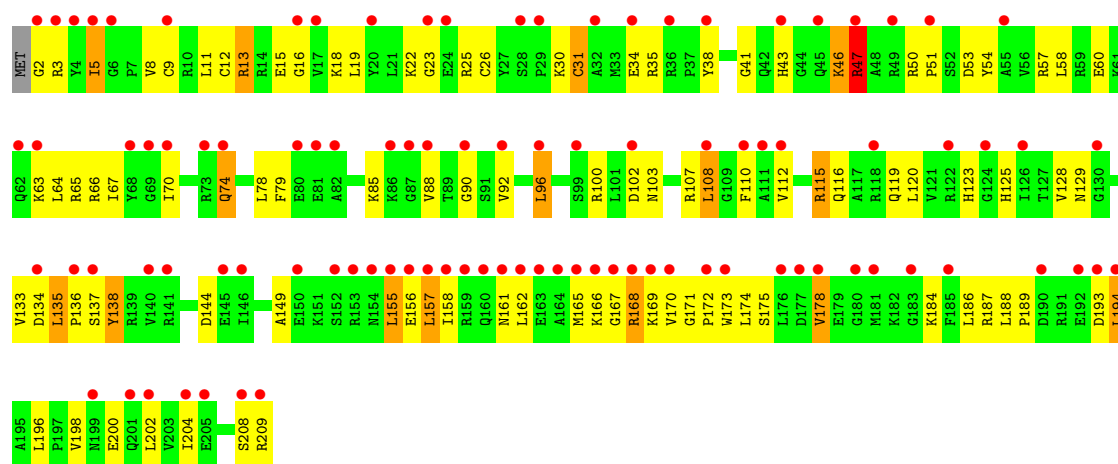


• Molecule 4: 30S ribosomal protein S4

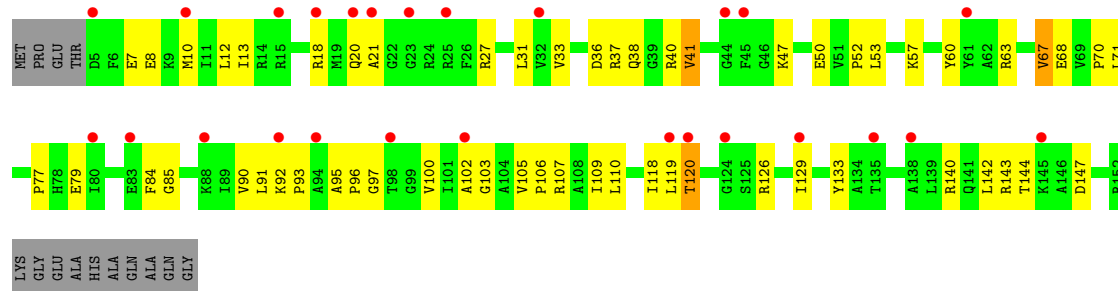




• Molecule 4: 30S ribosomal protein S4

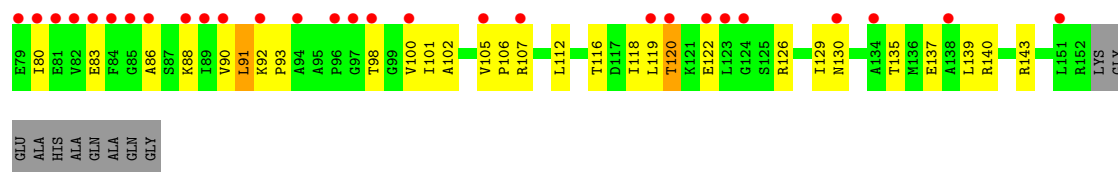


• Molecule 5: 30S ribosomal protein S5

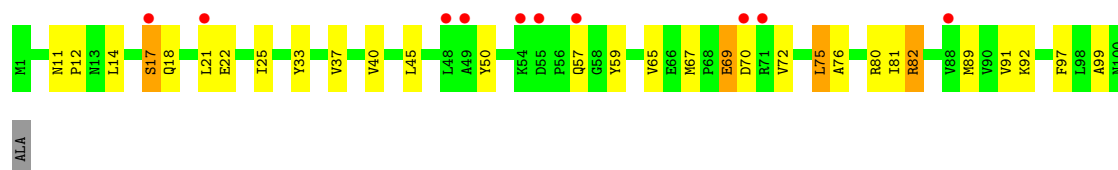


• Molecule 5: 30S ribosomal protein S5

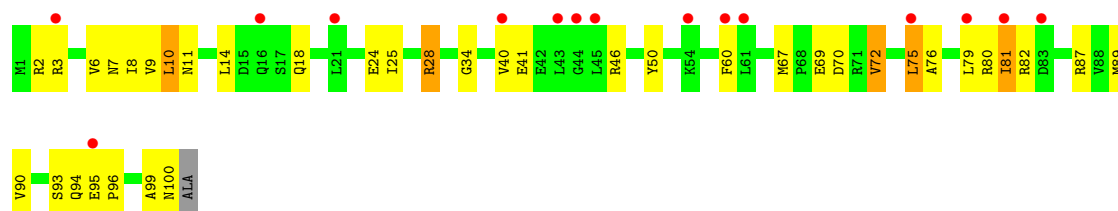




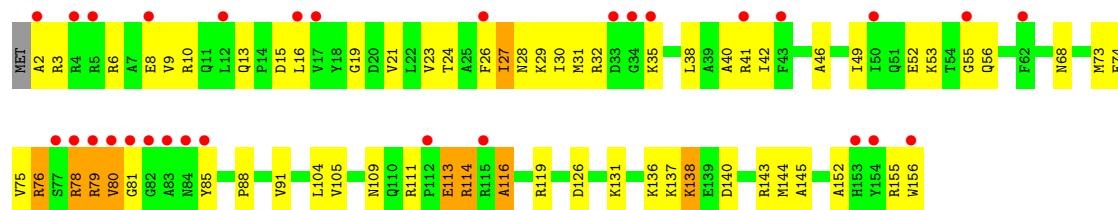
• Molecule 6: 30S ribosomal protein S6



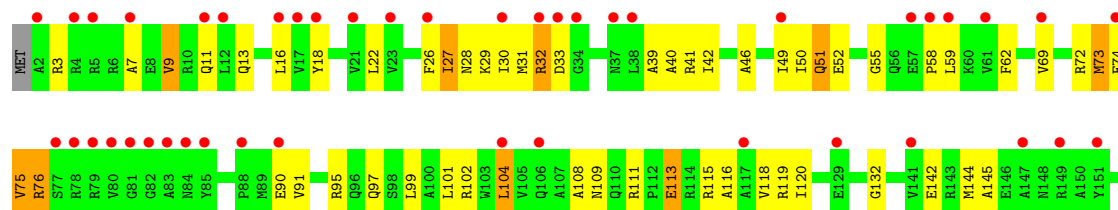
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

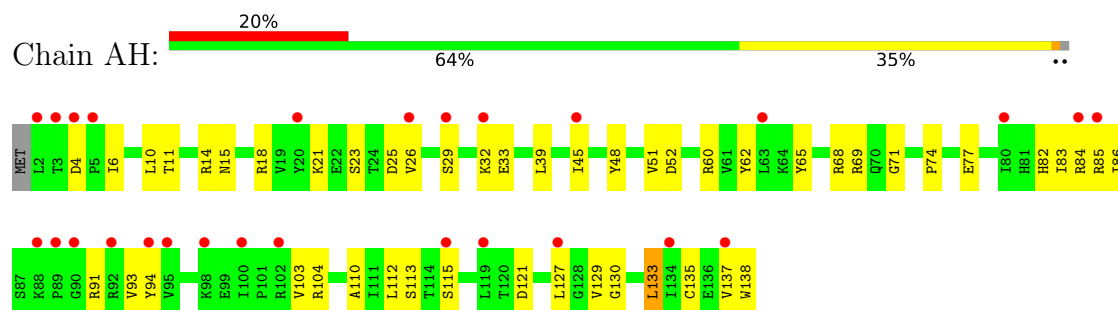


• Molecule 7: 30S ribosomal protein S7

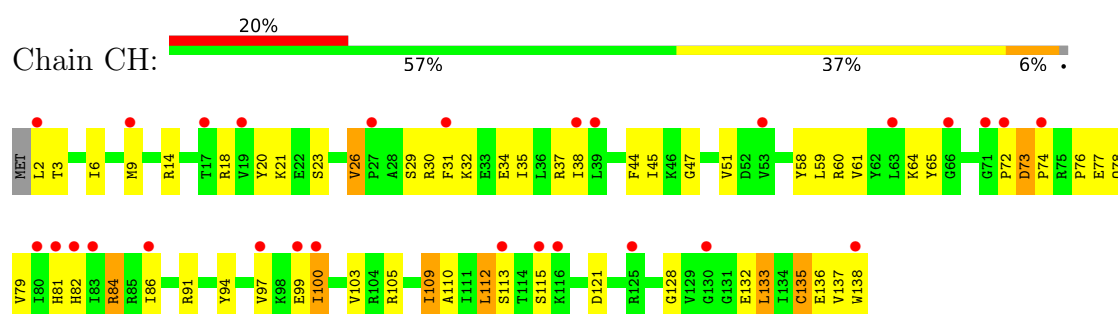


R155
W156

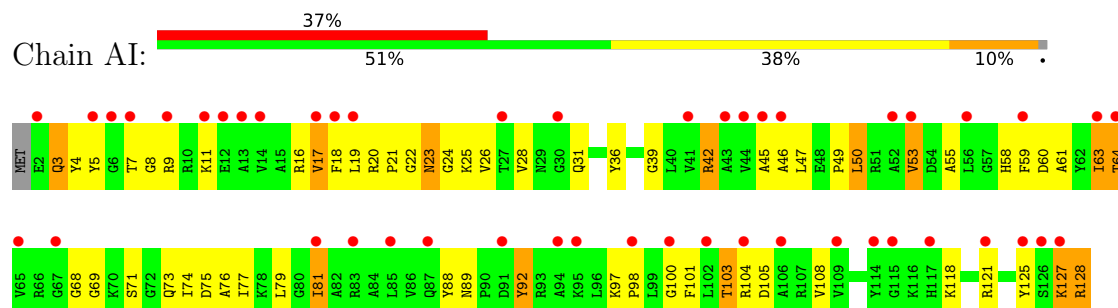
• Molecule 8: 30S ribosomal protein S8



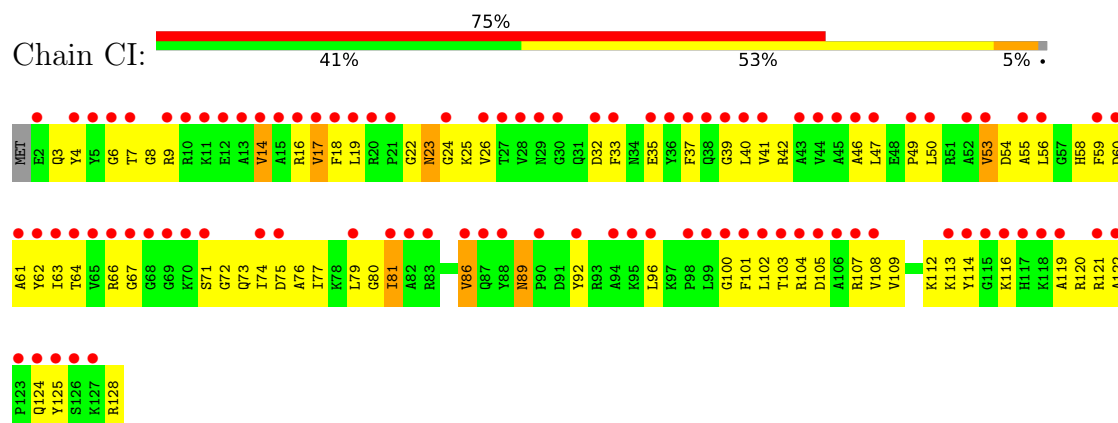
• Molecule 8: 30S ribosomal protein S8



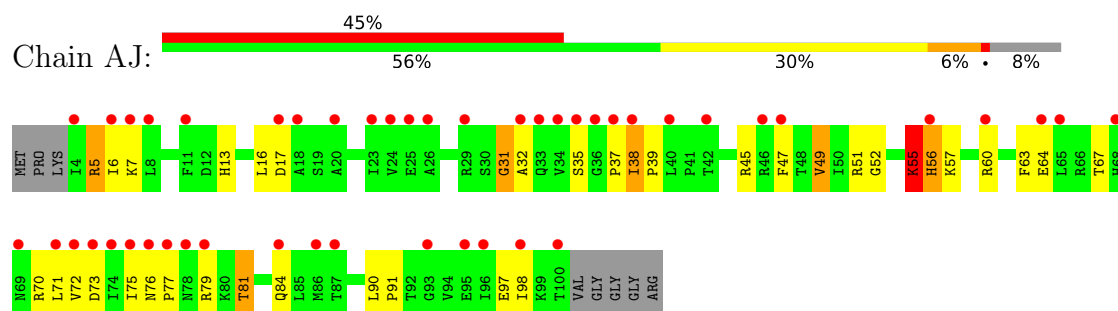
• Molecule 9: 30S ribosomal protein S9



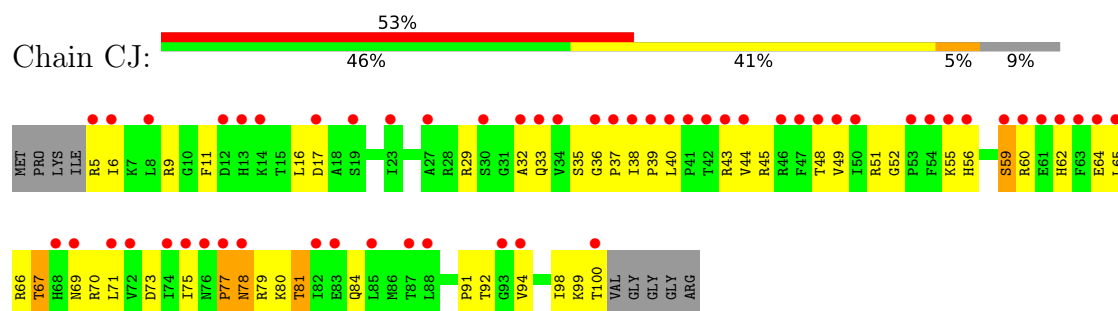
• Molecule 9: 30S ribosomal protein S9



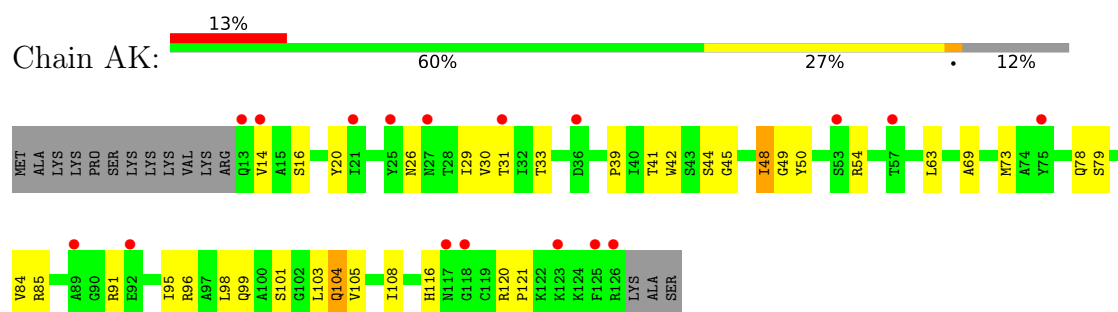
- Molecule 10: 30S ribosomal protein S10



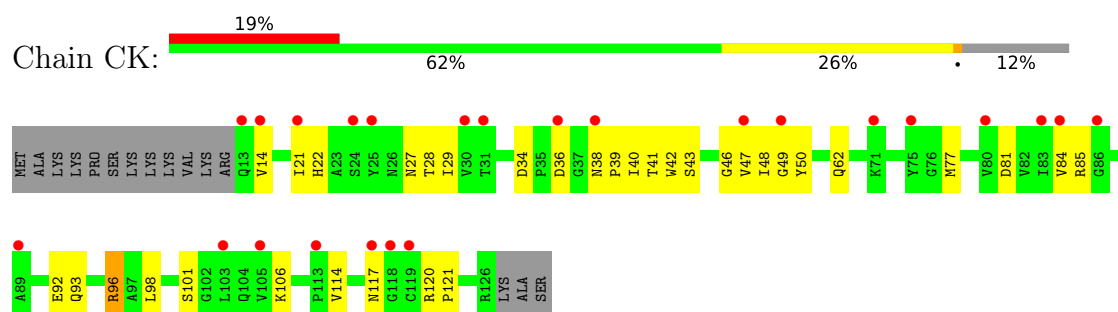
- Molecule 10: 30S ribosomal protein S10



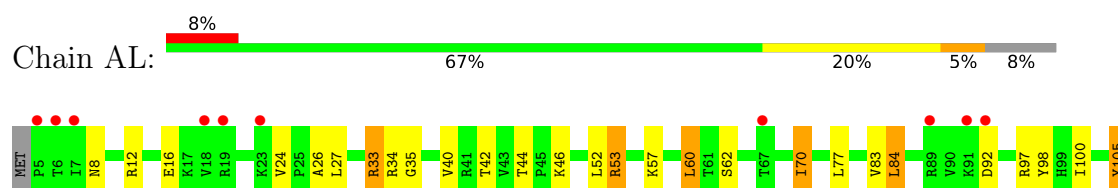
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

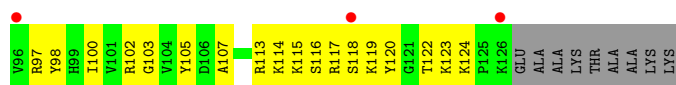
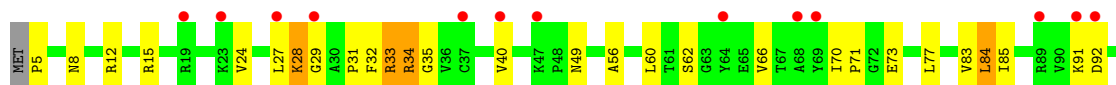


- Molecule 12: 30S ribosomal protein S12

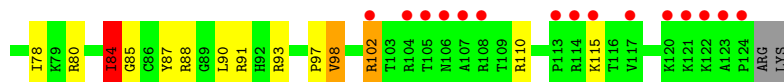
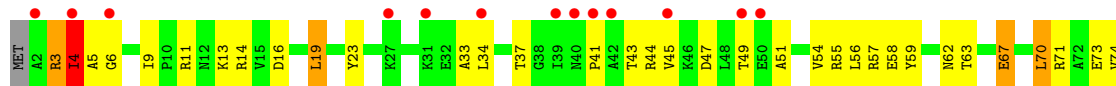




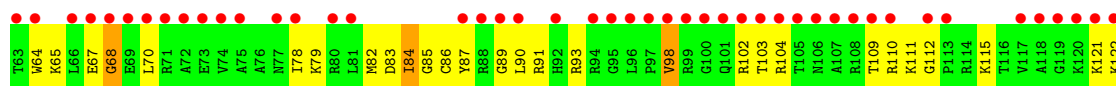
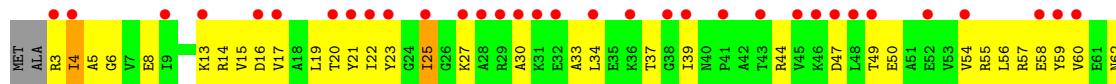
- Molecule 12: 30S ribosomal protein S12



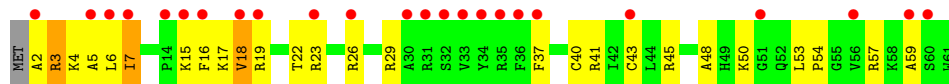
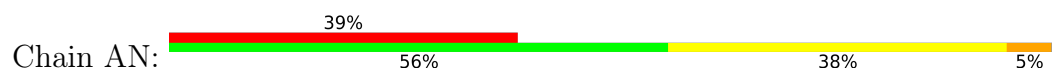
- Molecule 13: 30S ribosomal protein S13



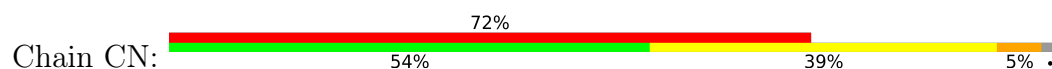
- Molecule 13: 30S ribosomal protein S13

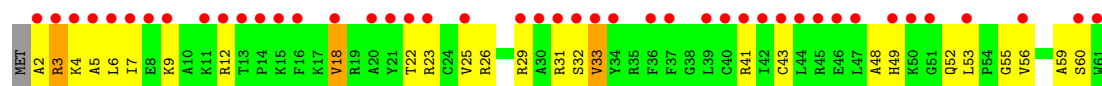


- Molecule 14: 30S ribosomal protein S14 type Z

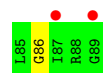
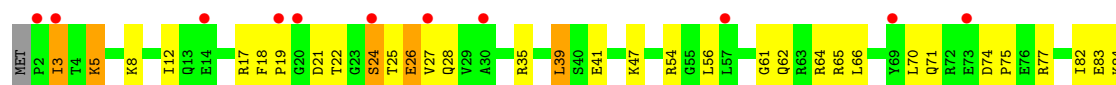


- Molecule 14: 30S ribosomal protein S14 type Z

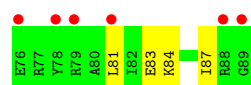




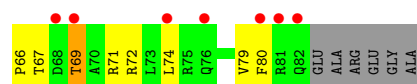
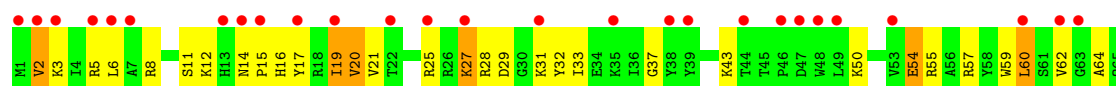
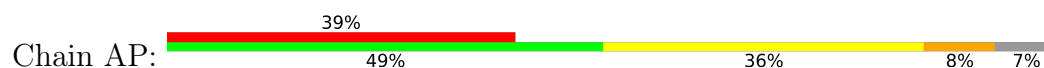
- Molecule 15: 30S ribosomal protein S15



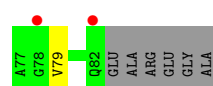
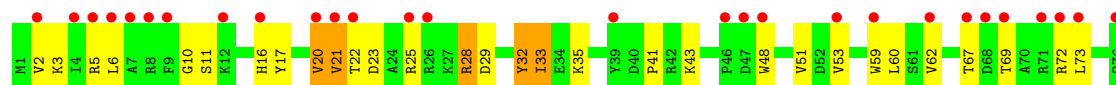
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

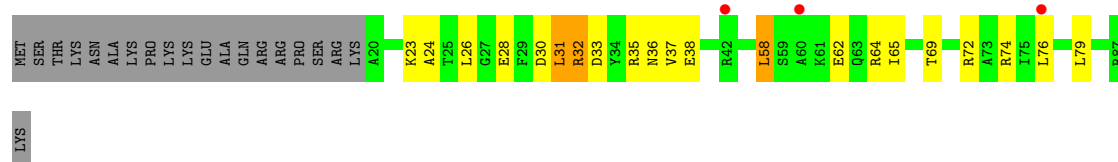




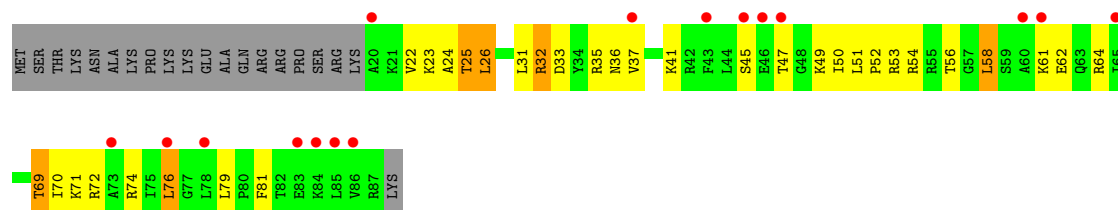
- Molecule 17: 30S ribosomal protein S17



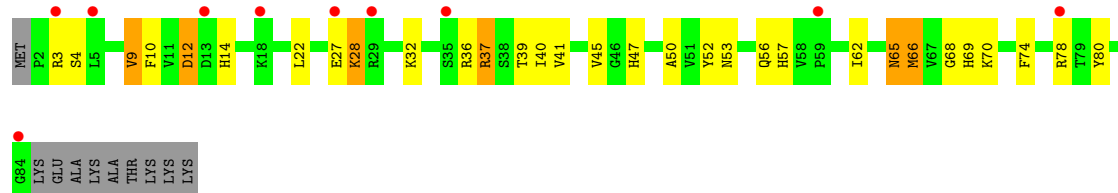
- Molecule 18: 30S ribosomal protein S18



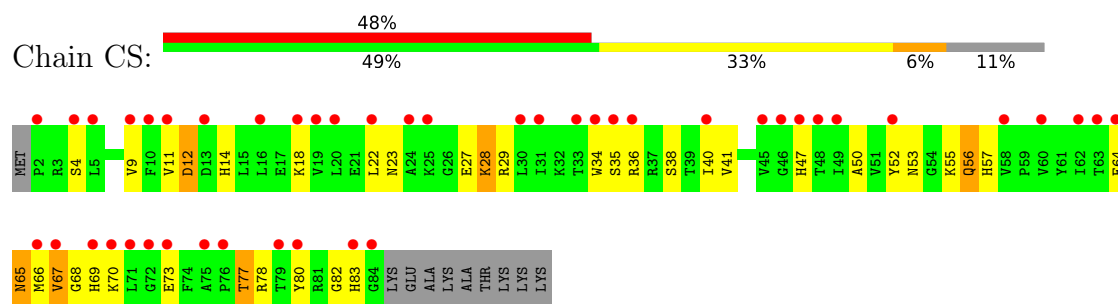
- Molecule 18: 30S ribosomal protein S18



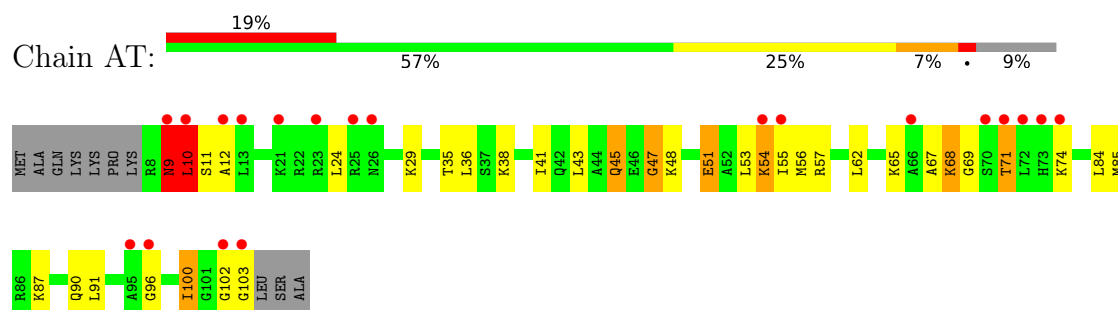
- Molecule 19: 30S ribosomal protein S19



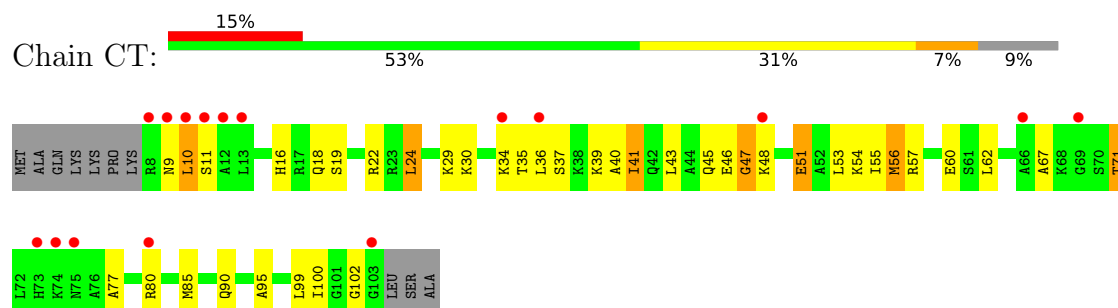
- Molecule 19: 30S ribosomal protein S19



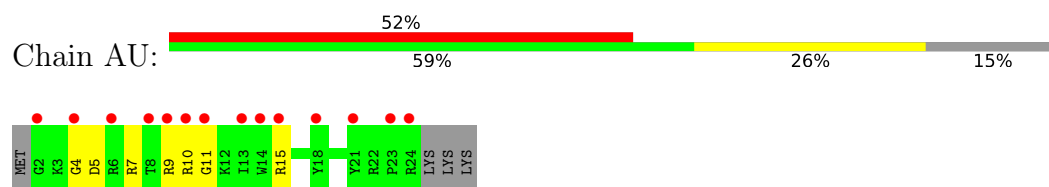
- Molecule 20: 30S ribosomal protein S20



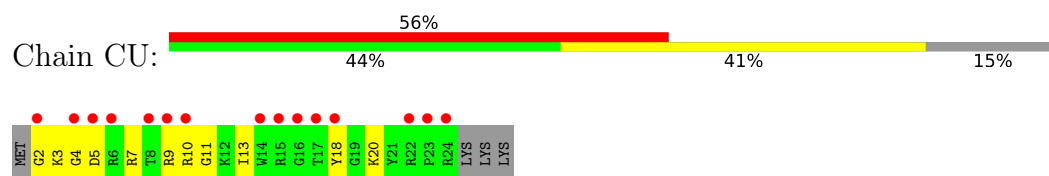
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx

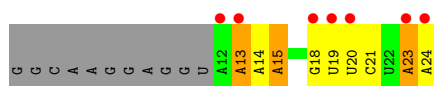


- Molecule 21: 30S ribosomal protein Thx

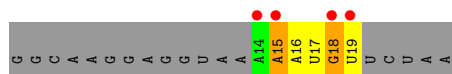


- Molecule 22: mRNA





● Molecule 22: mRNA



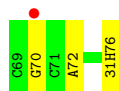
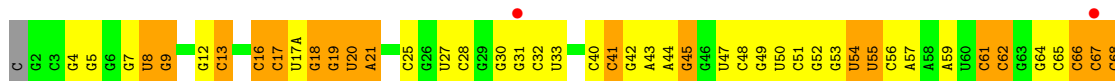
● Molecule 23: Cytidine-Puromycin



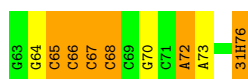
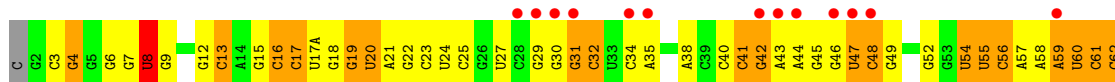
● Molecule 23: Cytidine-Puromycin



● Molecule 24: P-site tRNA



● Molecule 24: P-site tRNA



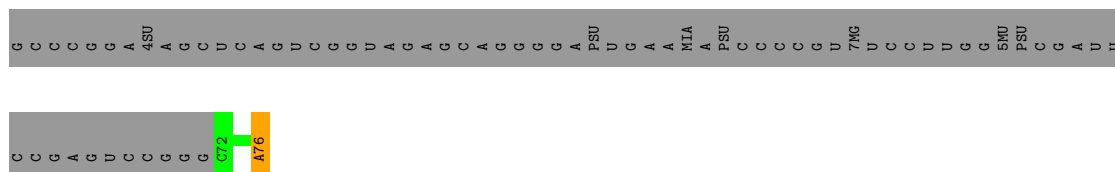
● Molecule 25: E-site tRNA





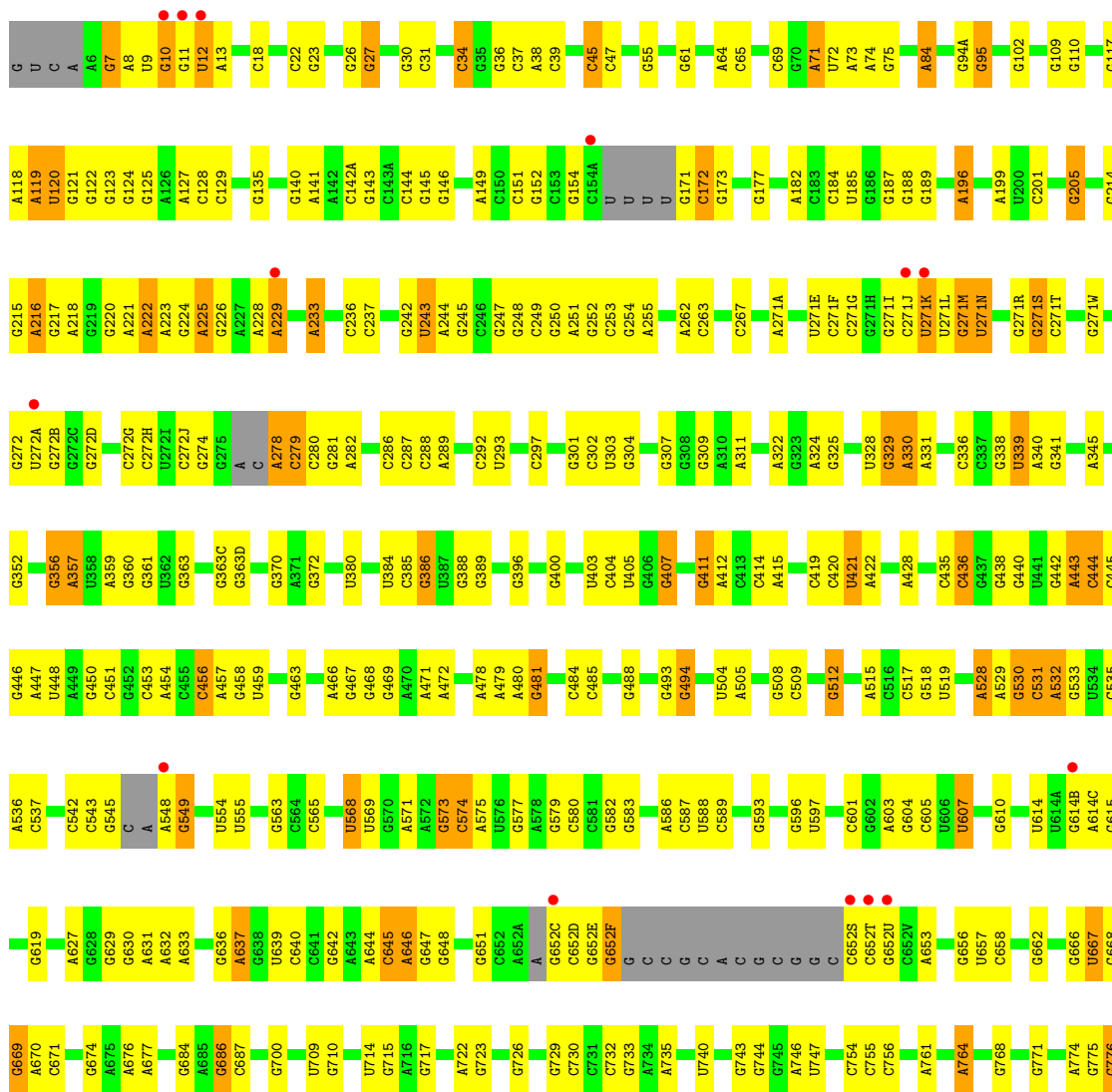
• Molecule 25: E-site tRNA

Chain CY: 5% 93%



• Molecule 26: 23S Ribosomal RNA

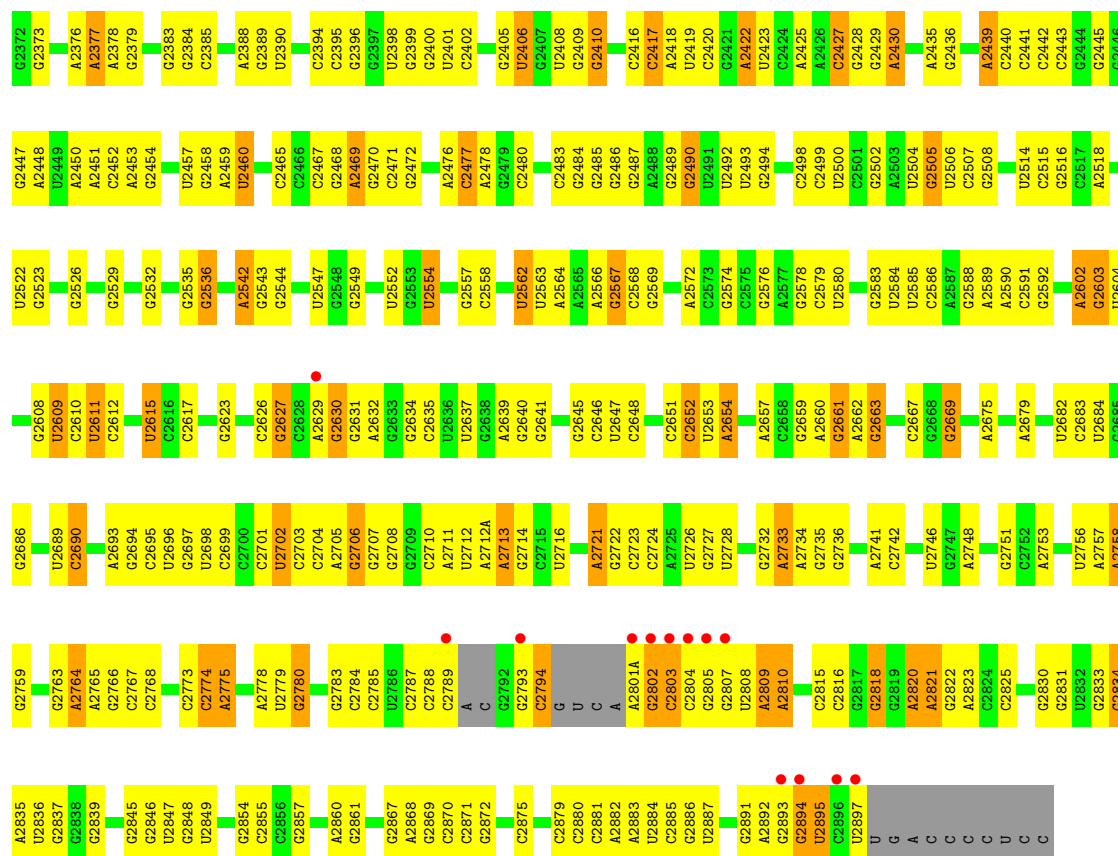
Chain BA: 4% 50% 37% 9%

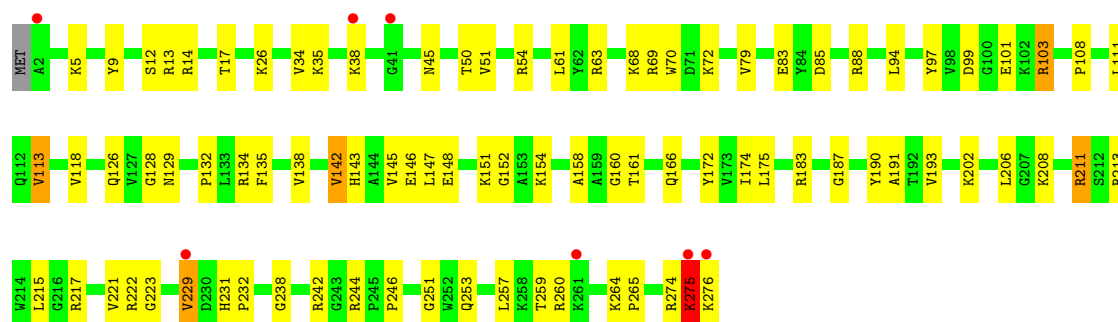


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G1973		A1784	A1676	A1568	G1491	A1309	G1120		A	C970	G791	G791
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G1992	G1907	A1791	A1691	A1583		A1318	G1219		A		G799	G799
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G2010	C1924	U1805	U1709	U1602		U1343	A1142		A		U905	
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G2012	A1927	A1812	C1711	A1608		U1345	A1144		U		U907	
A2013	A1928	G1813	G1713	A1609		G1346	C1145		U		A910	
A2014	G1929	A1814	G1714	A1610		U1347	A1148		A		A911	
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G1933	C1934	U1820	A1722	A1632		G1355	A1253		A		A1020	
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C1941	C1941	G1833	G1748	A1644		U1369	U1167		U		A941	
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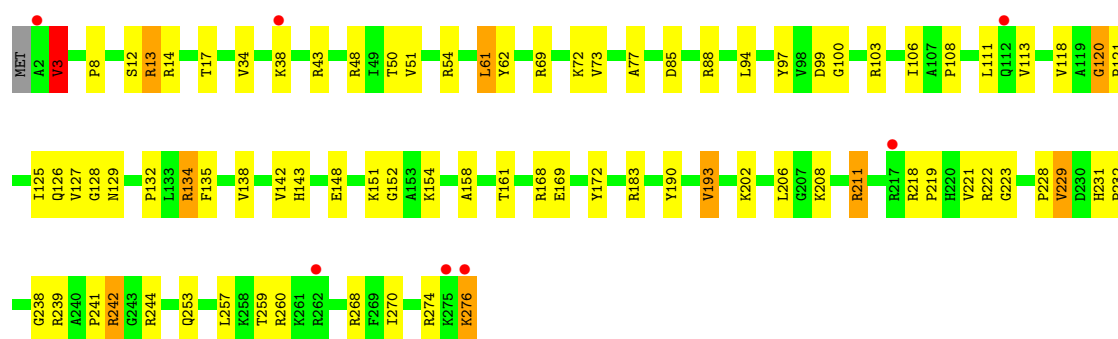
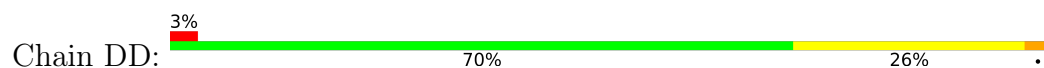


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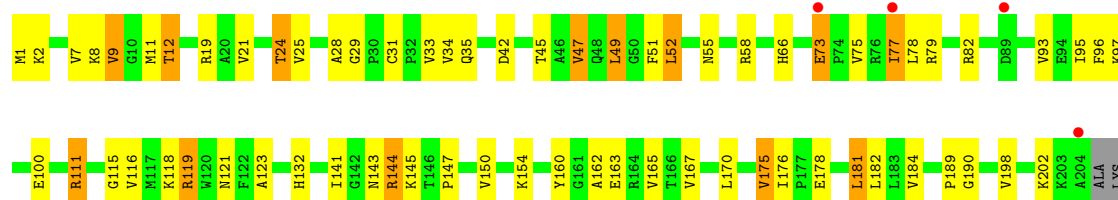




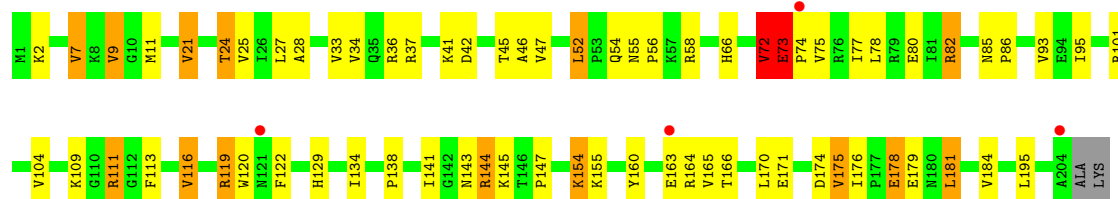
• Molecule 28: 50S ribosomal protein L2



• Molecule 29: 50S ribosomal protein L3

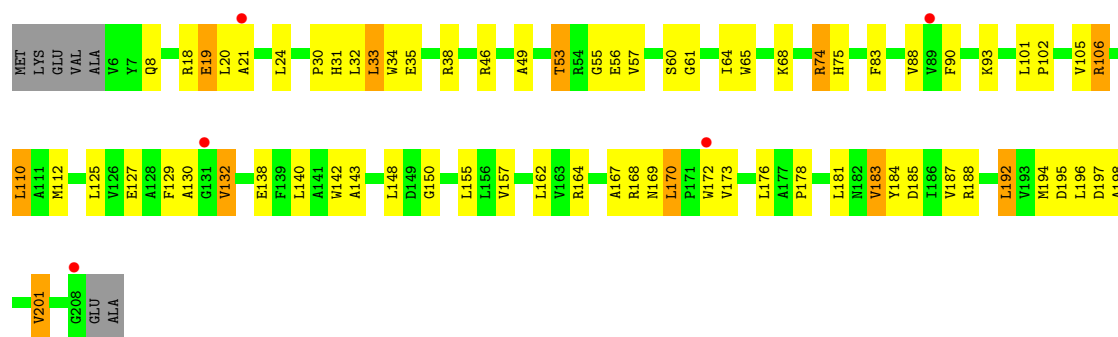


• Molecule 29: 50S ribosomal protein L3

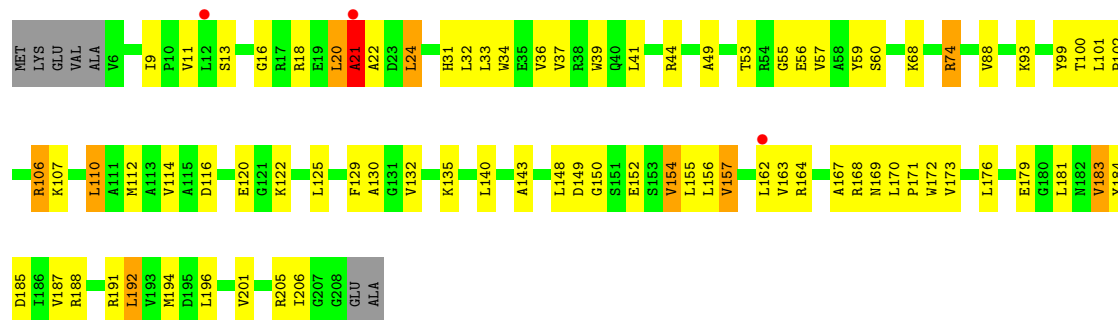


• Molecule 30: 50S ribosomal protein L4

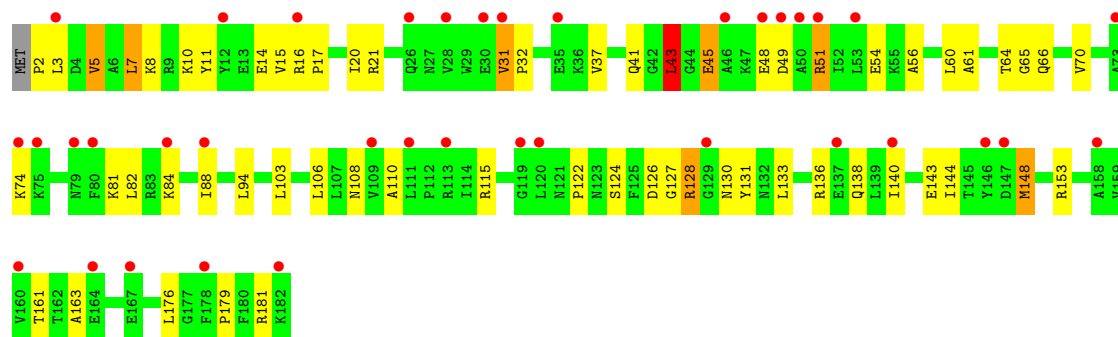




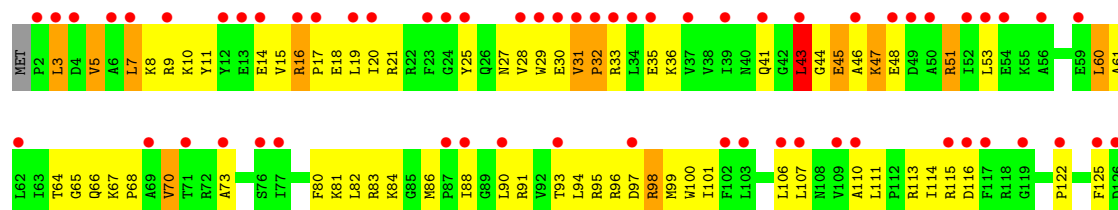
• Molecule 30: 50S ribosomal protein L4

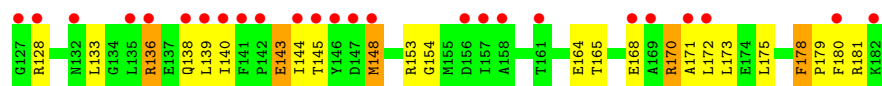


• Molecule 31: 50S ribosomal protein L5

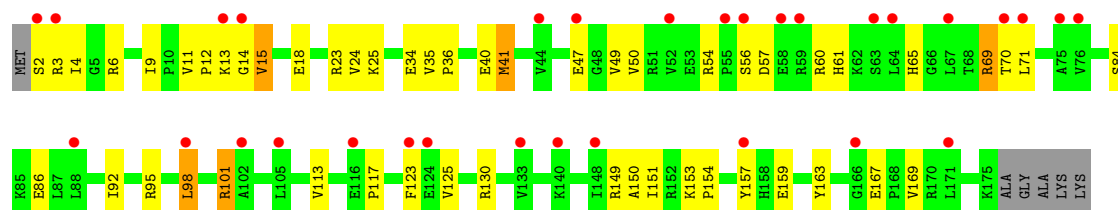


• Molecule 31: 50S ribosomal protein L5

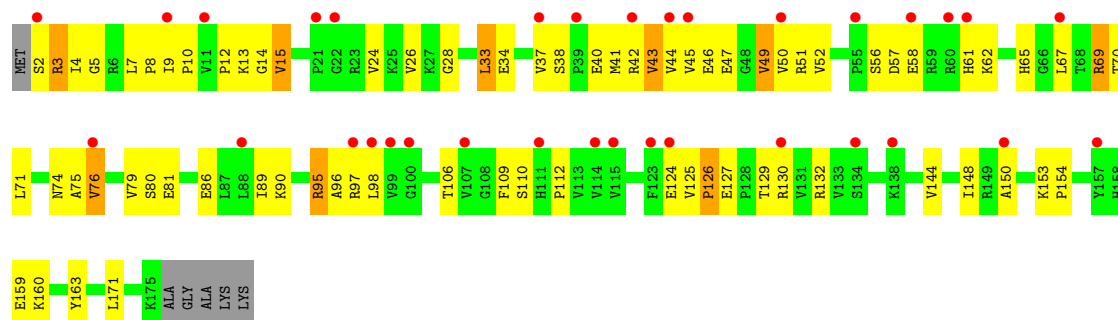




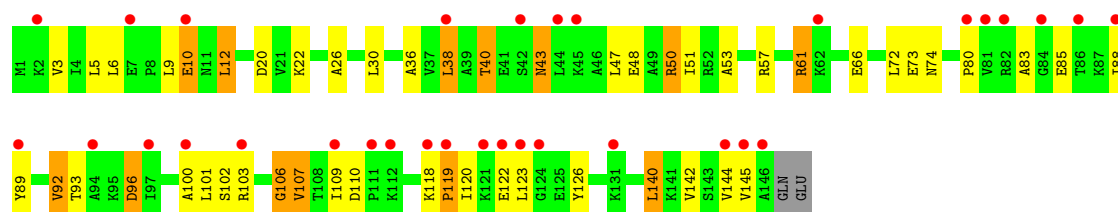
- Molecule 32: 50S ribosomal protein L6



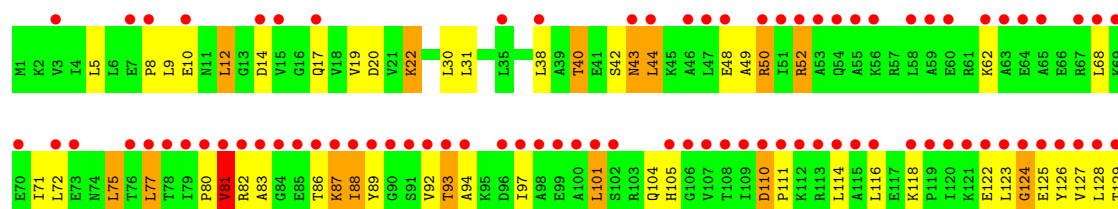
- Molecule 32: 50S ribosomal protein L6

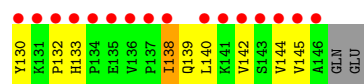


- Molecule 33: 50S ribosomal protein L9

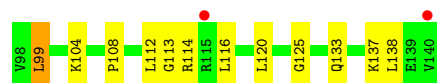
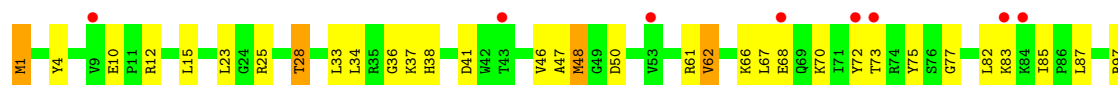


- Molecule 33: 50S ribosomal protein L9

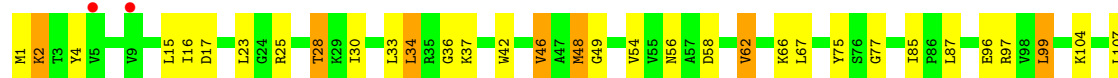
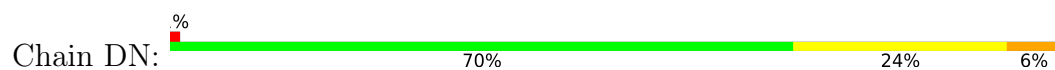




• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14

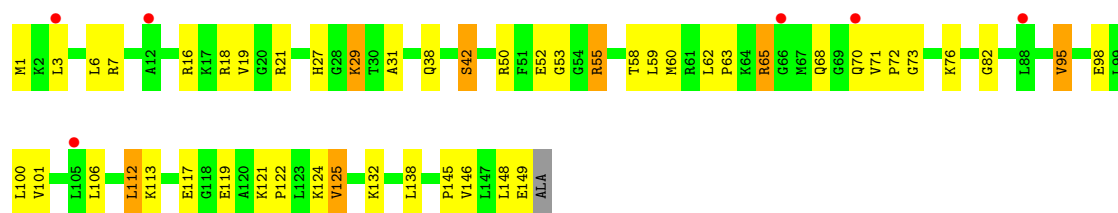


• Molecule 35: 50S ribosomal protein L14

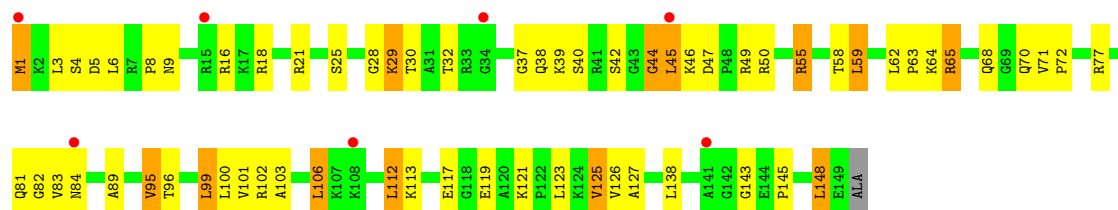


• Molecule 36: 50S ribosomal protein L15

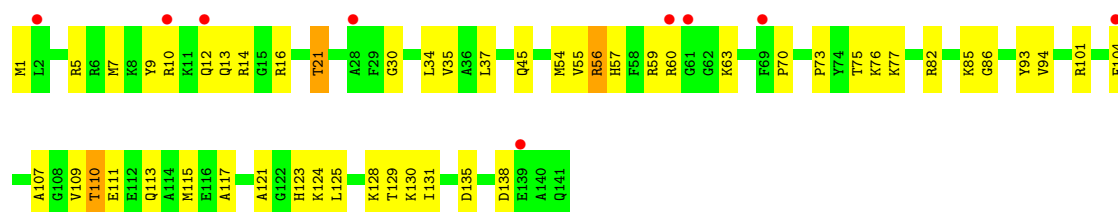




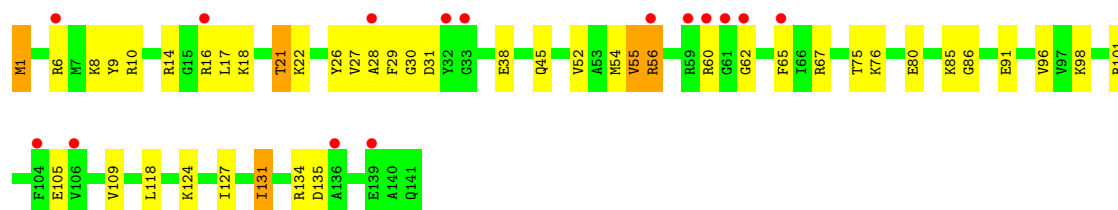
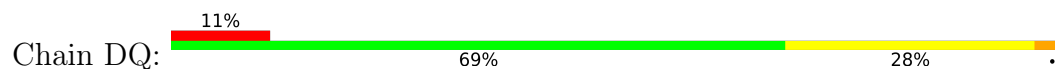
• Molecule 36: 50S ribosomal protein L15



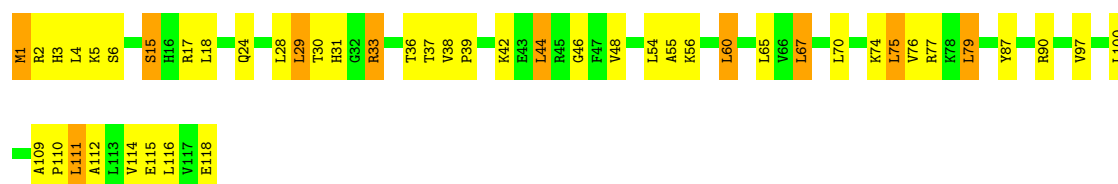
• Molecule 37: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L16

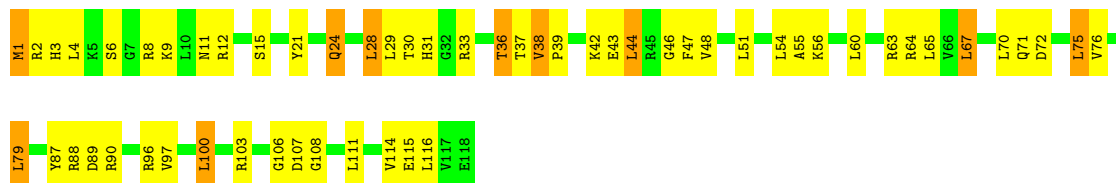


• Molecule 38: 50S ribosomal protein L17



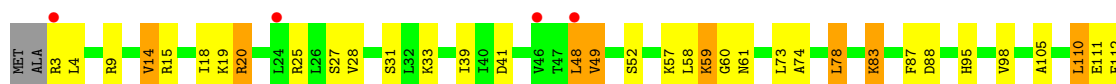
- Molecule 38: 50S ribosomal protein L17

Chain DR:  52% 40% 8%



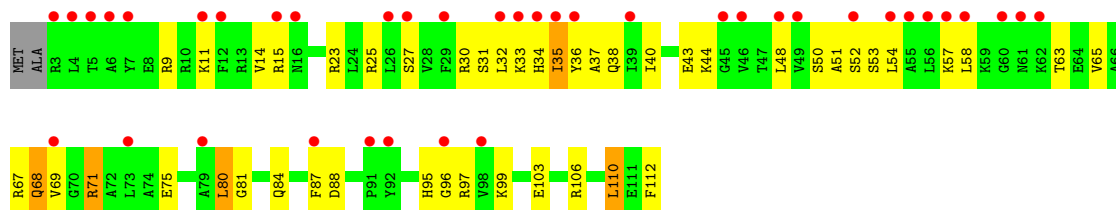
- Molecule 39: 50S ribosomal protein L18

Chain BS:  4% 67% 24% 7%



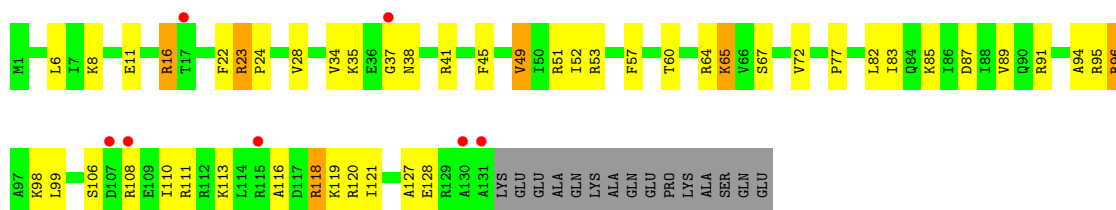
- Molecule 39: 50S ribosomal protein L18

Chain DS:  35% 56% 38%



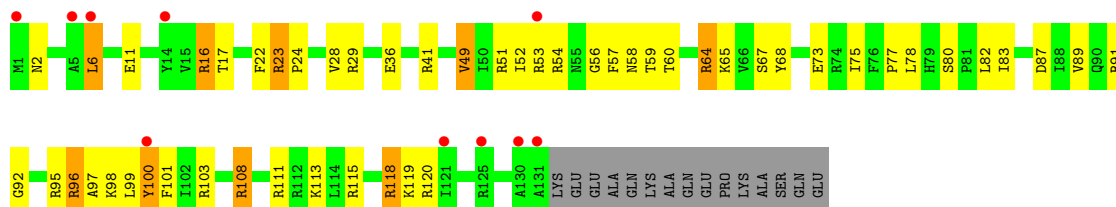
- Molecule 40: 50S ribosomal protein L19

Chain BT:  5% 57% 29% 10%

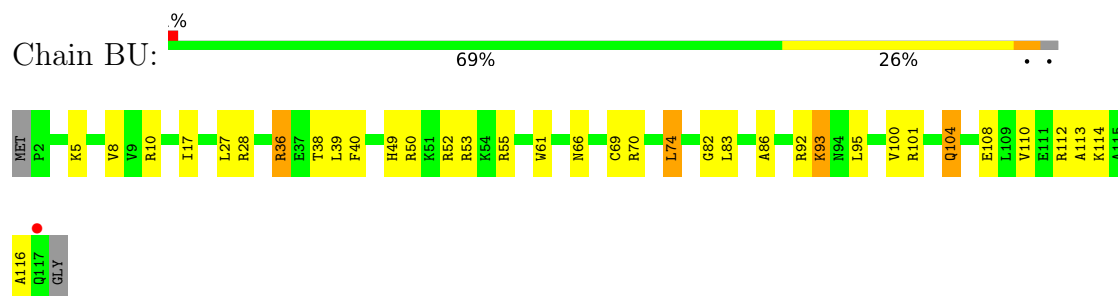


- Molecule 40: 50S ribosomal protein L19

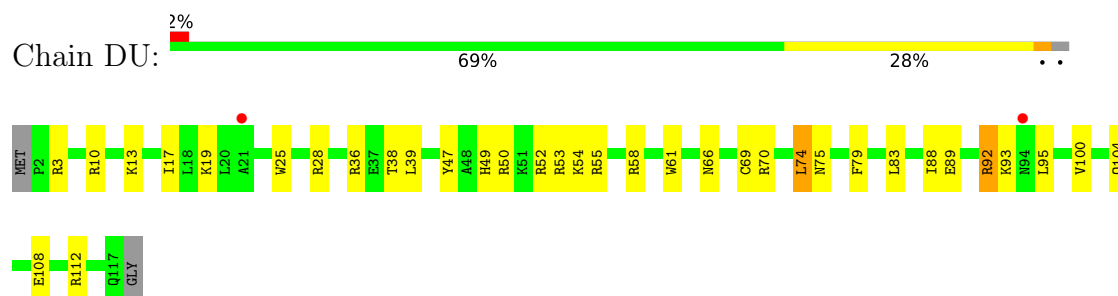
Chain DT:  7% 54% 29% 6% 10%



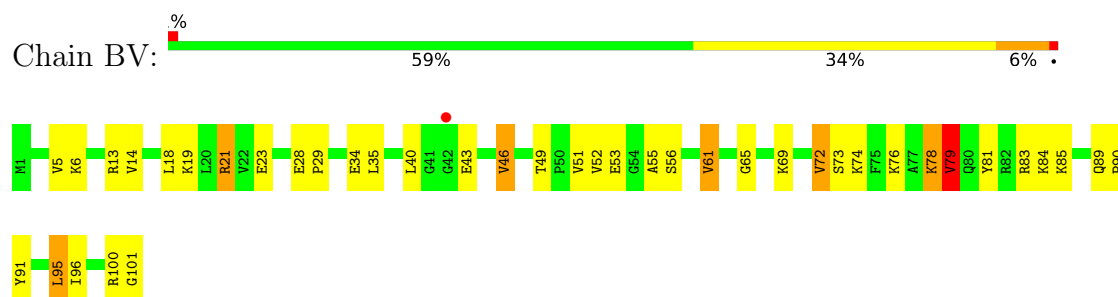
- Molecule 41: 50S ribosomal protein L20



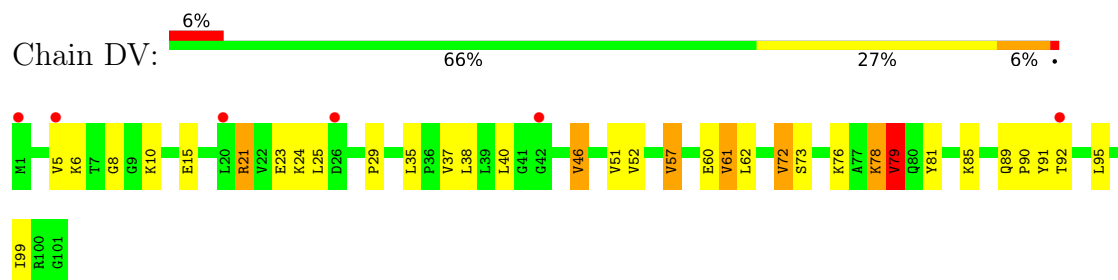
- Molecule 41: 50S ribosomal protein L20



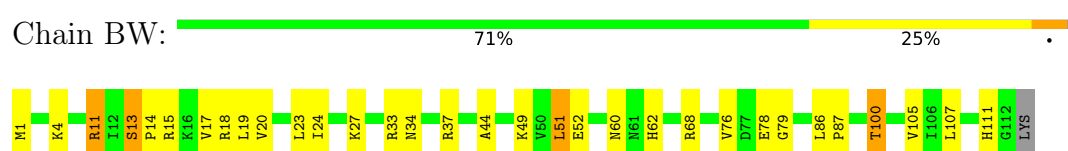
- Molecule 42: 50S ribosomal protein L21



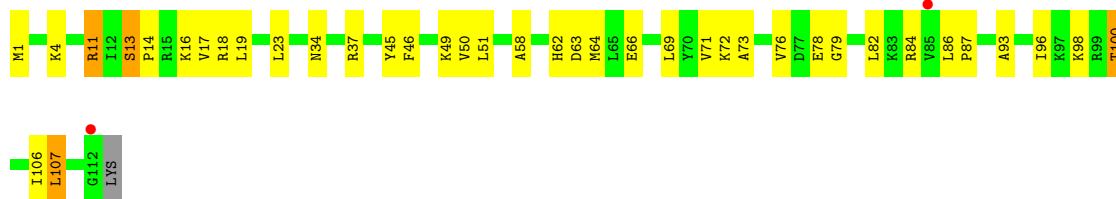
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23



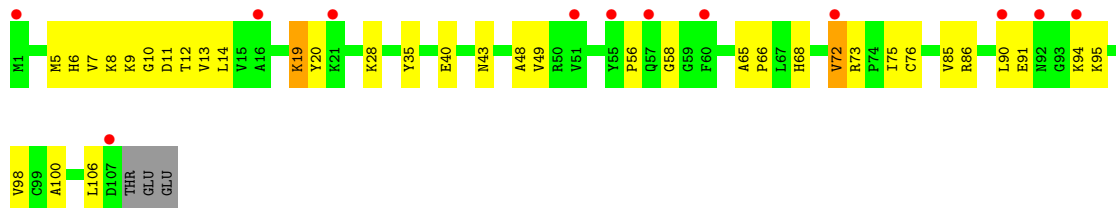
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24

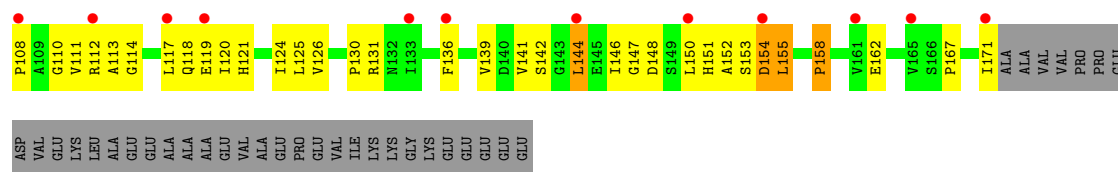


- Molecule 45: 50S ribosomal protein L24

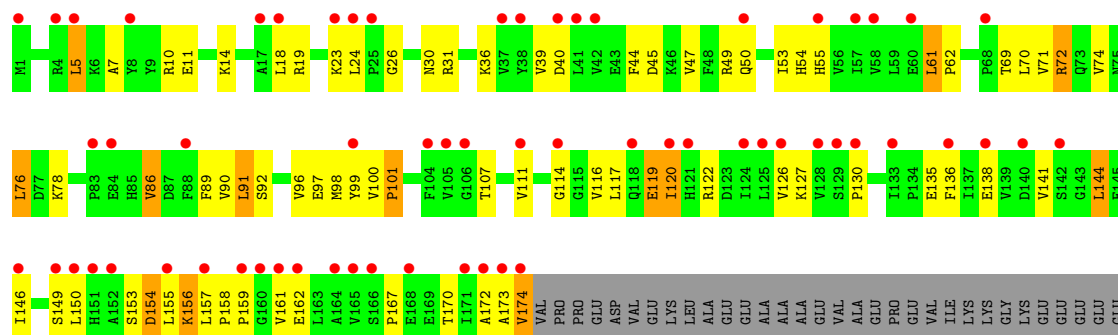


- Molecule 46: 50S ribosomal protein L25

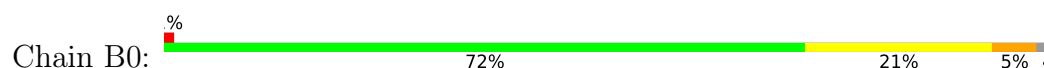




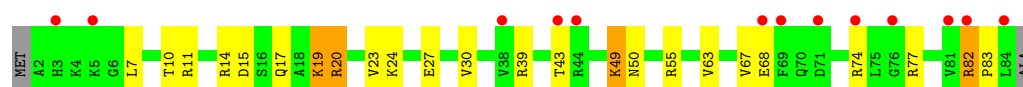
• Molecule 46: 50S ribosomal protein L25



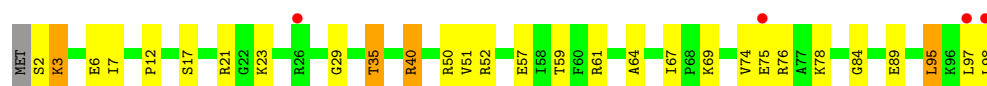
• Molecule 47: 50S ribosomal protein L27



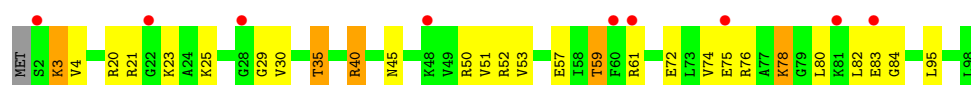
• Molecule 47: 50S ribosomal protein L27



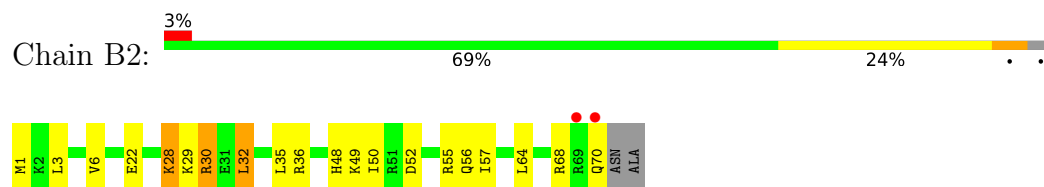
• Molecule 48: 50S ribosomal protein L28



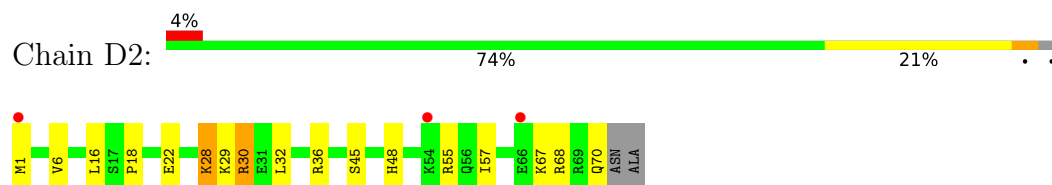
• Molecule 48: 50S ribosomal protein L28



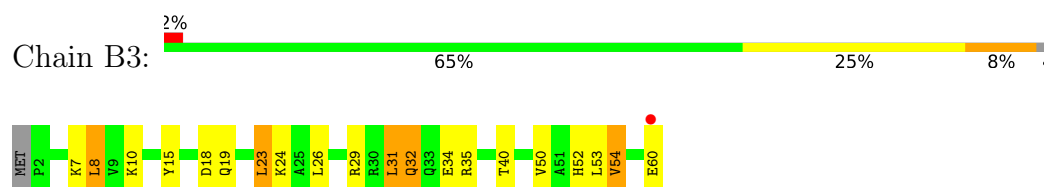
- Molecule 49: 50S ribosomal protein L29



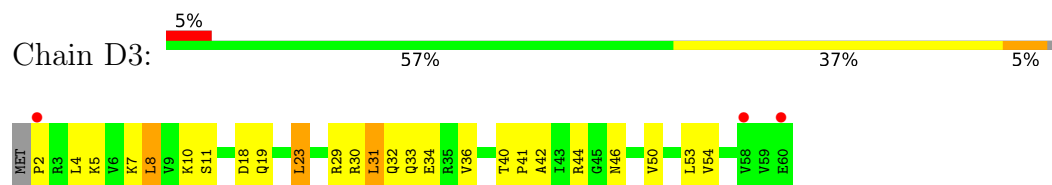
- Molecule 49: 50S ribosomal protein L29



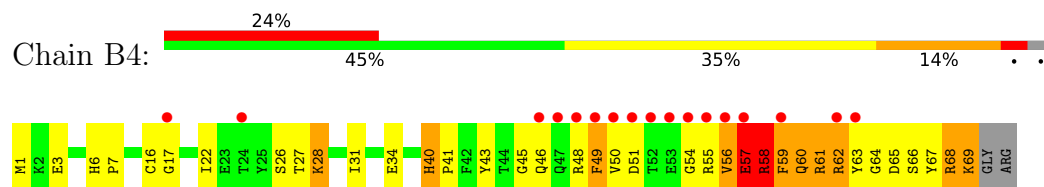
- Molecule 50: 50S ribosomal protein L30



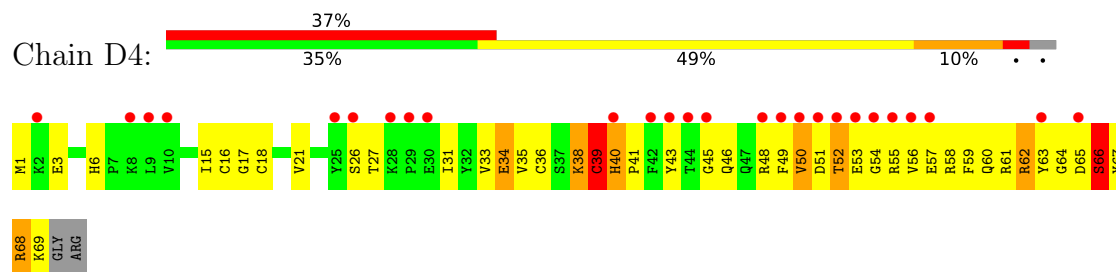
- Molecule 50: 50S ribosomal protein L30



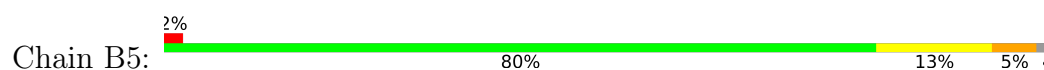
- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



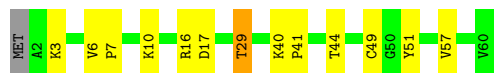
- Molecule 52: 50S ribosomal protein L32





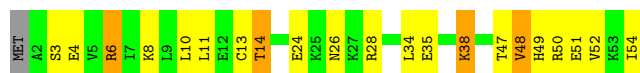
- Molecule 52: 50S ribosomal protein L32

Chain D5: 77% 20% ..



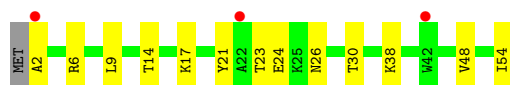
- Molecule 53: 50S ribosomal protein L33

Chain B6: 59% 31% 7% .



- Molecule 53: 50S ribosomal protein L33

Chain D6: 6% 74% 24% .



- Molecule 54: 50S ribosomal protein L34

Chain B7: 2% 59% 35% . .



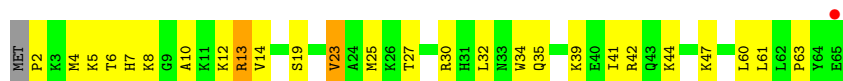
- Molecule 54: 50S ribosomal protein L34

Chain D7: 4% 51% 43% . .



- Molecule 55: 50S ribosomal protein L35

Chain B8: 2% 58% 37% . .



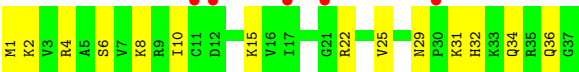
- Molecule 55: 50S ribosomal protein L35



• Molecule 56: 50S ribosomal protein L36



• Molecule 56: 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	207.56Å 444.23Å 613.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.38 – 2.80 150.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (150.38-2.80) 98.0 (150.38-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.280 0.234 , 0.279	Depositor DCC
R_{free} test set	67651 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290205	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: SF4, MG, PSU, K, 5MU, 5MC, 31H, ZN, PPU, 4SU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.23	0/36049	0.47	2/56261 (0.0%)
1	CA	0.24	0/36170	0.50	7/56452 (0.0%)
2	AB	0.39	0/1881	1.00	6/2542 (0.2%)
2	CB	0.44	0/1860	1.05	11/2518 (0.4%)
3	AC	0.39	0/1576	0.86	1/2130 (0.0%)
3	CC	0.40	0/1566	0.94	5/2119 (0.2%)
4	AD	0.38	0/1689	0.89	2/2267 (0.1%)
4	CD	0.39	0/1704	0.93	7/2284 (0.3%)
5	AE	0.39	0/1145	0.85	2/1543 (0.1%)
5	CE	0.40	0/1149	0.97	3/1548 (0.2%)
6	AF	0.35	0/819	0.79	0/1111
6	CF	0.36	0/829	0.81	0/1123
7	AG	0.36	0/1250	0.88	2/1679 (0.1%)
7	CG	0.37	0/1254	0.95	1/1683 (0.1%)
8	AH	0.36	0/1108	0.90	2/1494 (0.1%)
8	CH	0.35	0/1108	0.94	6/1494 (0.4%)
9	AI	0.38	0/1002	0.90	1/1346 (0.1%)
9	CI	0.42	0/997	0.92	3/1343 (0.2%)
10	AJ	0.38	0/722	1.06	7/982 (0.7%)
10	CJ	0.42	0/727	0.96	2/988 (0.2%)
11	AK	0.38	0/844	0.84	0/1145
11	CK	0.36	0/848	0.85	0/1149
12	AL	0.38	0/946	0.82	3/1274 (0.2%)
12	CL	0.36	0/946	0.85	2/1274 (0.2%)
13	AM	0.38	0/969	0.92	1/1302 (0.1%)
13	CM	0.41	0/961	0.95	3/1291 (0.2%)
14	AN	0.38	0/501	0.81	0/664
14	CN	0.41	0/501	0.86	1/664 (0.2%)
15	AO	0.38	0/739	0.86	1/985 (0.1%)
15	CO	0.40	0/739	0.88	2/985 (0.2%)
16	AP	0.39	0/697	0.86	1/939 (0.1%)
16	CP	0.38	0/693	0.82	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.34	0/836	0.84	0/1117
17	CQ	0.32	0/836	0.85	0/1117
18	AR	0.35	0/560	0.81	0/746
18	CR	0.37	0/560	0.83	0/746
19	AS	0.38	0/667	0.85	0/900
19	CS	0.40	0/661	1.04	1/893 (0.1%)
20	AT	0.36	0/730	0.94	0/965
20	CT	0.35	0/729	0.87	1/965 (0.1%)
21	AU	0.32	0/203	0.94	0/266
21	CU	0.38	0/203	0.80	0/266
22	AV	0.27	0/310	0.46	0/480
22	CV	0.61	0/144	0.83	0/222
23	AW	0.29	0/40	0.52	0/60
23	CW	0.21	0/40	0.51	0/60
24	AX	0.29	0/1700	0.50	0/2650
24	CX	0.30	0/1700	0.59	0/2650
25	AY	0.20	0/115	0.41	0/176
25	CY	0.19	0/115	0.36	0/176
26	BA	0.28	0/68013	0.45	2/106165 (0.0%)
26	DA	0.24	0/67542	0.45	1/105428 (0.0%)
27	BB	0.24	0/2878	0.48	0/4490
27	DB	0.23	0/2878	0.47	0/4490
28	BD	0.49	0/2186	0.87	2/2944 (0.1%)
28	DD	0.42	0/2186	0.92	5/2944 (0.2%)
29	BE	0.48	0/1592	0.87	0/2149
29	DE	0.43	0/1592	0.94	6/2149 (0.3%)
30	BF	0.46	0/1619	0.83	0/2193
30	DF	0.43	0/1615	0.93	5/2188 (0.2%)
31	BG	0.38	0/1450	0.90	4/1959 (0.2%)
31	DG	0.41	0/1449	1.01	4/1958 (0.2%)
32	BH	0.42	0/1356	0.86	1/1834 (0.1%)
32	DH	0.39	0/1356	0.92	3/1834 (0.2%)
33	BI	0.43	0/1100	0.98	7/1501 (0.5%)
33	DI	0.55	0/1076	1.27	12/1471 (0.8%)
34	BN	0.45	0/1144	0.90	2/1543 (0.1%)
34	DN	0.41	0/1144	0.95	2/1543 (0.1%)
35	BO	0.45	0/943	0.84	0/1269
35	DO	0.40	0/943	0.84	0/1269
36	BP	0.44	0/1152	0.84	0/1533
36	DP	0.40	0/1152	0.93	2/1533 (0.1%)
37	BQ	0.46	0/1143	0.84	0/1527
37	DQ	0.41	0/1143	0.83	0/1527
38	BR	0.48	0/982	0.84	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.40	0/982	0.86	2/1312 (0.2%)
39	BS	0.40	0/887	0.89	0/1180
39	DS	0.38	0/880	0.88	1/1172 (0.1%)
40	BT	0.43	0/1105	0.87	0/1477
40	DT	0.39	0/1097	0.79	0/1468
41	BU	0.46	0/977	0.79	0/1301
41	DU	0.37	0/977	0.82	0/1301
42	BV	0.45	0/782	0.80	0/1049
42	DV	0.37	0/782	0.79	0/1049
43	BW	0.48	0/897	0.89	2/1205 (0.2%)
43	DW	0.40	0/897	0.83	2/1205 (0.2%)
44	BX	0.47	0/764	0.87	0/1025
44	DX	0.37	0/764	0.79	0/1025
45	BY	0.44	0/819	0.93	2/1095 (0.2%)
45	DY	0.37	0/819	0.90	1/1095 (0.1%)
46	BZ	0.41	0/1379	0.96	4/1873 (0.2%)
46	DZ	0.36	0/1390	0.90	4/1890 (0.2%)
47	B0	0.44	0/662	0.87	1/881 (0.1%)
47	D0	0.36	0/662	0.82	2/881 (0.2%)
48	B1	0.42	0/762	0.85	1/1014 (0.1%)
48	D1	0.40	0/762	0.83	0/1014
49	B2	0.43	0/590	0.84	0/781
49	D2	0.35	0/590	0.80	0/781
50	B3	0.46	0/474	0.88	0/635
50	D3	0.39	0/469	0.94	0/630
51	B4	0.42	0/565	1.10	5/761 (0.7%)
51	D4	0.40	0/545	1.17	8/737 (1.1%)
52	B5	0.50	0/469	0.95	3/635 (0.5%)
52	D5	0.42	0/469	0.77	0/635
53	B6	0.47	0/460	0.78	0/613
53	D6	0.40	0/456	0.75	0/608
54	B7	0.48	0/426	0.85	0/561
54	D7	0.47	0/426	0.88	2/561 (0.4%)
55	B8	0.47	0/519	0.81	0/684
55	D8	0.40	0/525	0.75	0/691
56	B9	0.48	0/310	0.95	0/407
56	D9	0.36	0/310	0.89	0/407
All	All	0.31	0/310421	0.61	184/464361 (0.0%)

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
20	AT	0	1
29	DE	0	1
33	DI	0	1
39	BS	0	1
46	BZ	0	1
51	B4	0	2
51	D4	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	DI	88	ILE	N-CA-C	11.06	124.26	109.21
33	DI	71	ILE	N-CA-C	9.08	119.06	110.53
51	D4	52	THR	N-CA-C	-8.91	102.42	113.38
51	B4	60	GLN	N-CA-C	-8.37	103.17	112.72
3	CC	194	GLY	N-CA-C	8.30	120.91	110.29

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
20	AT	9	ASN	Peptide
39	BS	58	LEU	Peptide
46	BZ	158	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16255	758	1
1	CA	32312	0	16307	969	1

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1846	0	1867	75	0
2	CB	1825	0	1828	76	0
3	AC	1552	0	1546	51	0
3	CC	1542	0	1517	58	0
4	AD	1659	0	1676	77	0
4	CD	1674	0	1714	82	0
5	AE	1129	0	1184	35	0
5	CE	1133	0	1191	39	0
6	AF	806	0	793	20	0
6	CF	816	0	808	26	0
7	AG	1231	0	1238	39	0
7	CG	1235	0	1249	40	0
8	AH	1088	0	1126	36	0
8	CH	1088	0	1126	40	0
9	AI	983	0	986	49	0
9	CI	978	0	966	54	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	38	0
11	AK	829	0	825	23	0
11	CK	833	0	836	22	0
12	AL	930	0	980	22	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	38	0
13	CM	950	0	988	47	0
14	AN	492	0	529	28	0
14	CN	492	0	529	23	0
15	AO	728	0	760	23	0
15	CO	728	0	760	28	0
16	AP	681	0	697	28	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	24	0
17	CQ	823	0	891	18	0
18	AR	555	0	618	13	0
18	CR	555	0	618	25	0
19	AS	652	0	662	31	0
19	CS	646	0	644	40	0
20	AT	728	0	798	29	0
20	CT	727	0	796	24	0
21	AU	199	0	208	5	0
21	CU	199	0	208	7	0
22	AV	277	0	140	7	0
22	CV	129	0	65	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	74	0	51	5	0
23	CW	74	0	51	11	0
24	AX	1633	0	836	33	0
24	CX	1635	0	838	81	0
25	AY	104	0	56	3	0
25	CY	104	0	56	2	0
26	BA	60729	0	30620	968	0
26	DA	60311	0	30412	1244	1
27	BB	2573	0	1306	33	0
27	DB	2573	0	1306	87	0
28	BD	2136	0	2218	68	0
28	DD	2136	0	2218	75	0
29	BE	1559	0	1618	44	0
29	DE	1559	0	1618	53	0
30	BF	1584	0	1625	51	0
30	DF	1580	0	1619	57	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	74	0
32	BH	1330	0	1407	30	0
32	DH	1330	0	1407	47	0
33	BI	1085	0	1114	30	1
33	DI	1061	0	1080	51	0
34	BN	1117	0	1184	22	0
34	DN	1117	0	1184	29	0
35	BO	933	0	996	28	0
35	DO	933	0	996	42	0
36	BP	1135	0	1212	53	0
36	DP	1135	0	1212	65	0
37	BQ	1122	0	1179	40	0
37	DQ	1122	0	1179	34	0
38	BR	968	0	1033	28	1
38	DR	968	0	1033	37	0
39	BS	877	0	938	28	0
39	DS	870	0	923	29	0
40	BT	1091	0	1151	37	0
40	DT	1083	0	1136	40	0
41	BU	959	0	1019	25	0
41	DU	959	0	1018	28	0
42	BV	771	0	830	23	1
42	DV	771	0	830	25	0
43	BW	886	0	940	16	0
43	DW	886	0	940	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BX	750	0	814	25	0
44	DX	750	0	814	20	0
45	BY	806	0	881	23	0
45	DY	806	0	881	23	0
46	BZ	1349	0	1355	38	0
46	DZ	1360	0	1363	50	0
47	B0	653	0	674	21	0
47	D0	653	0	674	19	0
48	B1	755	0	826	19	0
48	D1	755	0	826	20	0
49	B2	588	0	643	9	0
49	D2	588	0	643	10	0
50	B3	469	0	518	15	0
50	D3	464	0	514	17	0
51	B4	552	0	533	34	0
51	D4	532	0	503	31	0
52	B5	455	0	465	9	0
52	D5	455	0	465	10	0
53	B6	453	0	473	14	0
53	D6	449	0	469	7	0
54	B7	418	0	467	20	0
54	D7	418	0	467	16	0
55	B8	511	0	571	30	0
55	D8	517	0	582	15	0
56	B9	307	0	335	7	0
56	D9	307	0	335	11	0
57	AA	207	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AF	1	0	0	0	0
57	AJ	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AS	1	0	0	0	0
57	AV	1	0	0	0	0
57	AW	1	0	0	0	0
57	AX	11	0	0	0	0
57	B0	4	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B5	2	0	0	0	0
57	B7	3	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	720	0	0	0	0
57	BB	20	0	0	0	0
57	BD	11	0	0	0	0
57	BE	7	0	0	0	0
57	BF	10	0	0	0	0
57	BG	2	0	0	0	0
57	BN	6	0	0	0	0
57	BO	1	0	0	0	0
57	BP	4	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	3	0	0	0	0
57	BU	8	0	0	0	0
57	BV	4	0	0	0	0
57	BW	5	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	160	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D8	2	0	0	0	0
57	DA	629	0	0	0	0
57	DB	10	0	0	0	0
57	DD	7	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DR	2	0	0	0	0
57	DU	4	0	0	0	0
57	DV	2	0	0	0	0
57	DW	2	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	170	0	0	16	0
61	AL	2	0	0	1	0
61	AO	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AW	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	5	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	0	0
61	BA	1102	0	0	59	0
61	BB	36	0	0	1	0
61	BD	8	0	0	1	0
61	BE	13	0	0	5	0
61	BF	4	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BP	15	0	0	1	0
61	BQ	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BR	1	0	0	1	0
61	BS	1	0	0	0	0
61	BT	3	0	0	0	0
61	BU	1	0	0	1	0
61	BV	4	0	0	0	0
61	BW	2	0	0	0	0
61	BX	2	0	0	0	0
61	CA	130	0	0	8	0
61	CE	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	1	0	0	0	0
61	CX	1	0	0	1	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	767	0	0	55	0
61	DB	9	0	0	0	0
61	DD	9	0	0	3	0
61	DE	5	0	0	0	0
61	DF	6	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	3	0
61	DR	2	0	0	1	0
61	DT	1	0	0	0	0
61	DU	2	0	0	0	0
61	DV	1	0	0	1	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0
All	All	290205	0	193167	6372	3

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 14.

The worst 5 of 6372 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:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.11
26:DA:2121:G:H1	26:DA:2177:C:N4	1.52	1.06
1:AA:1164:G:N2	1:AA:1165:C:C5	2.24	1.06
1:CA:72:C:N4	1:CA:97:G:N1	2.04	1.05
26:DA:2139:C:N4	26:DA:2152:G:H1	1.55	1.04

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1043:C:O2'	26:DA:2137:C:O2'[2_655]	2.08	0.12
33:BI:89:TYR:O	1:CA:357:G:O2'[3_654]	2.10	0.10
38:BR:33:ARG:NH2	42:BV:53:GLU:OE2[4_445]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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%)	21 (9%)	4 (2%)	7	25
2	CB	229/256 (90%)	204 (89%)	14 (6%)	11 (5%)	2	6
3	AC	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	12	38
3	CC	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24	55
4	AD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	55
4	CD	206/209 (99%)	196 (95%)	7 (3%)	3 (2%)	8	28
5	AE	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	18	47
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18	47
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	18	47
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	18	47
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	16	44
10	AJ	95/105 (90%)	83 (87%)	5 (5%)	7 (7%)	1	2
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	1	5
11	AK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	41
11	CK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	41
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	7	25
13	CM	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	16	44
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
15	CO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
16	CP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	16
20	AT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	1	3
20	CT	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	7
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	60
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
29	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	38
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	55
30	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	12	38
31	BG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	5	19
31	DG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	5	19
32	BH	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	10	34
32	DH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	10	34
33	BI	144/148 (97%)	132 (92%)	9 (6%)	3 (2%)	5	20
33	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	9	30
34	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
34	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	47
35	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	44
35	DO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	44
36	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18	47
36	DP	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	18	47
37	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
39	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	41
40	BT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
40	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	16	44
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
42	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	38
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	38
43	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	DX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
45	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
45	DY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
46	BZ	169/206 (82%)	148 (88%)	19 (11%)	2 (1%)	10	34
46	DZ	172/206 (84%)	156 (91%)	14 (8%)	2 (1%)	10	34
47	B0	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
47	D0	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	11	36
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	36
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	2
51	D4	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	3
52	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5	19
55	B8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10783 (94%)	516 (4%)	110 (1%)	12	38

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL

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Mol	Chain	Res	Type
10	AJ	55	LYS
20	AT	10	LEU

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%)	156 (81%)	36 (19%)	1	5
2	CB	187/220 (85%)	158 (84%)	29 (16%)	2	9
3	AC	143/188 (76%)	125 (87%)	18 (13%)	4	15
3	CC	140/188 (74%)	122 (87%)	18 (13%)	4	14
4	AD	170/181 (94%)	153 (90%)	17 (10%)	7	24
4	CD	173/181 (96%)	154 (89%)	19 (11%)	6	20
5	AE	113/123 (92%)	105 (93%)	8 (7%)	13	39
5	CE	114/123 (93%)	106 (93%)	8 (7%)	14	40
6	AF	83/90 (92%)	76 (92%)	7 (8%)	10	32
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	27
7	AG	119/127 (94%)	103 (87%)	16 (13%)	4	13
7	CG	120/127 (94%)	107 (89%)	13 (11%)	6	21
8	AH	114/119 (96%)	107 (94%)	7 (6%)	17	46
8	CH	114/119 (96%)	101 (89%)	13 (11%)	5	19
9	AI	90/99 (91%)	73 (81%)	17 (19%)	1	5
9	CI	89/99 (90%)	76 (85%)	13 (15%)	3	11
10	AJ	66/92 (72%)	59 (89%)	7 (11%)	6	22
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7	23
11	AK	82/99 (83%)	76 (93%)	6 (7%)	13	38
11	CK	83/99 (84%)	80 (96%)	3 (4%)	31	66
12	AL	97/109 (89%)	87 (90%)	10 (10%)	7	23
12	CL	97/109 (89%)	91 (94%)	6 (6%)	16	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AM	93/101 (92%)	80 (86%)	13 (14%)	3	12
13	CM	92/101 (91%)	79 (86%)	13 (14%)	3	12
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	16
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	16
15	AO	78/80 (98%)	67 (86%)	11 (14%)	3	12
15	CO	78/80 (98%)	68 (87%)	10 (13%)	4	15
16	AP	69/74 (93%)	57 (83%)	12 (17%)	2	7
16	CP	68/74 (92%)	58 (85%)	10 (15%)	3	10
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	26	60
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	31
18	AR	59/77 (77%)	51 (86%)	8 (14%)	3	13
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3	13
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	23
19	CS	67/80 (84%)	60 (90%)	7 (10%)	7	22
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3	11
20	CT	70/82 (85%)	60 (86%)	10 (14%)	3	11
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	8
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	20
28	BD	215/218 (99%)	200 (93%)	15 (7%)	14	40
28	DD	215/218 (99%)	194 (90%)	21 (10%)	7	25
29	BE	164/166 (99%)	140 (85%)	24 (15%)	3	11
29	DE	164/166 (99%)	140 (85%)	24 (15%)	3	11
30	BF	160/166 (96%)	140 (88%)	20 (12%)	4	15
30	DF	159/166 (96%)	143 (90%)	16 (10%)	7	23
31	BG	143/156 (92%)	127 (89%)	16 (11%)	6	19
31	DG	142/156 (91%)	121 (85%)	21 (15%)	3	10
32	BH	144/148 (97%)	133 (92%)	11 (8%)	12	36
32	DH	144/148 (97%)	132 (92%)	12 (8%)	10	32
33	BI	110/124 (89%)	90 (82%)	20 (18%)	2	6
33	DI	104/124 (84%)	88 (85%)	16 (15%)	2	10
34	BN	118/119 (99%)	98 (83%)	20 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	118/119 (99%)	104 (88%)	14 (12%)	5	17
35	BO	100/100 (100%)	92 (92%)	8 (8%)	11	34
35	DO	100/100 (100%)	95 (95%)	5 (5%)	22	54
36	BP	115/116 (99%)	102 (89%)	13 (11%)	5	19
36	DP	115/116 (99%)	99 (86%)	16 (14%)	3	12
37	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	28
37	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	28
38	BR	101/101 (100%)	82 (81%)	19 (19%)	1	5
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	6
39	BS	87/88 (99%)	75 (86%)	12 (14%)	3	12
39	DS	85/88 (97%)	70 (82%)	15 (18%)	2	7
40	BT	115/127 (91%)	104 (90%)	11 (10%)	8	26
40	DT	113/127 (89%)	101 (89%)	12 (11%)	6	22
41	BU	93/94 (99%)	84 (90%)	9 (10%)	8	25
41	DU	93/94 (99%)	87 (94%)	6 (6%)	15	43
42	BV	80/82 (98%)	65 (81%)	15 (19%)	1	5
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	8
43	BW	90/92 (98%)	81 (90%)	9 (10%)	7	24
43	DW	90/92 (98%)	81 (90%)	9 (10%)	7	24
44	BX	77/78 (99%)	72 (94%)	5 (6%)	15	43
44	DX	77/78 (99%)	69 (90%)	8 (10%)	7	22
45	BY	85/91 (93%)	74 (87%)	11 (13%)	4	14
45	DY	85/91 (93%)	79 (93%)	6 (7%)	13	39
46	BZ	145/179 (81%)	128 (88%)	17 (12%)	5	18
46	DZ	145/179 (81%)	122 (84%)	23 (16%)	2	9
47	B0	65/67 (97%)	59 (91%)	6 (9%)	8	27
47	D0	65/67 (97%)	59 (91%)	6 (9%)	8	27
48	B1	80/83 (96%)	73 (91%)	7 (9%)	9	29
48	D1	80/83 (96%)	73 (91%)	7 (9%)	9	29
49	B2	65/67 (97%)	57 (88%)	8 (12%)	4	16
49	D2	65/67 (97%)	59 (91%)	6 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	51/52 (98%)	44 (86%)	7 (14%)	3	13
50	D3	50/52 (96%)	45 (90%)	5 (10%)	7	24
51	B4	59/63 (94%)	46 (78%)	13 (22%)	1	3
51	D4	53/63 (84%)	46 (87%)	7 (13%)	4	14
52	B5	50/52 (96%)	47 (94%)	3 (6%)	17	47
52	D5	50/52 (96%)	47 (94%)	3 (6%)	17	47
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	13
53	D6	50/52 (96%)	47 (94%)	3 (6%)	17	47
54	B7	41/42 (98%)	39 (95%)	2 (5%)	22	55
54	D7	41/42 (98%)	39 (95%)	2 (5%)	22	55
55	B8	53/55 (96%)	48 (91%)	5 (9%)	8	27
55	D8	54/55 (98%)	50 (93%)	4 (7%)	13	37
56	B9	34/34 (100%)	31 (91%)	3 (9%)	9	29
56	D9	34/34 (100%)	33 (97%)	1 (3%)	37	73
All	All	9319/10066 (93%)	8250 (88%)	1069 (12%)	5	18

5 of 1069 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DR	63	ARG
40	DT	49	VAL
38	DR	60	LEU
49	D2	32	LEU
38	BR	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
10	CJ	13	HIS
31	DG	41	GLN
11	CK	93	GLN
20	CT	16	HIS
36	DP	38	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	407 (27%)	26 (1%)
1	CA	1501/1521 (98%)	413 (27%)	28 (1%)
22	AV	12/24 (50%)	7 (58%)	0
22	CV	5/24 (20%)	4 (80%)	0
23	AW	1/3 (33%)	0	0
23	CW	1/3 (33%)	0	0
24	AX	74/77 (96%)	26 (35%)	2 (2%)
24	CX	74/77 (96%)	31 (41%)	4 (5%)
25	AY	4/76 (5%)	1 (25%)	0
25	CY	4/76 (5%)	1 (25%)	0
26	BA	2811/2915 (96%)	531 (18%)	30 (1%)
26	DA	2791/2915 (95%)	598 (21%)	30 (1%)
27	BB	120/121 (99%)	16 (13%)	2 (1%)
27	DB	119/121 (98%)	31 (26%)	0
All	All	9012/9474 (95%)	2066 (22%)	122 (1%)

5 of 2066 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2893	G
26	DA	1913	A
1	CA	687	A
26	DA	1653	G
26	DA	2439	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	31H	AX	76	24,57	29,32,35	1.32	4 (13%)	34,45,50	2.54	12 (35%)
24	PSU	AX	55	24	18,21,22	1.37	2 (11%)	21,30,33	2.06	3 (14%)
24	5MU	AX	54	24	19,22,23	1.38	5 (26%)	27,32,35	2.21	6 (22%)
24	31H	CX	76	24,57,60	31,34,35	1.34	4 (12%)	35,47,50	2.46	13 (37%)
24	4SU	AX	8	24	18,21,22	2.24	5 (27%)	25,30,33	1.70	4 (16%)
24	5MC	AX	32	24	19,22,23	1.61	3 (15%)	26,32,35	1.27	3 (11%)
24	PSU	CX	55	24	18,21,22	1.33	2 (11%)	21,30,33	1.95	4 (19%)
23	PPU	AW	76	23,26	37,40,41	1.35	3 (8%)	47,57,60	2.10	14 (29%)
24	4SU	CX	8	24	18,21,22	1.99	5 (27%)	25,30,33	1.65	5 (20%)
24	5MC	CX	32	24	19,22,23	1.63	2 (10%)	26,32,35	1.06	2 (7%)
24	5MU	CX	54	24	19,22,23	1.35	5 (26%)	27,32,35	2.24	6 (22%)
23	PPU	CW	76	23,26	37,40,41	1.27	3 (8%)	47,57,60	2.27	15 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	31H	AX	76	24,57	-	7/19/37/41	0/3/3/3
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	31H	CX	76	24,57,60	-	9/22/40/41	0/3/3/3
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
23	PPU	AW	76	23,26	-	3/25/43/44	0/4/4/4
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
23	PPU	CW	76	23,26	-	6/25/43/44	0/4/4/4

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	32	5MC	C5-C4	5.90	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	32	5MC	C5-C4	5.59	1.48	1.44
23	AW	76	PPU	C5-C4	5.20	1.48	1.39
24	AX	8	4SU	C4-N3	-5.14	1.32	1.37
23	CW	76	PPU	C5-C4	4.93	1.47	1.39

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	76	31H	O4'-C1'-N9	7.99	123.44	108.09
23	CW	76	PPU	C5-C4-N3	-6.74	117.43	126.72
24	AX	76	31H	C5-C4-N3	-6.60	117.63	126.72
24	AX	55	PSU	N1-C2-N3	6.34	121.86	115.17
23	AW	76	PPU	C5-C4-N3	-6.33	118.00	126.72

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	CX	76	31H	C3'-C4'-C5'-O5'
24	CX	76	31H	C-CA-CB-CG
24	CX	76	31H	N-CA-CB-CG
24	CX	76	31H	OCN-CN-N-CA
23	AW	76	PPU	CE2-CZ-OC-CM

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	55	PSU	1	0
24	AX	54	5MU	1	0
24	CX	76	31H	4	0
24	AX	8	4SU	2	0
24	CX	55	PSU	1	0
23	AW	76	PPU	5	0
24	CX	8	4SU	2	0
24	CX	32	5MC	2	0
24	CX	54	5MU	1	0
23	CW	76	PPU	11	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1916 ligands modelled in this entry, 1914 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	AD	302	4	0,12,12	-	-	-		
58	SF4	CD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	AD	302	4	-	-	0/6/5/5
58	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AD	302	SF4	1	0
58	CD	501	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1498/1521 (98%)	0.93	99 (6%) 24 18	39, 73, 93, 105	0
1	CA	1503/1521 (98%)	1.22	236 (15%) 5 4	41, 75, 94, 106	0
2	AB	231/256 (90%)	1.54	50 (21%) 2 2	69, 82, 91, 101	0
2	CB	231/256 (90%)	1.90	99 (42%) 0 0	71, 84, 93, 101	0
3	AC	206/239 (86%)	1.47	46 (22%) 2 1	67, 79, 89, 95	0
3	CC	206/239 (86%)	1.83	75 (36%) 1 0	70, 81, 91, 95	0
4	AD	208/209 (99%)	1.52	57 (27%) 1 1	57, 74, 85, 91	0
4	CD	208/209 (99%)	1.98	97 (46%) 0 0	57, 75, 85, 92	0
5	AE	148/162 (91%)	1.25	26 (17%) 4 3	59, 71, 82, 90	0
5	CE	148/162 (91%)	1.60	42 (28%) 1 1	59, 73, 84, 91	0
6	AF	100/101 (99%)	1.03	10 (10%) 12 9	54, 69, 78, 83	0
6	CF	100/101 (99%)	1.20	15 (15%) 5 4	56, 71, 80, 83	0
7	AG	155/156 (99%)	1.29	30 (19%) 3 2	64, 76, 86, 92	0
7	CG	155/156 (99%)	1.68	44 (28%) 1 1	67, 78, 88, 92	0
8	AH	137/138 (99%)	1.37	27 (19%) 3 2	60, 72, 80, 85	0
8	CH	137/138 (99%)	1.49	28 (20%) 3 2	62, 74, 82, 85	0
9	AI	127/128 (99%)	1.80	47 (37%) 1 0	64, 83, 91, 96	0
9	CI	127/128 (99%)	2.85	96 (75%) 0 0	69, 84, 91, 98	0
10	AJ	97/105 (92%)	2.08	47 (48%) 0 0	66, 83, 92, 94	0
10	CJ	96/105 (91%)	2.32	56 (58%) 0 0	69, 85, 93, 94	0
11	AK	114/129 (88%)	1.12	17 (14%) 5 4	46, 70, 81, 85	0
11	CK	114/129 (88%)	1.42	24 (21%) 2 2	50, 71, 82, 85	0
12	AL	122/132 (92%)	0.90	11 (9%) 15 11	50, 64, 73, 81	0
12	CL	122/132 (92%)	1.22	16 (13%) 7 6	52, 65, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	1.44	28 (22%)	2	1	58, 72, 83, 90	0
13	CM	122/126 (96%)	2.43	81 (66%)	0	0	72, 85, 93, 100	0
14	AN	60/61 (98%)	1.88	24 (40%)	1	0	65, 75, 81, 82	0
14	CN	60/61 (98%)	2.73	44 (73%)	0	0	69, 78, 83, 86	0
15	AO	88/89 (98%)	1.20	13 (14%)	5	4	54, 69, 81, 85	0
15	CO	88/89 (98%)	1.31	16 (18%)	3	2	53, 71, 82, 87	0
16	AP	82/88 (93%)	2.00	34 (41%)	0	0	59, 72, 82, 85	0
16	CP	82/88 (93%)	1.73	30 (36%)	1	0	57, 71, 81, 85	0
17	AQ	99/105 (94%)	1.17	12 (12%)	8	6	58, 71, 80, 83	0
17	CQ	99/105 (94%)	1.28	17 (17%)	4	3	56, 72, 81, 83	0
18	AR	68/88 (77%)	0.89	3 (4%)	39	31	59, 70, 80, 84	0
18	CR	68/88 (77%)	1.38	16 (23%)	2	1	60, 71, 82, 85	0
19	AS	83/93 (89%)	1.32	10 (12%)	9	6	72, 82, 89, 93	0
19	CS	83/93 (89%)	2.14	45 (54%)	0	0	73, 84, 91, 95	0
20	AT	96/106 (90%)	1.36	20 (20%)	2	2	60, 71, 83, 85	0
20	CT	96/106 (90%)	1.24	16 (16%)	4	3	56, 71, 83, 85	0
21	AU	23/27 (85%)	2.09	14 (60%)	0	0	69, 74, 79, 85	0
21	CU	23/27 (85%)	2.77	15 (65%)	0	0	71, 76, 84, 86	0
22	AV	13/24 (54%)	2.20	7 (53%)	0	0	56, 88, 93, 97	0
22	CV	6/24 (25%)	3.09	4 (66%)	0	0	59, 76, 95, 96	0
23	AW	2/3 (66%)	0.01	0	100	100	30, 30, 30, 37	0
23	CW	2/3 (66%)	1.48	0	100	100	50, 50, 50, 57	0
24	AX	71/77 (92%)	0.94	3 (4%)	40	32	27, 70, 84, 92	0
24	CX	71/77 (92%)	1.34	13 (18%)	3	2	30, 75, 86, 93	0
25	AY	5/76 (6%)	1.51	2 (40%)	1	0	51, 76, 87, 94	0
25	CY	5/76 (6%)	1.38	0	100	100	60, 79, 90, 91	0
26	BA	2819/2915 (96%)	0.08	107 (3%)	44	35	20, 42, 89, 107	0
26	DA	2800/2915 (96%)	0.18	117 (4%)	40	32	22, 46, 90, 107	0
27	BB	120/121 (99%)	0.63	3 (2%)	58	48	37, 63, 77, 88	0
27	DB	120/121 (99%)	1.27	24 (20%)	3	2	42, 68, 80, 91	0
28	BD	275/276 (99%)	0.44	7 (2%)	58	48	21, 41, 58, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.47	7 (2%) 58 48	23, 43, 61, 80	0
29	BE	204/206 (99%)	0.46	4 (1%) 65 56	21, 46, 65, 82	0
29	DE	204/206 (99%)	0.42	4 (1%) 65 56	23, 48, 67, 84	0
30	BF	203/210 (96%)	0.53	5 (2%) 58 48	22, 51, 73, 87	0
30	DF	203/210 (96%)	0.48	3 (1%) 72 63	24, 54, 74, 86	0
31	BG	181/182 (99%)	1.37	37 (20%) 3 2	55, 70, 82, 93	0
31	DG	181/182 (99%)	2.03	86 (47%) 0 0	59, 74, 85, 93	0
32	BH	174/180 (96%)	1.34	31 (17%) 4 3	49, 65, 77, 81	0
32	DH	174/180 (96%)	1.32	33 (18%) 3 2	52, 70, 80, 84	0
33	BI	146/148 (98%)	1.50	32 (21%) 2 2	47, 81, 90, 95	0
33	DI	146/148 (98%)	3.16	100 (68%) 0 0	46, 84, 94, 99	0
34	BN	140/140 (100%)	0.70	10 (7%) 22 16	29, 49, 72, 82	0
34	DN	140/140 (100%)	0.71	2 (1%) 73 64	33, 53, 74, 83	0
35	BO	122/122 (100%)	0.24	4 (3%) 49 39	26, 42, 61, 65	0
35	DO	122/122 (100%)	0.72	4 (3%) 49 39	36, 57, 70, 79	0
36	BP	149/150 (99%)	0.65	6 (4%) 42 33	25, 52, 76, 85	0
36	DP	149/150 (99%)	0.79	7 (4%) 36 29	28, 54, 78, 86	0
37	BQ	141/141 (100%)	0.75	9 (6%) 25 18	29, 51, 65, 78	0
37	DQ	141/141 (100%)	0.95	15 (10%) 11 8	31, 55, 69, 79	0
38	BR	118/118 (100%)	0.02	0 100 100	23, 37, 56, 63	0
38	DR	118/118 (100%)	0.41	0 100 100	31, 50, 64, 71	0
39	BS	110/112 (98%)	0.43	4 (3%) 46 37	33, 51, 63, 76	0
39	DS	110/112 (98%)	1.78	39 (35%) 1 0	55, 76, 86, 89	0
40	BT	131/146 (89%)	0.38	7 (5%) 32 24	27, 44, 73, 86	0
40	DT	131/146 (89%)	0.95	10 (7%) 20 14	42, 59, 78, 86	0
41	BU	116/118 (98%)	-0.13	1 (0%) 81 74	18, 32, 52, 73	0
41	DU	116/118 (98%)	0.59	2 (1%) 69 60	37, 58, 75, 80	0
42	BV	101/101 (100%)	0.12	1 (0%) 79 72	20, 42, 61, 76	0
42	DV	101/101 (100%)	0.75	6 (5%) 28 21	36, 67, 81, 87	0
43	BW	112/113 (99%)	-0.17	0 100 100	20, 33, 51, 84	0
43	DW	112/113 (99%)	0.38	2 (1%) 67 58	32, 47, 65, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.02	1 (1%) 78 70	22, 37, 57, 82	0
44	DX	95/96 (98%)	0.79	9 (9%) 14 10	39, 59, 73, 82	0
45	BY	107/110 (97%)	0.52	2 (1%) 66 57	32, 48, 70, 81	0
45	DY	107/110 (97%)	1.14	12 (11%) 10 7	48, 68, 78, 89	0
46	BZ	171/206 (83%)	0.92	17 (9%) 13 9	40, 63, 83, 88	0
46	DZ	174/206 (84%)	1.75	62 (35%) 1 0	64, 82, 94, 97	0
47	B0	83/85 (97%)	0.13	1 (1%) 76 68	23, 38, 52, 66	0
47	D0	83/85 (97%)	1.17	13 (15%) 5 4	36, 61, 72, 81	0
48	B1	97/98 (98%)	0.34	4 (4%) 41 33	21, 42, 65, 74	0
48	D1	97/98 (98%)	0.83	9 (9%) 14 10	30, 54, 76, 82	0
49	B2	70/72 (97%)	0.36	2 (2%) 53 43	32, 48, 63, 87	0
49	D2	70/72 (97%)	0.76	3 (4%) 40 31	50, 67, 78, 83	0
50	B3	59/60 (98%)	0.06	1 (1%) 69 60	21, 37, 62, 81	0
50	D3	59/60 (98%)	0.72	3 (5%) 33 25	44, 60, 77, 87	0
51	B4	69/71 (97%)	1.29	17 (24%) 2 1	54, 76, 90, 98	0
51	D4	69/71 (97%)	1.97	26 (37%) 1 0	80, 90, 95, 99	0
52	B5	59/60 (98%)	-0.17	1 (1%) 69 60	19, 33, 53, 65	0
52	D5	59/60 (98%)	0.40	0 100 100	28, 48, 69, 72	0
53	B6	53/54 (98%)	-0.15	0 100 100	28, 40, 60, 64	0
53	D6	53/54 (98%)	0.90	3 (5%) 29 22	43, 59, 72, 82	0
54	B7	48/49 (97%)	-0.10	1 (2%) 63 54	18, 25, 54, 63	0
54	D7	48/49 (97%)	0.24	2 (4%) 40 32	29, 39, 63, 81	0
55	B8	64/65 (98%)	0.05	1 (1%) 70 61	23, 32, 46, 61	0
55	D8	64/65 (98%)	0.69	1 (1%) 70 61	37, 55, 66, 70	0
56	B9	37/37 (100%)	0.83	3 (8%) 18 13	27, 49, 67, 71	0
56	D9	37/37 (100%)	1.20	5 (13%) 7 5	46, 54, 67, 74	0
All	All	20640/21602 (95%)	0.84	2690 (13%) 7 6	18, 63, 89, 107	0

The worst 5 of 2690 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DI	65	ALA	8.9
9	CI	126	SER	8.6

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Mol	Chain	Res	Type	RSRZ
33	DI	111	PRO	8.3
7	AG	79	ARG	8.1
33	DI	96	ASP	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
24	5MC	CX	32	21/22	0.79	0.18	68,80,88,99	0
24	4SU	CX	8	20/21	0.84	0.14	61,80,93,118	0
24	5MU	CX	54	21/22	0.85	0.14	71,79,92,107	0
24	PSU	CX	55	20/21	0.85	0.12	61,72,81,89	0
24	PSU	AX	55	20/21	0.87	0.14	58,70,77,82	0
24	5MU	AX	54	21/22	0.89	0.14	57,67,82,96	0
24	31H	CX	76	32/33	0.92	0.15	23,42,61,84	10
24	4SU	AX	8	20/21	0.93	0.11	47,59,67,84	0
24	5MC	AX	32	21/22	0.94	0.12	46,55,75,77	0
24	31H	AX	76	30/33	0.95	0.14	14,31,55,77	8
23	PPU	CW	76	37/38	0.96	0.10	27,41,53,63	0
23	PPU	AW	76	37/38	0.97	0.09	12,29,37,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	DA	3553	1/1	0.17	0.34	75,75,75,75	0
57	MG	CA	3148	1/1	0.26	0.29	81,81,81,81	0
57	MG	BA	3502	1/1	0.45	0.23	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3175	1/1	0.49	0.24	55,55,55,55	0
57	MG	CA	3023	1/1	0.53	0.26	88,88,88,88	0
57	MG	CA	3129	1/1	0.54	0.35	83,83,83,83	0
57	MG	CA	3062	1/1	0.55	0.43	73,73,73,73	0
57	MG	AA	3166	1/1	0.55	0.21	70,70,70,70	0
57	MG	DA	3555	1/1	0.59	0.28	70,70,70,70	0
57	MG	CA	3116	1/1	0.60	0.21	74,74,74,74	0
57	MG	DA	3160	1/1	0.60	0.24	65,65,65,65	0
57	MG	CA	3060	1/1	0.61	0.30	78,78,78,78	0
57	MG	CA	3107	1/1	0.61	0.36	89,89,89,89	0
57	MG	CA	3106	1/1	0.62	0.21	65,65,65,65	0
57	MG	CA	3094	1/1	0.63	0.34	80,80,80,80	0
57	MG	AA	3080	1/1	0.63	0.35	82,82,82,82	0
57	MG	CA	3085	1/1	0.63	0.38	71,71,71,71	0
57	MG	DA	3491	1/1	0.64	0.21	43,43,43,43	0
57	MG	AA	3109	1/1	0.64	0.30	75,75,75,75	0
57	MG	CA	3082	1/1	0.64	0.27	71,71,71,71	0
57	MG	BA	3651	1/1	0.65	0.28	62,62,62,62	0
57	MG	CA	3158	1/1	0.65	0.28	66,66,66,66	0
57	MG	AA	3063	1/1	0.66	0.22	89,89,89,89	0
57	MG	CA	3120	1/1	0.66	0.35	72,72,72,72	0
57	MG	BA	3487	1/1	0.66	0.27	70,70,70,70	0
57	MG	DA	3595	1/1	0.66	0.15	65,65,65,65	0
57	MG	BA	3113	1/1	0.68	0.17	57,57,57,57	0
57	MG	CA	3139	1/1	0.68	0.20	82,82,82,82	0
57	MG	CA	3126	1/1	0.68	0.28	73,73,73,73	0
57	MG	AA	3014	1/1	0.69	0.23	73,73,73,73	0
57	MG	AX	3011	1/1	0.69	0.39	73,73,73,73	0
57	MG	DA	3565	1/1	0.69	0.23	49,49,49,49	0
57	MG	AA	3146	1/1	0.69	0.19	81,81,81,81	0
57	MG	BA	3091	1/1	0.70	0.17	56,56,56,56	0
57	MG	CA	3030	1/1	0.70	0.30	75,75,75,75	0
57	MG	DA	3609	1/1	0.70	0.24	55,55,55,55	0
57	MG	AA	3198	1/1	0.71	0.15	66,66,66,66	0
57	MG	AA	3069	1/1	0.71	0.29	75,75,75,75	0
57	MG	AA	3145	1/1	0.71	0.40	71,71,71,71	0
57	MG	DA	3374	1/1	0.71	0.15	42,42,42,42	0
57	MG	CA	3119	1/1	0.71	0.18	74,74,74,74	0
57	MG	DA	3533	1/1	0.72	0.30	47,47,47,47	0
57	MG	DA	3547	1/1	0.72	0.28	68,68,68,68	0
57	MG	DA	3548	1/1	0.72	0.14	58,58,58,58	0
57	MG	BA	3674	1/1	0.72	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3004	1/1	0.72	0.16	70,70,70,70	0
57	MG	DA	3303	1/1	0.72	0.20	57,57,57,57	0
57	MG	AA	3056	1/1	0.72	0.26	66,66,66,66	0
57	MG	CA	3152	1/1	0.72	0.21	66,66,66,66	0
57	MG	DB	3002	1/1	0.72	0.25	75,75,75,75	0
57	MG	DA	3162	1/1	0.74	0.27	58,58,58,58	0
57	MG	AA	3018	1/1	0.74	0.19	62,62,62,62	0
57	MG	DA	3001	1/1	0.74	0.22	45,45,45,45	0
57	MG	DA	3550	1/1	0.74	0.26	63,63,63,63	0
57	MG	CA	3154	1/1	0.74	0.32	68,68,68,68	0
57	MG	DR	3001	1/1	0.74	0.52	66,66,66,66	0
57	MG	AA	3064	1/1	0.75	0.23	65,65,65,65	0
57	MG	BA	3610	1/1	0.75	0.27	60,60,60,60	0
57	MG	CA	3113	1/1	0.75	0.23	75,75,75,75	0
57	MG	AA	3046	1/1	0.75	0.33	72,72,72,72	0
57	MG	DB	3008	1/1	0.75	0.15	59,59,59,59	0
57	MG	AA	3132	1/1	0.75	0.26	67,67,67,67	0
57	MG	DV	202	1/1	0.75	0.26	75,75,75,75	0
57	MG	D8	101	1/1	0.75	0.31	60,60,60,60	0
57	MG	BA	3625	1/1	0.76	0.16	46,46,46,46	0
57	MG	CA	3059	1/1	0.76	0.26	60,60,60,60	0
57	MG	AA	3123	1/1	0.76	0.27	59,59,59,59	0
57	MG	DA	3304	1/1	0.76	0.16	44,44,44,44	0
57	MG	DA	3608	1/1	0.76	0.18	61,61,61,61	0
57	MG	AA	3054	1/1	0.76	0.30	62,62,62,62	0
57	MG	BA	3519	1/1	0.76	0.15	26,26,26,26	0
57	MG	CA	3017	1/1	0.76	0.31	69,69,69,69	0
57	MG	BA	3470	1/1	0.76	0.16	69,69,69,69	0
57	MG	DA	3134	1/1	0.76	0.28	59,59,59,59	0
57	MG	DA	3135	1/1	0.76	0.26	61,61,61,61	0
57	MG	DA	3158	1/1	0.77	0.11	52,52,52,52	0
57	MG	BA	3577	1/1	0.77	0.24	35,35,35,35	0
57	MG	BA	3587	1/1	0.77	0.21	51,51,51,51	0
57	MG	CA	3098	1/1	0.77	0.16	76,76,76,76	0
57	MG	CA	3155	1/1	0.77	0.25	66,66,66,66	0
57	MG	DA	3342	1/1	0.77	0.16	49,49,49,49	0
57	MG	CA	3020	1/1	0.77	0.11	51,51,51,51	0
57	MG	DA	3390	1/1	0.77	0.21	54,54,54,54	0
57	MG	AA	3160	1/1	0.77	0.21	58,58,58,58	0
57	MG	DA	3003	1/1	0.77	0.12	56,56,56,56	0
57	MG	CA	3134	1/1	0.77	0.14	72,72,72,72	0
57	MG	CA	3027	1/1	0.77	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BG	3002	1/1	0.78	0.14	65,65,65,65	0
57	MG	CA	3042	1/1	0.78	0.29	68,68,68,68	0
57	MG	BA	3595	1/1	0.78	0.26	52,52,52,52	0
57	MG	DA	3610	1/1	0.78	0.18	42,42,42,42	0
57	MG	CX	3002	1/1	0.78	0.37	75,75,75,75	0
57	MG	BA	3416	1/1	0.78	0.15	73,73,73,73	0
57	MG	BA	3425	1/1	0.78	0.15	28,28,28,28	0
57	MG	AA	3127	1/1	0.78	0.25	73,73,73,73	0
57	MG	BA	3413	1/1	0.78	0.13	50,50,50,50	0
57	MG	DA	3417	1/1	0.79	0.20	46,46,46,46	0
57	MG	DA	3426	1/1	0.79	0.28	38,38,38,38	0
57	MG	DA	3439	1/1	0.79	0.12	44,44,44,44	0
57	MG	DA	3458	1/1	0.79	0.11	44,44,44,44	0
57	MG	BA	3630	1/1	0.79	0.29	72,72,72,72	0
57	MG	CA	3117	1/1	0.79	0.17	100,100,100,100	0
57	MG	BA	3412	1/1	0.79	0.27	44,44,44,44	0
57	MG	AA	3193	1/1	0.79	0.40	77,77,77,77	0
57	MG	BA	3533	1/1	0.79	0.23	45,45,45,45	0
57	MG	DA	3142	1/1	0.79	0.23	50,50,50,50	0
57	MG	BZ	3001	1/1	0.79	0.15	56,56,56,56	0
57	MG	CA	3084	1/1	0.79	0.27	58,58,58,58	0
57	MG	AA	3041	1/1	0.79	0.26	62,62,62,62	0
57	MG	DA	3601	1/1	0.79	0.16	43,43,43,43	0
57	MG	DA	3276	1/1	0.79	0.12	56,56,56,56	0
57	MG	DA	3291	1/1	0.79	0.18	56,56,56,56	0
57	MG	DA	3297	1/1	0.79	0.17	48,48,48,48	0
57	MG	BA	3579	1/1	0.79	0.16	44,44,44,44	0
57	MG	AA	3001	1/1	0.79	0.24	72,72,72,72	0
57	MG	BA	3235	1/1	0.79	0.15	52,52,52,52	0
57	MG	BA	3482	1/1	0.79	0.13	56,56,56,56	0
57	MG	BA	3281	1/1	0.79	0.14	46,46,46,46	0
57	MG	CA	3135	1/1	0.80	0.26	85,85,85,85	0
57	MG	DA	3461	1/1	0.80	0.20	55,55,55,55	0
57	MG	BA	3467	1/1	0.80	0.22	51,51,51,51	0
57	MG	DA	3509	1/1	0.80	0.23	42,42,42,42	0
57	MG	CA	3035	1/1	0.80	0.26	63,63,63,63	0
57	MG	DA	3193	1/1	0.80	0.16	43,43,43,43	0
57	MG	DA	3204	1/1	0.80	0.17	39,39,39,39	0
57	MG	DA	3223	1/1	0.80	0.24	56,56,56,56	0
57	MG	BF	309	1/1	0.80	0.15	61,61,61,61	0
57	MG	DA	3280	1/1	0.80	0.21	49,49,49,49	0
57	MG	BA	3604	1/1	0.80	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3569	1/1	0.80	0.13	42,42,42,42	0
57	MG	BA	3207	1/1	0.80	0.17	55,55,55,55	0
57	MG	AA	3068	1/1	0.80	0.18	64,64,64,64	0
57	MG	CA	3081	1/1	0.80	0.16	67,67,67,67	0
57	MG	DA	3328	1/1	0.80	0.16	66,66,66,66	0
57	MG	AA	3125	1/1	0.80	0.21	60,60,60,60	0
57	MG	DA	3615	1/1	0.80	0.12	36,36,36,36	0
57	MG	DA	3625	1/1	0.80	0.20	57,57,57,57	0
57	MG	BA	3631	1/1	0.80	0.15	53,53,53,53	0
57	MG	DA	3125	1/1	0.80	0.15	48,48,48,48	0
57	MG	CA	3127	1/1	0.80	0.33	76,76,76,76	0
57	MG	BA	3374	1/1	0.80	0.16	48,48,48,48	0
57	MG	BA	3656	1/1	0.80	0.20	57,57,57,57	0
57	MG	DA	3208	1/1	0.81	0.16	50,50,50,50	0
57	MG	BA	3598	1/1	0.81	0.18	54,54,54,54	0
57	MG	AX	3003	1/1	0.81	0.30	66,66,66,66	0
57	MG	BA	3530	1/1	0.81	0.18	20,20,20,20	0
57	MG	AA	3113	1/1	0.81	0.32	54,54,54,54	0
57	MG	CA	3008	1/1	0.81	0.41	67,67,67,67	0
57	MG	BA	3535	1/1	0.81	0.16	29,29,29,29	0
57	MG	DA	3064	1/1	0.81	0.16	52,52,52,52	0
57	MG	DA	3308	1/1	0.81	0.15	52,52,52,52	0
57	MG	DA	3314	1/1	0.81	0.17	56,56,56,56	0
57	MG	DA	3596	1/1	0.81	0.21	71,71,71,71	0
57	MG	DA	3087	1/1	0.81	0.23	65,65,65,65	0
57	MG	CA	3019	1/1	0.81	0.17	57,57,57,57	0
57	MG	AA	3180	1/1	0.81	0.10	61,61,61,61	0
57	MG	CA	3133	1/1	0.81	0.27	69,69,69,69	0
57	MG	DA	3409	1/1	0.81	0.18	70,70,70,70	0
57	MG	CA	3091	1/1	0.81	0.26	75,75,75,75	0
57	MG	AA	3150	1/1	0.81	0.20	65,65,65,65	0
57	MG	AA	3090	1/1	0.81	0.22	70,70,70,70	0
57	MG	CA	3146	1/1	0.81	0.22	74,74,74,74	0
57	MG	AF	3001	1/1	0.81	0.14	58,58,58,58	0
57	MG	BA	3700	1/1	0.81	0.41	69,69,69,69	0
57	MG	AX	3002	1/1	0.82	0.20	67,67,67,67	0
57	MG	DA	3447	1/1	0.82	0.16	48,48,48,48	0
57	MG	CA	3051	1/1	0.82	0.25	57,57,57,57	0
57	MG	CA	3053	1/1	0.82	0.26	59,59,59,59	0
57	MG	DA	3182	1/1	0.82	0.43	52,52,52,52	0
57	MG	BA	3263	1/1	0.82	0.28	50,50,50,50	0
57	MG	AA	3122	1/1	0.82	0.22	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3543	1/1	0.82	0.22	61,61,61,61	0
57	MG	BA	3350	1/1	0.82	0.11	43,43,43,43	0
57	MG	CA	3078	1/1	0.82	0.21	63,63,63,63	0
57	MG	DA	3252	1/1	0.82	0.12	63,63,63,63	0
57	MG	BB	3020	1/1	0.82	0.14	55,55,55,55	0
57	MG	BA	3351	1/1	0.82	0.12	62,62,62,62	0
57	MG	BA	3372	1/1	0.82	0.16	58,58,58,58	0
57	MG	AA	3134	1/1	0.82	0.15	59,59,59,59	0
57	MG	AA	3151	1/1	0.82	0.21	72,72,72,72	0
57	MG	BA	3105	1/1	0.82	0.17	45,45,45,45	0
57	MG	AA	3085	1/1	0.82	0.31	69,69,69,69	0
57	MG	DA	3602	1/1	0.82	0.20	50,50,50,50	0
57	MG	AA	3163	1/1	0.82	0.19	70,70,70,70	0
57	MG	BA	3204	1/1	0.82	0.24	61,61,61,61	0
57	MG	AN	502	1/1	0.82	0.16	61,61,61,61	0
57	MG	CA	3115	1/1	0.82	0.15	59,59,59,59	0
57	MG	DA	3624	1/1	0.82	0.21	66,66,66,66	0
57	MG	DA	3380	1/1	0.82	0.21	65,65,65,65	0
57	MG	BA	3216	1/1	0.82	0.13	35,35,35,35	0
57	MG	BA	3220	1/1	0.82	0.35	54,54,54,54	0
57	MG	DA	3412	1/1	0.82	0.15	60,60,60,60	0
57	MG	BA	3636	1/1	0.82	0.24	45,45,45,45	0
57	MG	DW	201	1/1	0.82	0.22	70,70,70,70	0
57	MG	CA	3038	1/1	0.82	0.12	68,68,68,68	0
57	MG	BA	3303	1/1	0.83	0.15	39,39,39,39	0
57	MG	DA	3499	1/1	0.83	0.10	47,47,47,47	0
57	MG	CA	3006	1/1	0.83	0.10	43,43,43,43	0
57	MG	CA	3140	1/1	0.83	0.15	48,48,48,48	0
57	MG	BA	3611	1/1	0.83	0.21	61,61,61,61	0
57	MG	DA	3544	1/1	0.83	0.15	59,59,59,59	0
57	MG	BA	3136	1/1	0.83	0.14	56,56,56,56	0
57	MG	BA	3514	1/1	0.83	0.24	36,36,36,36	0
57	MG	BA	3003	1/1	0.83	0.09	44,44,44,44	0
57	MG	BA	3634	1/1	0.83	0.18	58,58,58,58	0
57	MG	DA	3554	1/1	0.83	0.10	46,46,46,46	0
57	MG	CA	3105	1/1	0.83	0.27	76,76,76,76	0
57	MG	BA	3178	1/1	0.83	0.23	52,52,52,52	0
57	MG	BA	3639	1/1	0.83	0.12	46,46,46,46	0
57	MG	DA	3576	1/1	0.83	0.22	46,46,46,46	0
57	MG	BA	3011	1/1	0.83	0.13	32,32,32,32	0
57	MG	DA	3017	1/1	0.83	0.29	58,58,58,58	0
57	MG	DA	3059	1/1	0.83	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3064	1/1	0.83	0.14	38,38,38,38	0
57	MG	DA	3356	1/1	0.83	0.15	53,53,53,53	0
57	MG	BA	3066	1/1	0.83	0.29	53,53,53,53	0
57	MG	DA	3112	1/1	0.83	0.23	63,63,63,63	0
57	MG	CA	3043	1/1	0.83	0.30	68,68,68,68	0
57	MG	CA	3044	1/1	0.83	0.11	59,59,59,59	0
57	MG	BA	3688	1/1	0.83	0.20	46,46,46,46	0
57	MG	AA	3061	1/1	0.83	0.20	65,65,65,65	0
57	MG	BA	3221	1/1	0.83	0.34	59,59,59,59	0
57	MG	DO	5001	1/1	0.83	0.19	53,53,53,53	0
57	MG	AA	3066	1/1	0.83	0.14	66,66,66,66	0
57	MG	BA	3109	1/1	0.83	0.15	53,53,53,53	0
57	MG	AA	3006	1/1	0.83	0.12	62,62,62,62	0
57	MG	DA	3189	1/1	0.83	0.15	57,57,57,57	0
57	MG	AA	3011	1/1	0.84	0.12	67,67,67,67	0
57	MG	DA	3437	1/1	0.84	0.18	48,48,48,48	0
57	MG	CA	3005	1/1	0.84	0.24	81,81,81,81	0
57	MG	AA	3196	1/1	0.84	0.17	60,60,60,60	0
57	MG	BA	3266	1/1	0.84	0.24	53,53,53,53	0
57	MG	AA	3171	1/1	0.84	0.17	45,45,45,45	0
57	MG	CA	3110	1/1	0.84	0.18	56,56,56,56	0
57	MG	DA	3493	1/1	0.84	0.17	53,53,53,53	0
57	MG	AA	3199	1/1	0.84	0.17	58,58,58,58	0
57	MG	CA	3114	1/1	0.84	0.22	96,96,96,96	0
57	MG	DA	3526	1/1	0.84	0.11	41,41,41,41	0
57	MG	BA	3323	1/1	0.84	0.16	59,59,59,59	0
57	MG	BA	3347	1/1	0.84	0.19	32,32,32,32	0
57	MG	AA	3205	1/1	0.84	0.18	48,48,48,48	0
57	MG	BA	3032	1/1	0.84	0.17	30,30,30,30	0
57	MG	BA	3644	1/1	0.84	0.25	48,48,48,48	0
57	MG	CA	3125	1/1	0.84	0.14	64,64,64,64	0
57	MG	BA	3649	1/1	0.84	0.18	65,65,65,65	0
57	MG	BA	3359	1/1	0.84	0.14	56,56,56,56	0
57	MG	BA	3060	1/1	0.84	0.22	59,59,59,59	0
57	MG	BA	3671	1/1	0.84	0.21	55,55,55,55	0
57	MG	DA	3277	1/1	0.84	0.32	50,50,50,50	0
57	MG	AE	3001	1/1	0.84	0.12	85,85,85,85	0
57	MG	AA	3175	1/1	0.84	0.35	61,61,61,61	0
57	MG	CA	3055	1/1	0.84	0.20	66,66,66,66	0
57	MG	CA	3058	1/1	0.84	0.44	70,70,70,70	0
57	MG	BA	3585	1/1	0.84	0.12	45,45,45,45	0
57	MG	BB	3019	1/1	0.84	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3061	1/1	0.84	0.16	87,87,87,87	0
57	MG	BA	3088	1/1	0.84	0.30	59,59,59,59	0
57	MG	DA	3337	1/1	0.84	0.15	46,46,46,46	0
57	MG	DA	3619	1/1	0.84	0.23	63,63,63,63	0
57	MG	BA	3590	1/1	0.84	0.30	62,62,62,62	0
57	MG	AA	3043	1/1	0.84	0.28	59,59,59,59	0
57	MG	DA	3628	1/1	0.84	0.26	59,59,59,59	0
57	MG	CK	3001	1/1	0.84	0.20	57,57,57,57	0
57	MG	BN	3002	1/1	0.84	0.12	46,46,46,46	0
57	MG	DD	307	1/1	0.84	0.11	50,50,50,50	0
57	MG	BW	202	1/1	0.84	0.43	41,41,41,41	0
57	MG	BA	3419	1/1	0.84	0.29	58,58,58,58	0
57	MG	CA	3090	1/1	0.84	0.35	64,64,64,64	0
57	MG	CA	3003	1/1	0.84	0.17	74,74,74,74	0
57	MG	DA	3419	1/1	0.84	0.15	37,37,37,37	0
57	MG	BA	3222	1/1	0.85	0.14	52,52,52,52	0
57	MG	CA	3014	1/1	0.85	0.19	58,58,58,58	0
57	MG	DA	3381	1/1	0.85	0.24	55,55,55,55	0
57	MG	CA	3015	1/1	0.85	0.21	61,61,61,61	0
57	MG	DA	3069	1/1	0.85	0.35	59,59,59,59	0
57	MG	DA	3411	1/1	0.85	0.14	51,51,51,51	0
57	MG	DA	3074	1/1	0.85	0.18	38,38,38,38	0
57	MG	DA	3076	1/1	0.85	0.20	53,53,53,53	0
57	MG	AA	3114	1/1	0.85	0.31	57,57,57,57	0
57	MG	DA	3425	1/1	0.85	0.14	40,40,40,40	0
57	MG	DA	3111	1/1	0.85	0.15	54,54,54,54	0
57	MG	BA	3380	1/1	0.85	0.14	55,55,55,55	0
57	MG	DA	3117	1/1	0.85	0.10	40,40,40,40	0
57	MG	DA	3446	1/1	0.85	0.17	37,37,37,37	0
57	MG	BA	3540	1/1	0.85	0.13	24,24,24,24	0
57	MG	DA	3455	1/1	0.85	0.16	34,34,34,34	0
57	MG	BA	3543	1/1	0.85	0.14	69,69,69,69	0
57	MG	BA	3567	1/1	0.85	0.16	55,55,55,55	0
57	MG	BA	3241	1/1	0.85	0.30	53,53,53,53	0
57	MG	DA	3144	1/1	0.85	0.09	48,48,48,48	0
57	MG	AA	3093	1/1	0.85	0.29	56,56,56,56	0
57	MG	BA	3672	1/1	0.85	0.13	28,28,28,28	0
57	MG	CA	3041	1/1	0.85	0.23	62,62,62,62	0
57	MG	DA	3527	1/1	0.85	0.14	52,52,52,52	0
57	MG	DA	3168	1/1	0.85	0.29	50,50,50,50	0
57	MG	BA	3584	1/1	0.85	0.15	59,59,59,59	0
57	MG	DA	3187	1/1	0.85	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3683	1/1	0.85	0.17	44,44,44,44	0
57	MG	DA	3191	1/1	0.85	0.12	54,54,54,54	0
57	MG	BA	3155	1/1	0.85	0.20	44,44,44,44	0
57	MG	BA	3692	1/1	0.85	0.31	64,64,64,64	0
57	MG	AA	3133	1/1	0.85	0.20	59,59,59,59	0
57	MG	DA	3217	1/1	0.85	0.27	50,50,50,50	0
57	MG	BB	3008	1/1	0.85	0.15	60,60,60,60	0
57	MG	DA	3248	1/1	0.85	0.09	59,59,59,59	0
57	MG	AA	3189	1/1	0.85	0.17	69,69,69,69	0
57	MG	DA	3256	1/1	0.85	0.18	52,52,52,52	0
57	MG	DA	3259	1/1	0.85	0.09	39,39,39,39	0
57	MG	AA	3155	1/1	0.85	0.18	65,65,65,65	0
57	MG	BA	3328	1/1	0.85	0.13	55,55,55,55	0
57	MG	BA	3602	1/1	0.85	0.36	65,65,65,65	0
57	MG	DA	3283	1/1	0.85	0.12	40,40,40,40	0
57	MG	BA	3474	1/1	0.85	0.16	64,64,64,64	0
57	MG	CA	3071	1/1	0.85	0.30	49,49,49,49	0
57	MG	CA	3075	1/1	0.85	0.14	48,48,48,48	0
57	MG	BA	3337	1/1	0.85	0.17	51,51,51,51	0
57	MG	DA	3307	1/1	0.85	0.21	51,51,51,51	0
57	MG	AA	3004	1/1	0.85	0.38	61,61,61,61	0
57	MG	DA	3312	1/1	0.85	0.17	30,30,30,30	0
57	MG	DB	3005	1/1	0.85	0.24	54,54,54,54	0
57	MG	BA	3615	1/1	0.85	0.13	60,60,60,60	0
57	MG	DA	3319	1/1	0.85	0.26	45,45,45,45	0
57	MG	AX	3008	1/1	0.85	0.09	58,58,58,58	0
57	MG	AA	3137	1/1	0.85	0.46	66,66,66,66	0
57	MG	AA	3065	1/1	0.85	0.13	48,48,48,48	0
57	MG	DA	3353	1/1	0.85	0.14	42,42,42,42	0
57	MG	CA	3007	1/1	0.85	0.19	55,55,55,55	0
57	MG	DA	3457	1/1	0.86	0.14	45,45,45,45	0
57	MG	DA	3271	1/1	0.86	0.20	47,47,47,47	0
57	MG	AA	3142	1/1	0.86	0.27	53,53,53,53	0
57	MG	DA	3472	1/1	0.86	0.11	24,24,24,24	0
57	MG	DA	3481	1/1	0.86	0.17	69,69,69,69	0
57	MG	BA	3492	1/1	0.86	0.10	30,30,30,30	0
57	MG	DA	3066	1/1	0.86	0.09	55,55,55,55	0
57	MG	BA	3415	1/1	0.86	0.16	61,61,61,61	0
57	MG	AA	3170	1/1	0.86	0.15	70,70,70,70	0
57	MG	DA	3520	1/1	0.86	0.13	51,51,51,51	0
57	MG	BA	3107	1/1	0.86	0.25	49,49,49,49	0
57	MG	BA	3597	1/1	0.86	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3525	1/1	0.86	0.15	49,49,49,49	0
57	MG	BA	3666	1/1	0.86	0.16	79,79,79,79	0
57	MG	BA	3600	1/1	0.86	0.25	59,59,59,59	0
57	MG	AA	3126	1/1	0.86	0.15	52,52,52,52	0
57	MG	BA	3603	1/1	0.86	0.15	42,42,42,42	0
57	MG	BA	3679	1/1	0.86	0.10	38,38,38,38	0
57	MG	DA	3322	1/1	0.86	0.11	51,51,51,51	0
57	MG	BA	3426	1/1	0.86	0.14	30,30,30,30	0
57	MG	BA	3429	1/1	0.86	0.12	37,37,37,37	0
57	MG	DA	3561	1/1	0.86	0.14	51,51,51,51	0
57	MG	DA	3148	1/1	0.86	0.16	45,45,45,45	0
57	MG	DA	3346	1/1	0.86	0.11	39,39,39,39	0
57	MG	DA	3571	1/1	0.86	0.12	54,54,54,54	0
57	MG	BA	3451	1/1	0.86	0.16	59,59,59,59	0
57	MG	DA	3592	1/1	0.86	0.16	62,62,62,62	0
57	MG	CA	3025	1/1	0.86	0.17	66,66,66,66	0
57	MG	DA	3366	1/1	0.86	0.14	40,40,40,40	0
57	MG	DA	3370	1/1	0.86	0.24	72,72,72,72	0
57	MG	BA	3613	1/1	0.86	0.19	74,74,74,74	0
57	MG	CA	3147	1/1	0.86	0.14	56,56,56,56	0
57	MG	CA	3029	1/1	0.86	0.11	48,48,48,48	0
57	MG	AA	3047	1/1	0.86	0.14	59,59,59,59	0
57	MG	AA	3178	1/1	0.86	0.23	67,67,67,67	0
57	MG	DA	3410	1/1	0.86	0.13	37,37,37,37	0
57	MG	CA	3099	1/1	0.86	0.17	50,50,50,50	0
57	MG	CA	3102	1/1	0.86	0.14	56,56,56,56	0
57	MG	CJ	5001	1/1	0.86	0.07	51,51,51,51	0
57	MG	BA	3628	1/1	0.86	0.18	60,60,60,60	0
57	MG	BD	311	1/1	0.86	0.14	60,60,60,60	0
57	MG	DA	3220	1/1	0.86	0.19	54,54,54,54	0
57	MG	AA	3201	1/1	0.86	0.26	68,68,68,68	0
57	MG	DG	3001	1/1	0.86	0.08	49,49,49,49	0
57	MG	AA	3106	1/1	0.86	0.25	53,53,53,53	0
57	MG	DA	3443	1/1	0.86	0.13	27,27,27,27	0
57	MG	CA	3111	1/1	0.86	0.18	65,65,65,65	0
57	MG	DA	3043	1/1	0.86	0.14	44,44,44,44	0
57	MG	DA	3051	1/1	0.86	0.11	54,54,54,54	0
57	MG	BA	3052	1/1	0.87	0.23	44,44,44,44	0
57	MG	CA	3066	1/1	0.87	0.30	69,69,69,69	0
57	MG	DA	3444	1/1	0.87	0.15	37,37,37,37	0
57	MG	CA	3067	1/1	0.87	0.17	45,45,45,45	0
57	MG	CA	3068	1/1	0.87	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3453	1/1	0.87	0.13	44,44,44,44	0
57	MG	AA	3124	1/1	0.87	0.34	58,58,58,58	0
57	MG	DA	3456	1/1	0.87	0.30	59,59,59,59	0
57	MG	DA	3219	1/1	0.87	0.12	54,54,54,54	0
57	MG	BA	3549	1/1	0.87	0.22	55,55,55,55	0
57	MG	CA	3153	1/1	0.87	0.33	57,57,57,57	0
57	MG	DA	3226	1/1	0.87	0.26	54,54,54,54	0
57	MG	BA	3565	1/1	0.87	0.12	50,50,50,50	0
57	MG	BA	3316	1/1	0.87	0.21	49,49,49,49	0
57	MG	CA	3012	1/1	0.87	0.27	45,45,45,45	0
57	MG	DA	3495	1/1	0.87	0.10	48,48,48,48	0
57	MG	CE	3001	1/1	0.87	0.14	80,80,80,80	0
57	MG	DA	3260	1/1	0.87	0.11	43,43,43,43	0
57	MG	DA	3519	1/1	0.87	0.18	60,60,60,60	0
57	MG	BA	3061	1/1	0.87	0.17	58,58,58,58	0
57	MG	DA	3521	1/1	0.87	0.12	57,57,57,57	0
57	MG	BA	3199	1/1	0.87	0.27	60,60,60,60	0
57	MG	BA	3652	1/1	0.87	0.18	65,65,65,65	0
57	MG	AA	3188	1/1	0.87	0.12	62,62,62,62	0
57	MG	DA	3537	1/1	0.87	0.12	45,45,45,45	0
57	MG	DA	3539	1/1	0.87	0.21	52,52,52,52	0
57	MG	CA	3092	1/1	0.87	0.17	76,76,76,76	0
57	MG	BA	3454	1/1	0.87	0.10	45,45,45,45	0
57	MG	DA	3027	1/1	0.87	0.09	42,42,42,42	0
57	MG	DA	3038	1/1	0.87	0.12	39,39,39,39	0
57	MG	CA	3021	1/1	0.87	0.11	46,46,46,46	0
57	MG	CA	3022	1/1	0.87	0.27	55,55,55,55	0
57	MG	BA	3465	1/1	0.87	0.17	44,44,44,44	0
57	MG	BA	3344	1/1	0.87	0.19	48,48,48,48	0
57	MG	CA	3026	1/1	0.87	0.17	59,59,59,59	0
57	MG	AA	3008	1/1	0.87	0.19	65,65,65,65	0
57	MG	CA	3028	1/1	0.87	0.26	57,57,57,57	0
57	MG	BA	3349	1/1	0.87	0.13	55,55,55,55	0
57	MG	BA	3480	1/1	0.87	0.22	50,50,50,50	0
57	MG	DA	3584	1/1	0.87	0.17	63,63,63,63	0
57	MG	DA	3591	1/1	0.87	0.12	69,69,69,69	0
57	MG	DA	3090	1/1	0.87	0.12	52,52,52,52	0
57	MG	AA	3156	1/1	0.87	0.24	86,86,86,86	0
57	MG	BA	3002	1/1	0.87	0.18	45,45,45,45	0
57	MG	AA	3075	1/1	0.87	0.13	57,57,57,57	0
57	MG	AA	3040	1/1	0.87	0.29	67,67,67,67	0
57	MG	DA	3606	1/1	0.87	0.25	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3607	1/1	0.87	0.21	73,73,73,73	0
57	MG	DA	3130	1/1	0.87	0.16	55,55,55,55	0
57	MG	BA	3609	1/1	0.87	0.21	47,47,47,47	0
57	MG	BA	3224	1/1	0.87	0.25	48,48,48,48	0
57	MG	CA	3121	1/1	0.87	0.24	51,51,51,51	0
57	MG	BA	3515	1/1	0.87	0.14	44,44,44,44	0
57	MG	DA	3397	1/1	0.87	0.15	46,46,46,46	0
57	MG	BA	3024	1/1	0.87	0.11	42,42,42,42	0
57	MG	BA	3385	1/1	0.87	0.20	34,34,34,34	0
57	MG	BA	3621	1/1	0.87	0.11	18,18,18,18	0
57	MG	DB	3003	1/1	0.87	0.18	76,76,76,76	0
57	MG	CA	3131	1/1	0.87	0.15	57,57,57,57	0
57	MG	DA	3415	1/1	0.87	0.25	55,55,55,55	0
57	MG	DA	3165	1/1	0.87	0.21	54,54,54,54	0
57	MG	BA	3111	1/1	0.87	0.22	51,51,51,51	0
57	MG	AS	101	1/1	0.87	0.15	55,55,55,55	0
57	MG	BA	3050	1/1	0.87	0.11	44,44,44,44	0
57	MG	DA	3429	1/1	0.87	0.15	38,38,38,38	0
57	MG	DA	3430	1/1	0.87	0.13	26,26,26,26	0
57	MG	CA	3138	1/1	0.87	0.32	66,66,66,66	0
57	MG	DA	3228	1/1	0.88	0.19	49,49,49,49	0
57	MG	CW	101	1/1	0.88	0.12	43,43,43,43	0
57	MG	BB	3009	1/1	0.88	0.21	63,63,63,63	0
57	MG	DA	3254	1/1	0.88	0.27	42,42,42,42	0
57	MG	CA	3032	1/1	0.88	0.29	58,58,58,58	0
57	MG	DA	3002	1/1	0.88	0.23	44,44,44,44	0
57	MG	CA	3103	1/1	0.88	0.24	71,71,71,71	0
57	MG	CA	3104	1/1	0.88	0.16	37,37,37,37	0
57	MG	CA	3034	1/1	0.88	0.15	49,49,49,49	0
57	MG	BA	3614	1/1	0.88	0.18	64,64,64,64	0
57	MG	BA	3320	1/1	0.88	0.12	56,56,56,56	0
57	MG	CA	3109	1/1	0.88	0.21	61,61,61,61	0
57	MG	DA	3511	1/1	0.88	0.09	40,40,40,40	0
57	MG	DA	3284	1/1	0.88	0.17	51,51,51,51	0
57	MG	DA	3053	1/1	0.88	0.29	50,50,50,50	0
57	MG	BA	3322	1/1	0.88	0.15	40,40,40,40	0
57	MG	BA	3548	1/1	0.88	0.21	54,54,54,54	0
57	MG	BA	3188	1/1	0.88	0.22	48,48,48,48	0
57	MG	AA	3077	1/1	0.88	0.23	52,52,52,52	0
57	MG	DA	3072	1/1	0.88	0.22	46,46,46,46	0
57	MG	BQ	3003	1/1	0.88	0.15	68,68,68,68	0
57	MG	CA	3052	1/1	0.88	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	3108	1/1	0.88	0.18	54,54,54,54	0
57	MG	DA	3545	1/1	0.88	0.11	70,70,70,70	0
57	MG	CA	3054	1/1	0.88	0.27	53,53,53,53	0
57	MG	DA	3102	1/1	0.88	0.23	64,64,64,64	0
57	MG	DA	3331	1/1	0.88	0.25	54,54,54,54	0
57	MG	BA	3633	1/1	0.88	0.23	54,54,54,54	0
57	MG	CA	3056	1/1	0.88	0.15	56,56,56,56	0
57	MG	BA	3205	1/1	0.88	0.24	52,52,52,52	0
57	MG	DA	3351	1/1	0.88	0.24	45,45,45,45	0
57	MG	AA	3173	1/1	0.88	0.10	53,53,53,53	0
57	MG	DA	3355	1/1	0.88	0.12	48,48,48,48	0
57	MG	BA	3090	1/1	0.88	0.26	50,50,50,50	0
57	MG	DA	3362	1/1	0.88	0.24	48,48,48,48	0
57	MG	AA	3049	1/1	0.88	0.18	43,43,43,43	0
57	MG	DA	3586	1/1	0.88	0.12	21,21,21,21	0
57	MG	CA	3130	1/1	0.88	0.14	88,88,88,88	0
57	MG	AD	303	1/1	0.88	0.29	60,60,60,60	0
57	MG	BA	3017	1/1	0.88	0.19	48,48,48,48	0
57	MG	AA	3042	1/1	0.88	0.26	52,52,52,52	0
57	MG	BA	3031	1/1	0.88	0.21	51,51,51,51	0
57	MG	CA	3136	1/1	0.88	0.25	68,68,68,68	0
57	MG	DA	3605	1/1	0.88	0.11	64,64,64,64	0
57	MG	DA	3406	1/1	0.88	0.13	62,62,62,62	0
57	MG	DA	3408	1/1	0.88	0.09	44,44,44,44	0
57	MG	BA	3238	1/1	0.88	0.17	26,26,26,26	0
57	MG	BA	3599	1/1	0.88	0.14	43,43,43,43	0
57	MG	AA	3032	1/1	0.88	0.34	80,80,80,80	0
57	MG	DA	3170	1/1	0.88	0.34	47,47,47,47	0
57	MG	CA	3144	1/1	0.88	0.22	58,58,58,58	0
57	MG	BA	3409	1/1	0.88	0.18	27,27,27,27	0
57	MG	DA	3188	1/1	0.88	0.26	48,48,48,48	0
57	MG	BA	3116	1/1	0.88	0.35	54,54,54,54	0
57	MG	CA	3083	1/1	0.88	0.38	71,71,71,71	0
57	MG	DA	3428	1/1	0.88	0.15	46,46,46,46	0
57	MG	AA	3117	1/1	0.88	0.22	55,55,55,55	0
57	MG	AA	3121	1/1	0.88	0.18	66,66,66,66	0
57	MG	DD	306	1/1	0.88	0.20	44,44,44,44	0
57	MG	BA	3691	1/1	0.88	0.23	54,54,54,54	0
57	MG	DA	3209	1/1	0.88	0.20	53,53,53,53	0
57	MG	BA	3532	1/1	0.88	0.16	39,39,39,39	0
57	MG	AA	3059	1/1	0.88	0.29	61,61,61,61	0
57	MG	BB	3001	1/1	0.88	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3096	1/1	0.88	0.13	51,51,51,51	0
57	MG	AA	3097	1/1	0.88	0.11	45,45,45,45	0
59	ZN	D4	501	1/1	0.88	0.10	154,154,154,154	0
57	MG	BA	3560	1/1	0.89	0.17	54,54,54,54	0
57	MG	DA	3435	1/1	0.89	0.12	59,59,59,59	0
57	MG	DA	3185	1/1	0.89	0.36	57,57,57,57	0
57	MG	BA	3673	1/1	0.89	0.12	55,55,55,55	0
57	MG	BA	3223	1/1	0.89	0.08	38,38,38,38	0
57	MG	BA	3678	1/1	0.89	0.13	49,49,49,49	0
57	MG	AA	3031	1/1	0.89	0.07	41,41,41,41	0
57	MG	BA	3680	1/1	0.89	0.11	46,46,46,46	0
57	MG	DA	3449	1/1	0.89	0.12	52,52,52,52	0
57	MG	BA	3682	1/1	0.89	0.11	30,30,30,30	0
57	MG	AA	3120	1/1	0.89	0.15	53,53,53,53	0
57	MG	AA	3206	1/1	0.89	0.14	62,62,62,62	0
57	MG	DA	3210	1/1	0.89	0.34	57,57,57,57	0
57	MG	AA	3098	1/1	0.89	0.10	42,42,42,42	0
57	MG	BA	3261	1/1	0.89	0.16	52,52,52,52	0
57	MG	BA	3422	1/1	0.89	0.13	39,39,39,39	0
57	MG	BA	3135	1/1	0.89	0.13	48,48,48,48	0
57	MG	DA	3225	1/1	0.89	0.14	42,42,42,42	0
57	MG	BA	3264	1/1	0.89	0.13	47,47,47,47	0
57	MG	AA	3099	1/1	0.89	0.14	59,59,59,59	0
57	MG	DA	3496	1/1	0.89	0.20	63,63,63,63	0
57	MG	DA	3498	1/1	0.89	0.09	66,66,66,66	0
57	MG	DA	3245	1/1	0.89	0.13	46,46,46,46	0
57	MG	DA	3503	1/1	0.89	0.08	51,51,51,51	0
57	MG	DA	3506	1/1	0.89	0.27	38,38,38,38	0
57	MG	BA	3434	1/1	0.89	0.13	27,27,27,27	0
57	MG	CA	3064	1/1	0.89	0.27	64,64,64,64	0
57	MG	DA	3513	1/1	0.89	0.12	49,49,49,49	0
57	MG	DA	3514	1/1	0.89	0.14	34,34,34,34	0
57	MG	DA	3515	1/1	0.89	0.16	53,53,53,53	0
57	MG	BA	3442	1/1	0.89	0.15	51,51,51,51	0
57	MG	BA	3138	1/1	0.89	0.28	57,57,57,57	0
57	MG	BF	305	1/1	0.89	0.08	33,33,33,33	0
57	MG	AA	3100	1/1	0.89	0.26	69,69,69,69	0
57	MG	BA	3460	1/1	0.89	0.09	43,43,43,43	0
57	MG	DA	3529	1/1	0.89	0.12	43,43,43,43	0
57	MG	DA	3273	1/1	0.89	0.15	41,41,41,41	0
57	MG	BA	3304	1/1	0.89	0.21	49,49,49,49	0
57	MG	BA	3605	1/1	0.89	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CX	3003	1/1	0.89	0.10	53,53,53,53	0
57	MG	BA	3162	1/1	0.89	0.13	39,39,39,39	0
57	MG	BA	3317	1/1	0.89	0.16	49,49,49,49	0
57	MG	B7	102	1/1	0.89	0.12	53,53,53,53	0
57	MG	DA	3013	1/1	0.89	0.12	43,43,43,43	0
57	MG	BA	3166	1/1	0.89	0.23	45,45,45,45	0
57	MG	CA	3086	1/1	0.89	0.20	56,56,56,56	0
57	MG	DA	3034	1/1	0.89	0.32	46,46,46,46	0
57	MG	DA	3036	1/1	0.89	0.11	48,48,48,48	0
57	MG	CA	3088	1/1	0.89	0.20	61,61,61,61	0
57	MG	CA	3089	1/1	0.89	0.22	65,65,65,65	0
57	MG	DA	3315	1/1	0.89	0.23	57,57,57,57	0
57	MG	DA	3045	1/1	0.89	0.15	39,39,39,39	0
57	MG	DA	3572	1/1	0.89	0.13	46,46,46,46	0
57	MG	DA	3575	1/1	0.89	0.11	19,19,19,19	0
57	MG	AA	3104	1/1	0.89	0.12	47,47,47,47	0
57	MG	BA	3177	1/1	0.89	0.11	39,39,39,39	0
57	MG	BA	3324	1/1	0.89	0.18	61,61,61,61	0
57	MG	AA	3186	1/1	0.89	0.11	43,43,43,43	0
57	MG	BA	3623	1/1	0.89	0.09	42,42,42,42	0
57	MG	DA	3593	1/1	0.89	0.21	49,49,49,49	0
57	MG	CA	3010	1/1	0.89	0.27	56,56,56,56	0
57	MG	BA	3179	1/1	0.89	0.24	49,49,49,49	0
57	MG	DA	3600	1/1	0.89	0.16	45,45,45,45	0
57	MG	BA	3507	1/1	0.89	0.13	48,48,48,48	0
57	MG	AA	3003	1/1	0.89	0.20	53,53,53,53	0
57	MG	BA	3198	1/1	0.89	0.23	45,45,45,45	0
57	MG	AA	3062	1/1	0.89	0.27	57,57,57,57	0
57	MG	DA	3093	1/1	0.89	0.12	45,45,45,45	0
57	MG	DA	3097	1/1	0.89	0.13	50,50,50,50	0
57	MG	DA	3372	1/1	0.89	0.10	49,49,49,49	0
57	MG	BA	3068	1/1	0.89	0.23	46,46,46,46	0
57	MG	BA	3635	1/1	0.89	0.11	59,59,59,59	0
57	MG	BA	3526	1/1	0.89	0.16	48,48,48,48	0
57	MG	BA	3074	1/1	0.89	0.15	43,43,43,43	0
57	MG	DA	3396	1/1	0.89	0.14	43,43,43,43	0
57	MG	AA	3086	1/1	0.89	0.08	45,45,45,45	0
57	MG	BA	3370	1/1	0.89	0.12	32,32,32,32	0
57	MG	AA	3131	1/1	0.89	0.15	56,56,56,56	0
57	MG	AA	3039	1/1	0.89	0.40	62,62,62,62	0
57	MG	DA	3139	1/1	0.89	0.22	49,49,49,49	0
57	MG	AA	3057	1/1	0.89	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3660	1/1	0.89	0.15	62,62,62,62	0
57	MG	BA	3665	1/1	0.89	0.11	50,50,50,50	0
57	MG	CA	3033	1/1	0.89	0.21	67,67,67,67	0
57	MG	AA	3200	1/1	0.89	0.14	58,58,58,58	0
57	MG	CA	3122	1/1	0.89	0.12	50,50,50,50	0
57	MG	BA	3404	1/1	0.89	0.16	30,30,30,30	0
57	MG	CA	3036	1/1	0.89	0.18	47,47,47,47	0
57	MG	CA	3037	1/1	0.89	0.25	60,60,60,60	0
57	MG	DA	3448	1/1	0.90	0.16	36,36,36,36	0
57	MG	BA	3293	1/1	0.90	0.15	43,43,43,43	0
57	MG	BA	3302	1/1	0.90	0.12	50,50,50,50	0
57	MG	AA	3195	1/1	0.90	0.13	58,58,58,58	0
57	MG	BA	3558	1/1	0.90	0.19	63,63,63,63	0
57	MG	DA	3246	1/1	0.90	0.32	57,57,57,57	0
57	MG	BA	3559	1/1	0.90	0.12	36,36,36,36	0
57	MG	DA	3460	1/1	0.90	0.10	57,57,57,57	0
57	MG	BA	3196	1/1	0.90	0.28	51,51,51,51	0
57	MG	DA	3468	1/1	0.90	0.26	64,64,64,64	0
57	MG	DA	3469	1/1	0.90	0.19	41,41,41,41	0
57	MG	BA	3306	1/1	0.90	0.11	32,32,32,32	0
57	MG	DA	3479	1/1	0.90	0.20	45,45,45,45	0
57	MG	DA	3039	1/1	0.90	0.20	48,48,48,48	0
57	MG	BA	3428	1/1	0.90	0.19	54,54,54,54	0
57	MG	BA	3569	1/1	0.90	0.18	46,46,46,46	0
57	MG	DA	3262	1/1	0.90	0.11	39,39,39,39	0
57	MG	DA	3266	1/1	0.90	0.10	45,45,45,45	0
57	MG	DA	3497	1/1	0.90	0.15	61,61,61,61	0
57	MG	DA	3269	1/1	0.90	0.13	40,40,40,40	0
57	MG	BA	3197	1/1	0.90	0.12	32,32,32,32	0
57	MG	BA	3108	1/1	0.90	0.13	36,36,36,36	0
57	MG	DA	3056	1/1	0.90	0.07	35,35,35,35	0
57	MG	BA	3437	1/1	0.90	0.20	52,52,52,52	0
57	MG	AA	3115	1/1	0.90	0.25	38,38,38,38	0
57	MG	BA	3443	1/1	0.90	0.16	38,38,38,38	0
57	MG	BA	3445	1/1	0.90	0.15	35,35,35,35	0
57	MG	DA	3286	1/1	0.90	0.19	45,45,45,45	0
57	MG	DA	3287	1/1	0.90	0.12	58,58,58,58	0
57	MG	DA	3288	1/1	0.90	0.14	32,32,32,32	0
57	MG	DA	3289	1/1	0.90	0.28	50,50,50,50	0
57	MG	BA	3446	1/1	0.90	0.11	49,49,49,49	0
57	MG	BA	3689	1/1	0.90	0.10	46,46,46,46	0
57	MG	AA	3017	1/1	0.90	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3081	1/1	0.90	0.15	45,45,45,45	0
57	MG	DA	3082	1/1	0.90	0.15	47,47,47,47	0
57	MG	BA	3112	1/1	0.90	0.32	58,58,58,58	0
57	MG	BA	3696	1/1	0.90	0.11	41,41,41,41	0
57	MG	AA	3007	1/1	0.90	0.13	47,47,47,47	0
57	MG	AA	3140	1/1	0.90	0.18	56,56,56,56	0
57	MG	BA	3333	1/1	0.90	0.09	58,58,58,58	0
57	MG	DA	3110	1/1	0.90	0.09	60,60,60,60	0
57	MG	AA	3158	1/1	0.90	0.10	72,72,72,72	0
57	MG	BB	3018	1/1	0.90	0.07	43,43,43,43	0
57	MG	AA	3203	1/1	0.90	0.11	42,42,42,42	0
57	MG	DA	3118	1/1	0.90	0.08	46,46,46,46	0
57	MG	DA	3343	1/1	0.90	0.13	37,37,37,37	0
57	MG	DA	3122	1/1	0.90	0.14	58,58,58,58	0
57	MG	DA	3568	1/1	0.90	0.10	45,45,45,45	0
57	MG	AA	3141	1/1	0.90	0.09	54,54,54,54	0
57	MG	AA	3111	1/1	0.90	0.15	70,70,70,70	0
57	MG	CA	3132	1/1	0.90	0.12	51,51,51,51	0
57	MG	BE	3002	1/1	0.90	0.21	50,50,50,50	0
57	MG	DA	3136	1/1	0.90	0.30	62,62,62,62	0
57	MG	DA	3579	1/1	0.90	0.15	58,58,58,58	0
57	MG	DA	3581	1/1	0.90	0.12	53,53,53,53	0
57	MG	BA	3082	1/1	0.90	0.10	57,57,57,57	0
57	MG	DA	3369	1/1	0.90	0.14	36,36,36,36	0
57	MG	DA	3141	1/1	0.90	0.18	37,37,37,37	0
57	MG	BA	3229	1/1	0.90	0.37	52,52,52,52	0
57	MG	BA	3494	1/1	0.90	0.12	30,30,30,30	0
57	MG	DA	3376	1/1	0.90	0.18	40,40,40,40	0
57	MG	DA	3146	1/1	0.90	0.09	44,44,44,44	0
57	MG	BA	3499	1/1	0.90	0.31	51,51,51,51	0
57	MG	BA	3164	1/1	0.90	0.15	44,44,44,44	0
57	MG	DA	3394	1/1	0.90	0.11	48,48,48,48	0
57	MG	BU	201	1/1	0.90	0.09	36,36,36,36	0
57	MG	BU	202	1/1	0.90	0.10	45,45,45,45	0
57	MG	BA	3360	1/1	0.90	0.16	60,60,60,60	0
57	MG	BW	203	1/1	0.90	0.13	39,39,39,39	0
57	MG	AA	3021	1/1	0.90	0.24	58,58,58,58	0
57	MG	CA	3150	1/1	0.90	0.20	66,66,66,66	0
57	MG	DA	3184	1/1	0.90	0.09	44,44,44,44	0
57	MG	AA	3190	1/1	0.90	0.12	75,75,75,75	0
57	MG	BA	3247	1/1	0.90	0.13	37,37,37,37	0
57	MG	BA	3629	1/1	0.90	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3520	1/1	0.90	0.17	46,46,46,46	0
57	MG	BA	3257	1/1	0.90	0.14	40,40,40,40	0
57	MG	BA	3029	1/1	0.90	0.24	53,53,53,53	0
57	MG	BA	3100	1/1	0.90	0.14	40,40,40,40	0
57	MG	DA	3207	1/1	0.90	0.20	39,39,39,39	0
57	MG	DB	3009	1/1	0.90	0.27	55,55,55,55	0
57	MG	CA	3087	1/1	0.90	0.21	50,50,50,50	0
57	MG	CT	3001	1/1	0.90	0.14	59,59,59,59	0
57	MG	DE	303	1/1	0.90	0.20	49,49,49,49	0
57	MG	AA	3089	1/1	0.90	0.24	61,61,61,61	0
57	MG	BA	3180	1/1	0.90	0.11	32,32,32,32	0
57	MG	DA	3442	1/1	0.90	0.17	34,34,34,34	0
57	MG	DU	3001	1/1	0.90	0.32	56,56,56,56	0
57	MG	BA	3271	1/1	0.90	0.26	45,45,45,45	0
57	MG	BA	3537	1/1	0.90	0.08	35,35,35,35	0
57	MG	BA	3183	1/1	0.90	0.15	50,50,50,50	0
57	MG	DA	3224	1/1	0.90	0.29	60,60,60,60	0
57	MG	DA	3475	1/1	0.91	0.13	35,35,35,35	0
57	MG	DA	3105	1/1	0.91	0.13	37,37,37,37	0
57	MG	DA	3106	1/1	0.91	0.14	52,52,52,52	0
57	MG	BP	3001	1/1	0.91	0.26	49,49,49,49	0
57	MG	BA	3574	1/1	0.91	0.10	41,41,41,41	0
57	MG	BA	3575	1/1	0.91	0.12	30,30,30,30	0
57	MG	DA	3301	1/1	0.91	0.21	54,54,54,54	0
57	MG	BA	3369	1/1	0.91	0.15	57,57,57,57	0
57	MG	AA	3058	1/1	0.91	0.16	48,48,48,48	0
57	MG	DA	3120	1/1	0.91	0.17	55,55,55,55	0
57	MG	DA	3502	1/1	0.91	0.11	51,51,51,51	0
57	MG	AA	3053	1/1	0.91	0.12	54,54,54,54	0
57	MG	DA	3504	1/1	0.91	0.09	46,46,46,46	0
57	MG	DA	3310	1/1	0.91	0.10	43,43,43,43	0
57	MG	BA	3284	1/1	0.91	0.10	41,41,41,41	0
57	MG	DA	3313	1/1	0.91	0.11	51,51,51,51	0
57	MG	B0	102	1/1	0.91	0.11	53,53,53,53	0
57	MG	DA	3132	1/1	0.91	0.12	53,53,53,53	0
57	MG	B1	101	1/1	0.91	0.22	37,37,37,37	0
57	MG	BA	3378	1/1	0.91	0.17	45,45,45,45	0
57	MG	CA	3145	1/1	0.91	0.10	49,49,49,49	0
57	MG	CA	3069	1/1	0.91	0.33	56,56,56,56	0
57	MG	DA	3335	1/1	0.91	0.09	48,48,48,48	0
57	MG	B7	103	1/1	0.91	0.13	51,51,51,51	0
57	MG	DA	3528	1/1	0.91	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3073	1/1	0.91	0.13	57,57,57,57	0
57	MG	CA	3074	1/1	0.91	0.26	51,51,51,51	0
57	MG	CA	3001	1/1	0.91	0.10	53,53,53,53	0
57	MG	AA	3016	1/1	0.91	0.12	52,52,52,52	0
57	MG	DA	3542	1/1	0.91	0.11	44,44,44,44	0
57	MG	BA	3297	1/1	0.91	0.11	36,36,36,36	0
57	MG	BA	3669	1/1	0.91	0.11	34,34,34,34	0
57	MG	BA	3301	1/1	0.91	0.19	43,43,43,43	0
57	MG	DA	3358	1/1	0.91	0.26	45,45,45,45	0
57	MG	BA	3072	1/1	0.91	0.10	32,32,32,32	0
57	MG	AA	3191	1/1	0.91	0.19	56,56,56,56	0
57	MG	DA	3551	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3020	1/1	0.91	0.25	55,55,55,55	0
57	MG	BA	3677	1/1	0.91	0.14	30,30,30,30	0
57	MG	BA	3144	1/1	0.91	0.15	42,42,42,42	0
57	MG	BA	3148	1/1	0.91	0.22	44,44,44,44	0
57	MG	DA	3564	1/1	0.91	0.11	48,48,48,48	0
57	MG	BA	3084	1/1	0.91	0.13	37,37,37,37	0
57	MG	DA	3566	1/1	0.91	0.09	40,40,40,40	0
57	MG	AA	3084	1/1	0.91	0.10	43,43,43,43	0
57	MG	AA	3172	1/1	0.91	0.25	54,54,54,54	0
57	MG	BA	3684	1/1	0.91	0.10	47,47,47,47	0
57	MG	DA	3007	1/1	0.91	0.10	48,48,48,48	0
57	MG	DA	3010	1/1	0.91	0.13	51,51,51,51	0
57	MG	DA	3011	1/1	0.91	0.10	36,36,36,36	0
57	MG	AA	3154	1/1	0.91	0.13	46,46,46,46	0
57	MG	BA	3233	1/1	0.91	0.20	55,55,55,55	0
57	MG	BA	3094	1/1	0.91	0.08	46,46,46,46	0
57	MG	BA	3099	1/1	0.91	0.14	36,36,36,36	0
57	MG	DA	3587	1/1	0.91	0.10	35,35,35,35	0
57	MG	DA	3589	1/1	0.91	0.11	52,52,52,52	0
57	MG	AA	3197	1/1	0.91	0.09	50,50,50,50	0
57	MG	BA	3618	1/1	0.91	0.13	64,64,64,64	0
57	MG	BA	3707	1/1	0.91	0.28	34,34,34,34	0
57	MG	BA	3717	1/1	0.91	0.36	40,40,40,40	0
57	MG	CA	3031	1/1	0.91	0.13	55,55,55,55	0
57	MG	BA	3619	1/1	0.91	0.19	54,54,54,54	0
57	MG	DA	3227	1/1	0.91	0.14	57,57,57,57	0
57	MG	BB	3005	1/1	0.91	0.16	42,42,42,42	0
57	MG	DA	3234	1/1	0.91	0.16	34,34,34,34	0
57	MG	DA	3239	1/1	0.91	0.25	51,51,51,51	0
57	MG	DA	3432	1/1	0.91	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3338	1/1	0.91	0.08	50,50,50,50	0
57	MG	BA	3244	1/1	0.91	0.26	29,29,29,29	0
57	MG	DA	3062	1/1	0.91	0.11	49,49,49,49	0
57	MG	DA	3611	1/1	0.91	0.18	58,58,58,58	0
57	MG	DA	3612	1/1	0.91	0.16	64,64,64,64	0
57	MG	DA	3441	1/1	0.91	0.21	43,43,43,43	0
57	MG	BA	3104	1/1	0.91	0.14	54,54,54,54	0
57	MG	BA	3033	1/1	0.91	0.10	39,39,39,39	0
57	MG	DA	3255	1/1	0.91	0.22	34,34,34,34	0
57	MG	DA	3445	1/1	0.91	0.12	59,59,59,59	0
57	MG	DA	3068	1/1	0.91	0.12	48,48,48,48	0
57	MG	AA	3036	1/1	0.91	0.11	51,51,51,51	0
57	MG	BD	302	1/1	0.91	0.14	38,38,38,38	0
57	MG	BD	308	1/1	0.91	0.19	41,41,41,41	0
57	MG	AA	3051	1/1	0.91	0.27	51,51,51,51	0
57	MG	BE	3001	1/1	0.91	0.23	48,48,48,48	0
57	MG	CA	3045	1/1	0.91	0.15	53,53,53,53	0
57	MG	DE	301	1/1	0.91	0.16	52,52,52,52	0
57	MG	AA	3073	1/1	0.91	0.30	59,59,59,59	0
57	MG	AA	3105	1/1	0.91	0.12	59,59,59,59	0
57	MG	DA	3091	1/1	0.91	0.12	37,37,37,37	0
57	MG	DP	201	1/1	0.91	0.15	61,61,61,61	0
57	MG	DQ	3001	1/1	0.91	0.14	58,58,58,58	0
57	MG	BA	3466	1/1	0.91	0.16	57,57,57,57	0
57	MG	DR	3002	1/1	0.91	0.13	51,51,51,51	0
57	MG	DA	3462	1/1	0.91	0.25	35,35,35,35	0
57	MG	BA	3366	1/1	0.91	0.11	38,38,38,38	0
57	MG	BA	3571	1/1	0.91	0.11	24,24,24,24	0
57	MG	DA	3104	1/1	0.91	0.16	47,47,47,47	0
57	MG	DA	3473	1/1	0.91	0.11	32,32,32,32	0
57	MG	CA	3143	1/1	0.92	0.11	59,59,59,59	0
57	MG	AA	3079	1/1	0.92	0.15	62,62,62,62	0
57	MG	AV	3001	1/1	0.92	0.25	59,59,59,59	0
57	MG	BA	3570	1/1	0.92	0.09	48,48,48,48	0
57	MG	BA	3318	1/1	0.92	0.13	39,39,39,39	0
57	MG	DA	3190	1/1	0.92	0.22	52,52,52,52	0
57	MG	BA	3127	1/1	0.92	0.19	41,41,41,41	0
57	MG	BA	3685	1/1	0.92	0.18	40,40,40,40	0
57	MG	DA	3201	1/1	0.92	0.14	42,42,42,42	0
57	MG	BA	3132	1/1	0.92	0.15	52,52,52,52	0
57	MG	BA	3576	1/1	0.92	0.13	29,29,29,29	0
57	MG	DA	3450	1/1	0.92	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	3152	1/1	0.92	0.12	64,64,64,64	0
57	MG	AA	3139	1/1	0.92	0.11	51,51,51,51	0
57	MG	CA	3157	1/1	0.92	0.22	61,61,61,61	0
57	MG	DA	3212	1/1	0.92	0.07	47,47,47,47	0
57	MG	BA	3583	1/1	0.92	0.09	54,54,54,54	0
57	MG	BA	3073	1/1	0.92	0.16	39,39,39,39	0
57	MG	CF	3001	1/1	0.92	0.13	51,51,51,51	0
57	MG	AA	3174	1/1	0.92	0.13	64,64,64,64	0
57	MG	BA	3712	1/1	0.92	0.08	30,30,30,30	0
57	MG	BA	3334	1/1	0.92	0.11	37,37,37,37	0
57	MG	BA	3335	1/1	0.92	0.08	26,26,26,26	0
57	MG	BB	3002	1/1	0.92	0.17	44,44,44,44	0
57	MG	BA	3462	1/1	0.92	0.18	51,51,51,51	0
57	MG	DA	3476	1/1	0.92	0.12	49,49,49,49	0
57	MG	AA	3119	1/1	0.92	0.22	50,50,50,50	0
57	MG	BA	3230	1/1	0.92	0.21	45,45,45,45	0
57	MG	DA	3485	1/1	0.92	0.07	41,41,41,41	0
57	MG	DA	3488	1/1	0.92	0.12	47,47,47,47	0
57	MG	DA	3242	1/1	0.92	0.12	48,48,48,48	0
57	MG	DA	3492	1/1	0.92	0.08	45,45,45,45	0
57	MG	BB	3015	1/1	0.92	0.10	42,42,42,42	0
57	MG	DA	3494	1/1	0.92	0.17	56,56,56,56	0
57	MG	BA	3340	1/1	0.92	0.12	59,59,59,59	0
57	MG	BA	3468	1/1	0.92	0.08	42,42,42,42	0
57	MG	DA	3250	1/1	0.92	0.16	41,41,41,41	0
57	MG	BA	3601	1/1	0.92	0.17	69,69,69,69	0
57	MG	BA	3153	1/1	0.92	0.10	53,53,53,53	0
57	MG	AA	3035	1/1	0.92	0.30	52,52,52,52	0
57	MG	AA	3179	1/1	0.92	0.11	56,56,56,56	0
57	MG	DA	3028	1/1	0.92	0.20	52,52,52,52	0
57	MG	AA	3101	1/1	0.92	0.24	53,53,53,53	0
57	MG	DA	3035	1/1	0.92	0.12	45,45,45,45	0
57	MG	DA	3510	1/1	0.92	0.19	52,52,52,52	0
57	MG	DA	3263	1/1	0.92	0.17	47,47,47,47	0
57	MG	DA	3265	1/1	0.92	0.08	33,33,33,33	0
57	MG	AA	3202	1/1	0.92	0.19	60,60,60,60	0
57	MG	DA	3268	1/1	0.92	0.09	35,35,35,35	0
57	MG	CA	3076	1/1	0.92	0.27	59,59,59,59	0
57	MG	BA	3353	1/1	0.92	0.07	46,46,46,46	0
57	MG	DA	3042	1/1	0.92	0.23	37,37,37,37	0
57	MG	DA	3274	1/1	0.92	0.14	45,45,45,45	0
57	MG	BF	306	1/1	0.92	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BF	308	1/1	0.92	0.14	46,46,46,46	0
57	MG	DA	3046	1/1	0.92	0.22	50,50,50,50	0
57	MG	DA	3048	1/1	0.92	0.16	53,53,53,53	0
57	MG	DA	3534	1/1	0.92	0.08	30,30,30,30	0
57	MG	BA	3172	1/1	0.92	0.09	27,27,27,27	0
57	MG	DA	3538	1/1	0.92	0.12	77,77,77,77	0
57	MG	BG	3001	1/1	0.92	0.23	44,44,44,44	0
57	MG	BA	3612	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3497	1/1	0.92	0.15	41,41,41,41	0
57	MG	AA	3183	1/1	0.92	0.12	43,43,43,43	0
57	MG	BA	3097	1/1	0.92	0.13	44,44,44,44	0
57	MG	DA	3296	1/1	0.92	0.13	46,46,46,46	0
57	MG	AA	3204	1/1	0.92	0.21	64,64,64,64	0
57	MG	DA	3300	1/1	0.92	0.11	38,38,38,38	0
57	MG	BA	3509	1/1	0.92	0.23	34,34,34,34	0
57	MG	BA	3511	1/1	0.92	0.13	41,41,41,41	0
57	MG	BA	3622	1/1	0.92	0.07	24,24,24,24	0
57	MG	CA	3093	1/1	0.92	0.18	69,69,69,69	0
57	MG	AA	3143	1/1	0.92	0.09	32,32,32,32	0
57	MG	DA	3078	1/1	0.92	0.15	49,49,49,49	0
57	MG	DA	3080	1/1	0.92	0.19	64,64,64,64	0
57	MG	BA	3102	1/1	0.92	0.19	43,43,43,43	0
57	MG	CA	3097	1/1	0.92	0.11	43,43,43,43	0
57	MG	B0	103	1/1	0.92	0.10	38,38,38,38	0
57	MG	B0	104	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3516	1/1	0.92	0.12	32,32,32,32	0
57	MG	DA	3574	1/1	0.92	0.08	59,59,59,59	0
57	MG	DA	3327	1/1	0.92	0.08	49,49,49,49	0
57	MG	AA	3162	1/1	0.92	0.10	40,40,40,40	0
57	MG	DA	3578	1/1	0.92	0.14	63,63,63,63	0
57	MG	BA	3375	1/1	0.92	0.15	46,46,46,46	0
57	MG	DA	3332	1/1	0.92	0.14	52,52,52,52	0
57	MG	BA	3521	1/1	0.92	0.19	32,32,32,32	0
57	MG	CA	3002	1/1	0.92	0.10	66,66,66,66	0
57	MG	BA	3632	1/1	0.92	0.10	43,43,43,43	0
57	MG	BA	3523	1/1	0.92	0.09	31,31,31,31	0
57	MG	BA	3185	1/1	0.92	0.41	34,34,34,34	0
57	MG	AA	3207	1/1	0.92	0.18	57,57,57,57	0
57	MG	BA	3381	1/1	0.92	0.11	30,30,30,30	0
57	MG	BA	3638	1/1	0.92	0.08	41,41,41,41	0
57	MG	BA	3287	1/1	0.92	0.23	42,42,42,42	0
57	MG	AA	3013	1/1	0.92	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3648	1/1	0.92	0.12	50,50,50,50	0
57	MG	BA	3534	1/1	0.92	0.20	23,23,23,23	0
57	MG	DA	3604	1/1	0.92	0.21	61,61,61,61	0
57	MG	DA	3367	1/1	0.92	0.09	24,24,24,24	0
57	MG	CA	3016	1/1	0.92	0.13	52,52,52,52	0
57	MG	BA	3408	1/1	0.92	0.13	42,42,42,42	0
57	MG	AA	3027	1/1	0.92	0.11	55,55,55,55	0
57	MG	BA	3298	1/1	0.92	0.19	50,50,50,50	0
57	MG	BA	3659	1/1	0.92	0.13	47,47,47,47	0
57	MG	DA	3138	1/1	0.92	0.12	39,39,39,39	0
57	MG	AA	3034	1/1	0.92	0.21	47,47,47,47	0
57	MG	DA	3613	1/1	0.92	0.17	45,45,45,45	0
57	MG	DA	3614	1/1	0.92	0.39	56,56,56,56	0
57	MG	DA	3383	1/1	0.92	0.07	45,45,45,45	0
57	MG	DA	3617	1/1	0.92	0.12	40,40,40,40	0
57	MG	BA	3664	1/1	0.92	0.13	66,66,66,66	0
57	MG	DA	3621	1/1	0.92	0.15	61,61,61,61	0
57	MG	BA	3544	1/1	0.92	0.11	52,52,52,52	0
57	MG	BA	3545	1/1	0.92	0.12	34,34,34,34	0
57	MG	DA	3626	1/1	0.92	0.14	38,38,38,38	0
57	MG	DA	3627	1/1	0.92	0.12	56,56,56,56	0
57	MG	BA	3547	1/1	0.92	0.09	33,33,33,33	0
57	MG	DA	3404	1/1	0.92	0.11	48,48,48,48	0
57	MG	AJ	201	1/1	0.92	0.36	67,67,67,67	0
57	MG	DA	3407	1/1	0.92	0.12	67,67,67,67	0
57	MG	DB	3006	1/1	0.92	0.12	44,44,44,44	0
57	MG	DA	3149	1/1	0.92	0.13	42,42,42,42	0
57	MG	DA	3152	1/1	0.92	0.16	38,38,38,38	0
57	MG	DD	305	1/1	0.92	0.15	48,48,48,48	0
57	MG	BA	3200	1/1	0.92	0.22	39,39,39,39	0
57	MG	DA	3159	1/1	0.92	0.16	32,32,32,32	0
57	MG	BA	3203	1/1	0.92	0.25	56,56,56,56	0
57	MG	AA	3192	1/1	0.92	0.15	72,72,72,72	0
57	MG	DF	3003	1/1	0.92	0.13	36,36,36,36	0
57	MG	DF	3004	1/1	0.92	0.15	56,56,56,56	0
57	MG	DA	3164	1/1	0.92	0.14	44,44,44,44	0
57	MG	CA	3137	1/1	0.92	0.11	81,81,81,81	0
57	MG	DA	3420	1/1	0.92	0.10	41,41,41,41	0
57	MG	BA	3675	1/1	0.92	0.12	41,41,41,41	0
57	MG	BA	3310	1/1	0.92	0.24	43,43,43,43	0
57	MG	DA	3171	1/1	0.92	0.17	38,38,38,38	0
57	MG	DA	3177	1/1	0.92	0.26	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DU	3002	1/1	0.92	0.14	67,67,67,67	0
57	MG	DA	3178	1/1	0.92	0.17	39,39,39,39	0
57	MG	DA	3181	1/1	0.92	0.17	36,36,36,36	0
57	MG	DA	3434	1/1	0.92	0.08	48,48,48,48	0
57	MG	BA	3313	1/1	0.92	0.12	30,30,30,30	0
57	MG	BA	3464	1/1	0.93	0.10	26,26,26,26	0
57	MG	BB	3012	1/1	0.93	0.11	33,33,33,33	0
57	MG	DA	3019	1/1	0.93	0.18	54,54,54,54	0
57	MG	DA	3021	1/1	0.93	0.11	50,50,50,50	0
57	MG	DA	3230	1/1	0.93	0.25	46,46,46,46	0
57	MG	DA	3232	1/1	0.93	0.08	48,48,48,48	0
57	MG	BA	3062	1/1	0.93	0.20	52,52,52,52	0
57	MG	DA	3235	1/1	0.93	0.29	48,48,48,48	0
57	MG	DA	3236	1/1	0.93	0.07	45,45,45,45	0
57	MG	DA	3238	1/1	0.93	0.32	31,31,31,31	0
57	MG	CA	3070	1/1	0.93	0.23	42,42,42,42	0
57	MG	DA	3241	1/1	0.93	0.13	40,40,40,40	0
57	MG	AA	3144	1/1	0.93	0.20	44,44,44,44	0
57	MG	BA	3336	1/1	0.93	0.12	47,47,47,47	0
57	MG	AA	3038	1/1	0.93	0.24	58,58,58,58	0
57	MG	DA	3477	1/1	0.93	0.08	37,37,37,37	0
57	MG	DA	3478	1/1	0.93	0.16	57,57,57,57	0
57	MG	DA	3037	1/1	0.93	0.10	41,41,41,41	0
57	MG	BA	3225	1/1	0.93	0.07	45,45,45,45	0
57	MG	DA	3484	1/1	0.93	0.07	41,41,41,41	0
57	MG	BA	3339	1/1	0.93	0.23	52,52,52,52	0
57	MG	DA	3487	1/1	0.93	0.13	44,44,44,44	0
57	MG	CA	3077	1/1	0.93	0.21	63,63,63,63	0
57	MG	BA	3606	1/1	0.93	0.15	39,39,39,39	0
57	MG	CA	3079	1/1	0.93	0.13	42,42,42,42	0
57	MG	AA	3020	1/1	0.93	0.16	62,62,62,62	0
57	MG	DA	3047	1/1	0.93	0.19	44,44,44,44	0
57	MG	BA	3069	1/1	0.93	0.26	48,48,48,48	0
57	MG	BF	302	1/1	0.93	0.10	59,59,59,59	0
57	MG	BA	3486	1/1	0.93	0.08	32,32,32,32	0
57	MG	DA	3054	1/1	0.93	0.10	40,40,40,40	0
57	MG	BA	3143	1/1	0.93	0.18	41,41,41,41	0
57	MG	BA	3070	1/1	0.93	0.10	44,44,44,44	0
57	MG	DA	3270	1/1	0.93	0.24	57,57,57,57	0
57	MG	AA	3129	1/1	0.93	0.13	37,37,37,37	0
57	MG	BA	3151	1/1	0.93	0.12	42,42,42,42	0
57	MG	DA	3508	1/1	0.93	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3152	1/1	0.93	0.13	45,45,45,45	0
57	MG	BA	3357	1/1	0.93	0.10	31,31,31,31	0
57	MG	BO	5001	1/1	0.93	0.09	49,49,49,49	0
57	MG	BA	3620	1/1	0.93	0.09	35,35,35,35	0
57	MG	AA	3067	1/1	0.93	0.09	47,47,47,47	0
57	MG	AA	3048	1/1	0.93	0.13	42,42,42,42	0
57	MG	DA	3077	1/1	0.93	0.35	58,58,58,58	0
57	MG	BA	3075	1/1	0.93	0.36	45,45,45,45	0
57	MG	DA	3079	1/1	0.93	0.11	41,41,41,41	0
57	MG	DA	3524	1/1	0.93	0.11	40,40,40,40	0
57	MG	BA	3079	1/1	0.93	0.27	55,55,55,55	0
57	MG	DA	3290	1/1	0.93	0.13	43,43,43,43	0
57	MG	BA	3626	1/1	0.93	0.16	48,48,48,48	0
57	MG	BA	3627	1/1	0.93	0.07	28,28,28,28	0
57	MG	AA	3176	1/1	0.93	0.07	43,43,43,43	0
57	MG	BA	3171	1/1	0.93	0.17	44,44,44,44	0
57	MG	AA	3177	1/1	0.93	0.23	66,66,66,66	0
57	MG	BA	3277	1/1	0.93	0.20	34,34,34,34	0
57	MG	DA	3095	1/1	0.93	0.12	45,45,45,45	0
57	MG	BA	3279	1/1	0.93	0.24	48,48,48,48	0
57	MG	BA	3005	1/1	0.93	0.11	44,44,44,44	0
57	MG	AA	3153	1/1	0.93	0.09	46,46,46,46	0
57	MG	AA	3118	1/1	0.93	0.19	50,50,50,50	0
57	MG	DA	3546	1/1	0.93	0.09	41,41,41,41	0
57	MG	BA	3386	1/1	0.93	0.17	30,30,30,30	0
57	MG	DA	3107	1/1	0.93	0.14	39,39,39,39	0
57	MG	DA	3109	1/1	0.93	0.10	45,45,45,45	0
57	MG	DA	3317	1/1	0.93	0.17	42,42,42,42	0
57	MG	DA	3318	1/1	0.93	0.09	39,39,39,39	0
57	MG	BA	3531	1/1	0.93	0.17	20,20,20,20	0
57	MG	DA	3320	1/1	0.93	0.06	19,19,19,19	0
57	MG	DA	3558	1/1	0.93	0.07	45,45,45,45	0
57	MG	DA	3559	1/1	0.93	0.13	31,31,31,31	0
57	MG	DA	3321	1/1	0.93	0.11	40,40,40,40	0
57	MG	BA	3387	1/1	0.93	0.09	29,29,29,29	0
57	MG	DA	3324	1/1	0.93	0.12	42,42,42,42	0
57	MG	DA	3326	1/1	0.93	0.08	40,40,40,40	0
57	MG	DA	3567	1/1	0.93	0.08	49,49,49,49	0
57	MG	BA	3642	1/1	0.93	0.12	50,50,50,50	0
57	MG	DA	3114	1/1	0.93	0.08	51,51,51,51	0
57	MG	DA	3329	1/1	0.93	0.24	54,54,54,54	0
57	MG	DA	3330	1/1	0.93	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3388	1/1	0.93	0.09	31,31,31,31	0
57	MG	BA	3397	1/1	0.93	0.09	33,33,33,33	0
57	MG	DA	3119	1/1	0.93	0.13	52,52,52,52	0
57	MG	CA	3118	1/1	0.93	0.08	69,69,69,69	0
57	MG	BA	3398	1/1	0.93	0.20	36,36,36,36	0
57	MG	CA	3011	1/1	0.93	0.27	39,39,39,39	0
57	MG	DA	3128	1/1	0.93	0.23	45,45,45,45	0
57	MG	BA	3019	1/1	0.93	0.08	30,30,30,30	0
57	MG	CA	3013	1/1	0.93	0.22	45,45,45,45	0
57	MG	BA	3406	1/1	0.93	0.12	24,24,24,24	0
57	MG	DA	3590	1/1	0.93	0.12	58,58,58,58	0
57	MG	BA	3407	1/1	0.93	0.13	29,29,29,29	0
57	MG	AA	3005	1/1	0.93	0.10	66,66,66,66	0
57	MG	CA	3128	1/1	0.93	0.14	43,43,43,43	0
57	MG	DA	3594	1/1	0.93	0.17	51,51,51,51	0
57	MG	DA	3365	1/1	0.93	0.15	54,54,54,54	0
57	MG	BA	3098	1/1	0.93	0.38	50,50,50,50	0
57	MG	BA	3299	1/1	0.93	0.12	27,27,27,27	0
57	MG	BA	3300	1/1	0.93	0.10	55,55,55,55	0
57	MG	BA	3021	1/1	0.93	0.11	35,35,35,35	0
57	MG	DA	3603	1/1	0.93	0.12	40,40,40,40	0
57	MG	BA	3555	1/1	0.93	0.12	62,62,62,62	0
57	MG	AA	3024	1/1	0.93	0.20	49,49,49,49	0
57	MG	DA	3375	1/1	0.93	0.12	30,30,30,30	0
57	MG	BA	3417	1/1	0.93	0.12	49,49,49,49	0
57	MG	BA	3027	1/1	0.93	0.51	36,36,36,36	0
57	MG	DA	3157	1/1	0.93	0.19	44,44,44,44	0
57	MG	BA	3103	1/1	0.93	0.38	62,62,62,62	0
57	MG	DA	3385	1/1	0.93	0.07	47,47,47,47	0
57	MG	BA	3566	1/1	0.93	0.14	31,31,31,31	0
57	MG	DA	3391	1/1	0.93	0.10	39,39,39,39	0
57	MG	AA	3184	1/1	0.93	0.18	56,56,56,56	0
57	MG	BA	3307	1/1	0.93	0.20	31,31,31,31	0
57	MG	AA	3107	1/1	0.93	0.18	50,50,50,50	0
57	MG	DA	3618	1/1	0.93	0.09	46,46,46,46	0
57	MG	AD	301	1/1	0.93	0.11	47,47,47,47	0
57	MG	BA	3681	1/1	0.93	0.17	42,42,42,42	0
57	MG	DA	3622	1/1	0.93	0.43	58,58,58,58	0
57	MG	BA	3573	1/1	0.93	0.12	29,29,29,29	0
57	MG	BA	3430	1/1	0.93	0.10	54,54,54,54	0
57	MG	DA	3173	1/1	0.93	0.18	42,42,42,42	0
57	MG	BA	3433	1/1	0.93	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3201	1/1	0.93	0.10	44,44,44,44	0
57	MG	AA	3019	1/1	0.93	0.25	52,52,52,52	0
57	MG	BA	3035	1/1	0.93	0.08	28,28,28,28	0
57	MG	BA	3581	1/1	0.93	0.09	55,55,55,55	0
57	MG	AA	3029	1/1	0.93	0.08	42,42,42,42	0
57	MG	AA	3110	1/1	0.93	0.29	52,52,52,52	0
57	MG	BA	3698	1/1	0.93	0.18	51,51,51,51	0
57	MG	CA	3159	1/1	0.93	0.13	46,46,46,46	0
57	MG	CA	3046	1/1	0.93	0.17	53,53,53,53	0
57	MG	BA	3214	1/1	0.93	0.20	48,48,48,48	0
57	MG	BA	3702	1/1	0.93	0.07	41,41,41,41	0
57	MG	DE	302	1/1	0.93	0.27	51,51,51,51	0
57	MG	DA	3195	1/1	0.93	0.16	42,42,42,42	0
57	MG	DF	3001	1/1	0.93	0.07	36,36,36,36	0
57	MG	DA	3196	1/1	0.93	0.12	46,46,46,46	0
57	MG	BA	3448	1/1	0.93	0.07	42,42,42,42	0
57	MG	DA	3436	1/1	0.93	0.08	61,61,61,61	0
57	MG	BA	3709	1/1	0.93	0.23	45,45,45,45	0
57	MG	BA	3589	1/1	0.93	0.10	35,35,35,35	0
57	MG	DP	202	1/1	0.93	0.12	48,48,48,48	0
57	MG	BA	3713	1/1	0.93	0.19	63,63,63,63	0
57	MG	BA	3715	1/1	0.93	0.10	33,33,33,33	0
57	MG	AA	3164	1/1	0.93	0.17	54,54,54,54	0
57	MG	BA	3325	1/1	0.93	0.07	38,38,38,38	0
57	MG	BA	3596	1/1	0.93	0.06	56,56,56,56	0
57	MG	DA	3006	1/1	0.93	0.17	40,40,40,40	0
57	MG	BB	3004	1/1	0.93	0.06	43,43,43,43	0
57	MG	DY	502	1/1	0.93	0.15	56,56,56,56	0
57	MG	AA	3055	1/1	0.93	0.28	53,53,53,53	0
59	ZN	B9	501	1/1	0.93	0.09	59,59,59,59	0
57	MG	BA	3126	1/1	0.93	0.17	34,34,34,34	0
57	MG	BU	208	1/1	0.94	0.30	39,39,39,39	0
57	MG	BA	3217	1/1	0.94	0.41	57,57,57,57	0
57	MG	BA	3018	1/1	0.94	0.17	58,58,58,58	0
57	MG	BW	205	1/1	0.94	0.09	30,30,30,30	0
57	MG	AA	3187	1/1	0.94	0.15	47,47,47,47	0
57	MG	BA	3312	1/1	0.94	0.15	44,44,44,44	0
57	MG	DA	3483	1/1	0.94	0.23	41,41,41,41	0
57	MG	AA	3023	1/1	0.94	0.07	60,60,60,60	0
57	MG	DA	3084	1/1	0.94	0.17	42,42,42,42	0
57	MG	DA	3486	1/1	0.94	0.14	37,37,37,37	0
57	MG	DA	3086	1/1	0.94	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3156	1/1	0.94	0.08	43,43,43,43	0
57	MG	DA	3490	1/1	0.94	0.11	62,62,62,62	0
57	MG	DA	3088	1/1	0.94	0.14	41,41,41,41	0
57	MG	DA	3278	1/1	0.94	0.06	38,38,38,38	0
57	MG	BA	3643	1/1	0.94	0.15	47,47,47,47	0
57	MG	BA	3161	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3542	1/1	0.94	0.10	40,40,40,40	0
57	MG	AA	3168	1/1	0.94	0.07	56,56,56,56	0
57	MG	AX	3005	1/1	0.94	0.32	57,57,57,57	0
57	MG	DA	3098	1/1	0.94	0.11	32,32,32,32	0
57	MG	CA	3112	1/1	0.94	0.07	31,31,31,31	0
57	MG	DA	3500	1/1	0.94	0.08	32,32,32,32	0
57	MG	DA	3501	1/1	0.94	0.09	47,47,47,47	0
57	MG	AX	3006	1/1	0.94	0.26	59,59,59,59	0
57	MG	BA	3654	1/1	0.94	0.16	42,42,42,42	0
57	MG	DA	3293	1/1	0.94	0.11	41,41,41,41	0
57	MG	BA	3421	1/1	0.94	0.14	29,29,29,29	0
57	MG	BA	3657	1/1	0.94	0.14	55,55,55,55	0
57	MG	BA	3028	1/1	0.94	0.14	31,31,31,31	0
57	MG	AA	3026	1/1	0.94	0.09	61,61,61,61	0
57	MG	BA	3550	1/1	0.94	0.16	60,60,60,60	0
57	MG	BA	3174	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3113	1/1	0.94	0.12	42,42,42,42	0
57	MG	BA	3556	1/1	0.94	0.13	52,52,52,52	0
57	MG	DA	3115	1/1	0.94	0.11	58,58,58,58	0
57	MG	AX	3009	1/1	0.94	0.11	50,50,50,50	0
57	MG	BA	3331	1/1	0.94	0.14	39,39,39,39	0
57	MG	DA	3522	1/1	0.94	0.09	41,41,41,41	0
57	MG	BA	3243	1/1	0.94	0.18	46,46,46,46	0
57	MG	BA	3431	1/1	0.94	0.12	25,25,25,25	0
57	MG	DA	3121	1/1	0.94	0.07	39,39,39,39	0
57	MG	AA	3094	1/1	0.94	0.15	54,54,54,54	0
57	MG	CA	3018	1/1	0.94	0.10	47,47,47,47	0
57	MG	DA	3530	1/1	0.94	0.07	43,43,43,43	0
57	MG	DA	3531	1/1	0.94	0.09	40,40,40,40	0
57	MG	DA	3532	1/1	0.94	0.09	43,43,43,43	0
57	MG	BA	3245	1/1	0.94	0.28	37,37,37,37	0
57	MG	DA	3129	1/1	0.94	0.13	41,41,41,41	0
57	MG	DA	3536	1/1	0.94	0.10	48,48,48,48	0
57	MG	BA	3435	1/1	0.94	0.11	31,31,31,31	0
57	MG	BA	3076	1/1	0.94	0.17	34,34,34,34	0
57	MG	BA	3441	1/1	0.94	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3114	1/1	0.94	0.17	41,41,41,41	0
57	MG	BA	3258	1/1	0.94	0.07	35,35,35,35	0
57	MG	DA	3137	1/1	0.94	0.17	48,48,48,48	0
57	MG	BA	3259	1/1	0.94	0.20	40,40,40,40	0
57	MG	BA	3260	1/1	0.94	0.14	45,45,45,45	0
57	MG	BA	3447	1/1	0.94	0.10	44,44,44,44	0
57	MG	BA	3342	1/1	0.94	0.15	38,38,38,38	0
57	MG	BA	3450	1/1	0.94	0.06	45,45,45,45	0
57	MG	BA	3115	1/1	0.94	0.33	49,49,49,49	0
57	MG	DA	3552	1/1	0.94	0.08	43,43,43,43	0
57	MG	BA	3690	1/1	0.94	0.14	49,49,49,49	0
57	MG	AA	3044	1/1	0.94	0.14	46,46,46,46	0
57	MG	DA	3347	1/1	0.94	0.10	32,32,32,32	0
57	MG	BA	3457	1/1	0.94	0.07	41,41,41,41	0
57	MG	DA	3155	1/1	0.94	0.11	34,34,34,34	0
57	MG	BA	3693	1/1	0.94	0.09	48,48,48,48	0
57	MG	DA	3563	1/1	0.94	0.16	55,55,55,55	0
57	MG	BA	3119	1/1	0.94	0.14	41,41,41,41	0
57	MG	BA	3123	1/1	0.94	0.10	56,56,56,56	0
57	MG	DA	3360	1/1	0.94	0.09	54,54,54,54	0
57	MG	BA	3463	1/1	0.94	0.09	43,43,43,43	0
57	MG	DA	3364	1/1	0.94	0.09	49,49,49,49	0
57	MG	BA	3267	1/1	0.94	0.25	33,33,33,33	0
57	MG	DA	3163	1/1	0.94	0.18	43,43,43,43	0
57	MG	BA	3703	1/1	0.94	0.13	47,47,47,47	0
57	MG	DA	3573	1/1	0.94	0.08	49,49,49,49	0
57	MG	DA	3368	1/1	0.94	0.07	58,58,58,58	0
57	MG	BA	3189	1/1	0.94	0.17	33,33,33,33	0
57	MG	BA	3356	1/1	0.94	0.08	36,36,36,36	0
57	MG	BA	3710	1/1	0.94	0.08	21,21,21,21	0
57	MG	BA	3711	1/1	0.94	0.24	46,46,46,46	0
57	MG	CA	3160	1/1	0.94	0.27	49,49,49,49	0
57	MG	DA	3582	1/1	0.94	0.08	24,24,24,24	0
57	MG	CA	3048	1/1	0.94	0.18	48,48,48,48	0
57	MG	DA	3585	1/1	0.94	0.15	45,45,45,45	0
57	MG	DA	3379	1/1	0.94	0.09	37,37,37,37	0
57	MG	CA	3050	1/1	0.94	0.18	56,56,56,56	0
57	MG	BA	3272	1/1	0.94	0.25	38,38,38,38	0
57	MG	BA	3358	1/1	0.94	0.07	35,35,35,35	0
57	MG	BA	3080	1/1	0.94	0.29	51,51,51,51	0
57	MG	DA	3389	1/1	0.94	0.07	31,31,31,31	0
57	MG	BA	3471	1/1	0.94	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3186	1/1	0.94	0.07	33,33,33,33	0
57	MG	DA	3392	1/1	0.94	0.16	40,40,40,40	0
57	MG	DA	3393	1/1	0.94	0.14	41,41,41,41	0
57	MG	BA	3720	1/1	0.94	0.14	48,48,48,48	0
57	MG	BA	3278	1/1	0.94	0.08	38,38,38,38	0
57	MG	BA	3364	1/1	0.94	0.10	37,37,37,37	0
57	MG	DA	3398	1/1	0.94	0.09	37,37,37,37	0
57	MG	DA	3402	1/1	0.94	0.10	47,47,47,47	0
57	MG	AA	3078	1/1	0.94	0.07	66,66,66,66	0
57	MG	BA	3280	1/1	0.94	0.21	46,46,46,46	0
57	MG	BA	3130	1/1	0.94	0.22	39,39,39,39	0
57	MG	BA	3042	1/1	0.94	0.15	34,34,34,34	0
57	MG	CA	3063	1/1	0.94	0.23	59,59,59,59	0
57	MG	BA	3286	1/1	0.94	0.12	33,33,33,33	0
57	MG	DA	3203	1/1	0.94	0.10	46,46,46,46	0
57	MG	CA	3065	1/1	0.94	0.15	60,60,60,60	0
57	MG	DA	3205	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3134	1/1	0.94	0.14	43,43,43,43	0
57	MG	DA	3418	1/1	0.94	0.10	41,41,41,41	0
57	MG	BA	3377	1/1	0.94	0.19	58,58,58,58	0
57	MG	BA	3500	1/1	0.94	0.07	54,54,54,54	0
57	MG	DA	3422	1/1	0.94	0.15	40,40,40,40	0
57	MG	BA	3043	1/1	0.94	0.09	44,44,44,44	0
57	MG	BA	3504	1/1	0.94	0.16	33,33,33,33	0
57	MG	DA	3623	1/1	0.94	0.06	31,31,31,31	0
57	MG	DA	3032	1/1	0.94	0.07	34,34,34,34	0
57	MG	BA	3616	1/1	0.94	0.08	32,32,32,32	0
57	MG	BA	3617	1/1	0.94	0.09	59,59,59,59	0
57	MG	DA	3431	1/1	0.94	0.13	56,56,56,56	0
57	MG	BA	3379	1/1	0.94	0.19	69,69,69,69	0
57	MG	BA	3295	1/1	0.94	0.11	56,56,56,56	0
57	MG	BE	3006	1/1	0.94	0.12	72,72,72,72	0
57	MG	DB	3004	1/1	0.94	0.06	38,38,38,38	0
57	MG	BA	3510	1/1	0.94	0.11	20,20,20,20	0
57	MG	BA	3047	1/1	0.94	0.08	44,44,44,44	0
57	MG	BA	3513	1/1	0.94	0.11	55,55,55,55	0
57	MG	DA	3440	1/1	0.94	0.16	44,44,44,44	0
57	MG	DD	304	1/1	0.94	0.08	40,40,40,40	0
57	MG	CA	3080	1/1	0.94	0.21	61,61,61,61	0
57	MG	BF	307	1/1	0.94	0.18	25,25,25,25	0
57	MG	AA	3087	1/1	0.94	0.10	57,57,57,57	0
57	MG	BA	3007	1/1	0.94	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3055	1/1	0.94	0.12	43,43,43,43	0
57	MG	BA	3213	1/1	0.94	0.10	48,48,48,48	0
57	MG	DE	304	1/1	0.94	0.14	47,47,47,47	0
57	MG	BN	3001	1/1	0.94	0.26	46,46,46,46	0
57	MG	DA	3055	1/1	0.94	0.09	35,35,35,35	0
57	MG	BA	3389	1/1	0.94	0.09	57,57,57,57	0
57	MG	DA	3244	1/1	0.94	0.11	43,43,43,43	0
57	MG	DN	5001	1/1	0.94	0.08	53,53,53,53	0
57	MG	BN	3004	1/1	0.94	0.33	49,49,49,49	0
57	MG	DA	3454	1/1	0.94	0.10	28,28,28,28	0
57	MG	DA	3060	1/1	0.94	0.16	50,50,50,50	0
57	MG	DA	3061	1/1	0.94	0.17	36,36,36,36	0
57	MG	AN	503	1/1	0.94	0.23	61,61,61,61	0
57	MG	DA	3251	1/1	0.94	0.25	34,34,34,34	0
57	MG	BA	3215	1/1	0.94	0.14	53,53,53,53	0
57	MG	BA	3401	1/1	0.94	0.20	31,31,31,31	0
57	MG	DU	3004	1/1	0.94	0.16	69,69,69,69	0
57	MG	BR	203	1/1	0.94	0.17	31,31,31,31	0
57	MG	DA	3467	1/1	0.94	0.07	28,28,28,28	0
57	MG	BA	3402	1/1	0.94	0.14	39,39,39,39	0
57	MG	D3	3001	1/1	0.94	0.09	54,54,54,54	0
57	MG	AA	3030	1/1	0.94	0.15	41,41,41,41	0
57	MG	CA	3095	1/1	0.94	0.16	52,52,52,52	0
57	MG	DA	3075	1/1	0.94	0.07	40,40,40,40	0
60	K	AX	3001	1/1	0.94	0.09	39,39,39,39	0
57	MG	BA	3015	1/1	0.95	0.11	50,50,50,50	0
57	MG	BA	3373	1/1	0.95	0.23	46,46,46,46	0
57	MG	BA	3483	1/1	0.95	0.09	36,36,36,36	0
57	MG	DA	3471	1/1	0.95	0.12	23,23,23,23	0
57	MG	BA	3191	1/1	0.95	0.04	22,22,22,22	0
57	MG	DA	3249	1/1	0.95	0.19	48,48,48,48	0
57	MG	BB	3011	1/1	0.95	0.06	40,40,40,40	0
57	MG	BA	3607	1/1	0.95	0.09	41,41,41,41	0
57	MG	BA	3608	1/1	0.95	0.08	50,50,50,50	0
57	MG	DA	3253	1/1	0.95	0.16	34,34,34,34	0
57	MG	DA	3058	1/1	0.95	0.08	47,47,47,47	0
57	MG	BB	3016	1/1	0.95	0.06	39,39,39,39	0
57	MG	BA	3193	1/1	0.95	0.18	30,30,30,30	0
57	MG	BA	3282	1/1	0.95	0.12	44,44,44,44	0
57	MG	BA	3195	1/1	0.95	0.11	46,46,46,46	0
57	MG	DA	3261	1/1	0.95	0.14	38,38,38,38	0
57	MG	DA	3063	1/1	0.95	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3495	1/1	0.95	0.25	47,47,47,47	0
57	MG	BD	306	1/1	0.95	0.13	30,30,30,30	0
57	MG	DA	3067	1/1	0.95	0.16	54,54,54,54	0
57	MG	DA	3267	1/1	0.95	0.18	45,45,45,45	0
57	MG	BA	3496	1/1	0.95	0.19	33,33,33,33	0
57	MG	BD	310	1/1	0.95	0.20	34,34,34,34	0
57	MG	DA	3070	1/1	0.95	0.10	35,35,35,35	0
57	MG	BA	3118	1/1	0.95	0.21	28,28,28,28	0
57	MG	AE	3002	1/1	0.95	0.14	61,61,61,61	0
57	MG	BA	3120	1/1	0.95	0.26	52,52,52,52	0
57	MG	BA	3501	1/1	0.95	0.06	67,67,67,67	0
57	MG	BA	3383	1/1	0.95	0.09	37,37,37,37	0
57	MG	BF	304	1/1	0.95	0.13	35,35,35,35	0
57	MG	DA	3279	1/1	0.95	0.18	50,50,50,50	0
57	MG	BA	3294	1/1	0.95	0.18	37,37,37,37	0
57	MG	BA	3506	1/1	0.95	0.07	39,39,39,39	0
57	MG	DA	3505	1/1	0.95	0.09	41,41,41,41	0
57	MG	AA	3015	1/1	0.95	0.08	28,28,28,28	0
57	MG	DA	3285	1/1	0.95	0.10	50,50,50,50	0
57	MG	BA	3508	1/1	0.95	0.15	52,52,52,52	0
57	MG	BA	3125	1/1	0.95	0.22	30,30,30,30	0
57	MG	BF	310	1/1	0.95	0.07	51,51,51,51	0
57	MG	AA	3194	1/1	0.95	0.18	41,41,41,41	0
57	MG	AA	3028	1/1	0.95	0.12	58,58,58,58	0
57	MG	DA	3089	1/1	0.95	0.14	36,36,36,36	0
57	MG	DA	3517	1/1	0.95	0.10	36,36,36,36	0
57	MG	DA	3518	1/1	0.95	0.06	42,42,42,42	0
57	MG	DA	3292	1/1	0.95	0.07	29,29,29,29	0
57	MG	BA	3391	1/1	0.95	0.18	30,30,30,30	0
57	MG	BA	3392	1/1	0.95	0.12	27,27,27,27	0
57	MG	BN	3003	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3129	1/1	0.95	0.05	30,30,30,30	0
57	MG	BN	3006	1/1	0.95	0.32	47,47,47,47	0
57	MG	CA	3100	1/1	0.95	0.08	48,48,48,48	0
57	MG	AA	3002	1/1	0.95	0.07	58,58,58,58	0
57	MG	DA	3103	1/1	0.95	0.16	55,55,55,55	0
57	MG	BA	3517	1/1	0.95	0.07	20,20,20,20	0
57	MG	DA	3309	1/1	0.95	0.08	34,34,34,34	0
57	MG	BA	3399	1/1	0.95	0.08	26,26,26,26	0
57	MG	BR	201	1/1	0.95	0.20	30,30,30,30	0
57	MG	BA	3131	1/1	0.95	0.26	31,31,31,31	0
57	MG	DA	3535	1/1	0.95	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3210	1/1	0.95	0.08	42,42,42,42	0
57	MG	BA	3211	1/1	0.95	0.19	50,50,50,50	0
57	MG	DA	3316	1/1	0.95	0.11	39,39,39,39	0
57	MG	BU	206	1/1	0.95	0.12	39,39,39,39	0
57	MG	AA	3012	1/1	0.95	0.28	61,61,61,61	0
57	MG	BW	201	1/1	0.95	0.17	48,48,48,48	0
57	MG	AA	3009	1/1	0.95	0.12	40,40,40,40	0
57	MG	BA	3529	1/1	0.95	0.22	29,29,29,29	0
57	MG	BA	3640	1/1	0.95	0.09	53,53,53,53	0
57	MG	BA	3641	1/1	0.95	0.09	33,33,33,33	0
57	MG	BA	3308	1/1	0.95	0.08	14,14,14,14	0
57	MG	DA	3549	1/1	0.95	0.16	47,47,47,47	0
57	MG	BA	3078	1/1	0.95	0.17	55,55,55,55	0
57	MG	BA	3410	1/1	0.95	0.10	40,40,40,40	0
57	MG	BA	3645	1/1	0.95	0.10	43,43,43,43	0
57	MG	DA	3123	1/1	0.95	0.17	45,45,45,45	0
57	MG	B3	3001	1/1	0.95	0.10	43,43,43,43	0
57	MG	DA	3126	1/1	0.95	0.13	39,39,39,39	0
57	MG	DA	3334	1/1	0.95	0.06	31,31,31,31	0
57	MG	B3	3002	1/1	0.95	0.09	58,58,58,58	0
57	MG	DA	3560	1/1	0.95	0.18	48,48,48,48	0
57	MG	DA	3336	1/1	0.95	0.15	38,38,38,38	0
57	MG	DA	3562	1/1	0.95	0.07	58,58,58,58	0
57	MG	CA	3123	1/1	0.95	0.14	53,53,53,53	0
57	MG	CA	3124	1/1	0.95	0.16	57,57,57,57	0
57	MG	B5	101	1/1	0.95	0.09	30,30,30,30	0
57	MG	DA	3345	1/1	0.95	0.08	28,28,28,28	0
57	MG	DA	3133	1/1	0.95	0.11	52,52,52,52	0
57	MG	BA	3411	1/1	0.95	0.10	24,24,24,24	0
57	MG	AA	3157	1/1	0.95	0.09	38,38,38,38	0
57	MG	AA	3088	1/1	0.95	0.16	40,40,40,40	0
57	MG	BA	3536	1/1	0.95	0.09	42,42,42,42	0
57	MG	BA	3315	1/1	0.95	0.09	42,42,42,42	0
57	MG	DA	3357	1/1	0.95	0.07	29,29,29,29	0
57	MG	BA	3655	1/1	0.95	0.16	68,68,68,68	0
57	MG	BA	3219	1/1	0.95	0.27	42,42,42,42	0
57	MG	DA	3577	1/1	0.95	0.09	25,25,25,25	0
57	MG	BA	3541	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3139	1/1	0.95	0.19	45,45,45,45	0
57	MG	AA	3071	1/1	0.95	0.25	41,41,41,41	0
57	MG	CA	3009	1/1	0.95	0.07	44,44,44,44	0
57	MG	DA	3583	1/1	0.95	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3661	1/1	0.95	0.19	56,56,56,56	0
57	MG	DA	3151	1/1	0.95	0.22	48,48,48,48	0
57	MG	BA	3662	1/1	0.95	0.27	62,62,62,62	0
57	MG	AA	3060	1/1	0.95	0.26	49,49,49,49	0
57	MG	DA	3156	1/1	0.95	0.16	46,46,46,46	0
57	MG	AX	3007	1/1	0.95	0.22	54,54,54,54	0
57	MG	CA	3141	1/1	0.95	0.20	69,69,69,69	0
57	MG	BA	3424	1/1	0.95	0.13	29,29,29,29	0
57	MG	DA	3378	1/1	0.95	0.11	33,33,33,33	0
57	MG	BA	3668	1/1	0.95	0.17	39,39,39,39	0
57	MG	BA	3149	1/1	0.95	0.07	40,40,40,40	0
57	MG	AA	3050	1/1	0.95	0.20	49,49,49,49	0
57	MG	BA	3228	1/1	0.95	0.15	33,33,33,33	0
57	MG	DA	3384	1/1	0.95	0.09	41,41,41,41	0
57	MG	BA	3038	1/1	0.95	0.06	38,38,38,38	0
57	MG	DA	3388	1/1	0.95	0.08	33,33,33,33	0
57	MG	DA	3166	1/1	0.95	0.19	47,47,47,47	0
57	MG	CA	3149	1/1	0.95	0.08	49,49,49,49	0
57	MG	DA	3169	1/1	0.95	0.12	45,45,45,45	0
57	MG	BA	3329	1/1	0.95	0.05	21,21,21,21	0
57	MG	BA	3093	1/1	0.95	0.10	23,23,23,23	0
57	MG	DA	3172	1/1	0.95	0.05	32,32,32,32	0
57	MG	AA	3076	1/1	0.95	0.31	62,62,62,62	0
57	MG	DA	3174	1/1	0.95	0.16	38,38,38,38	0
57	MG	AX	3010	1/1	0.95	0.08	61,61,61,61	0
57	MG	BA	3561	1/1	0.95	0.13	37,37,37,37	0
57	MG	BA	3564	1/1	0.95	0.17	44,44,44,44	0
57	MG	BA	3158	1/1	0.95	0.15	48,48,48,48	0
57	MG	BA	3240	1/1	0.95	0.27	52,52,52,52	0
57	MG	BA	3045	1/1	0.95	0.19	33,33,33,33	0
57	MG	AA	3165	1/1	0.95	0.13	47,47,47,47	0
57	MG	BA	3048	1/1	0.95	0.08	44,44,44,44	0
57	MG	BA	3686	1/1	0.95	0.20	36,36,36,36	0
57	MG	BA	3165	1/1	0.95	0.18	34,34,34,34	0
57	MG	DA	3413	1/1	0.95	0.18	30,30,30,30	0
57	MG	BA	3049	1/1	0.95	0.19	53,53,53,53	0
57	MG	AX	3012	1/1	0.95	0.08	15,15,15,15	0
57	MG	AA	3025	1/1	0.95	0.19	46,46,46,46	0
57	MG	BA	3173	1/1	0.95	0.19	28,28,28,28	0
57	MG	DA	3629	1/1	0.95	0.10	40,40,40,40	0
57	MG	DB	3001	1/1	0.95	0.08	50,50,50,50	0
57	MG	BA	3054	1/1	0.95	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3198	1/1	0.95	0.10	41,41,41,41	0
57	MG	DA	3424	1/1	0.95	0.09	56,56,56,56	0
57	MG	CA	3039	1/1	0.95	0.09	52,52,52,52	0
57	MG	DA	3202	1/1	0.95	0.31	41,41,41,41	0
57	MG	DB	3007	1/1	0.95	0.07	55,55,55,55	0
57	MG	DA	3427	1/1	0.95	0.07	26,26,26,26	0
57	MG	BA	3694	1/1	0.95	0.12	11,11,11,11	0
57	MG	DB	3010	1/1	0.95	0.17	55,55,55,55	0
57	MG	DD	301	1/1	0.95	0.08	31,31,31,31	0
57	MG	DD	302	1/1	0.95	0.12	50,50,50,50	0
57	MG	DA	3005	1/1	0.95	0.15	29,29,29,29	0
57	MG	BA	3452	1/1	0.95	0.07	15,15,15,15	0
57	MG	AA	3033	1/1	0.95	0.19	43,43,43,43	0
57	MG	BA	3455	1/1	0.95	0.10	44,44,44,44	0
57	MG	BA	3262	1/1	0.95	0.14	38,38,38,38	0
57	MG	BA	3059	1/1	0.95	0.27	50,50,50,50	0
57	MG	BA	3704	1/1	0.95	0.09	31,31,31,31	0
57	MG	DA	3213	1/1	0.95	0.09	51,51,51,51	0
57	MG	BA	3705	1/1	0.95	0.15	32,32,32,32	0
57	MG	AA	3148	1/1	0.95	0.10	61,61,61,61	0
57	MG	DA	3022	1/1	0.95	0.06	27,27,27,27	0
57	MG	DA	3026	1/1	0.95	0.16	41,41,41,41	0
57	MG	BA	3006	1/1	0.95	0.09	38,38,38,38	0
57	MG	AA	3130	1/1	0.95	0.17	52,52,52,52	0
57	MG	BA	3181	1/1	0.95	0.09	49,49,49,49	0
57	MG	BA	3063	1/1	0.95	0.08	39,39,39,39	0
57	MG	BA	3273	1/1	0.95	0.12	30,30,30,30	0
57	MG	DQ	3002	1/1	0.95	0.10	45,45,45,45	0
57	MG	DQ	3003	1/1	0.95	0.22	59,59,59,59	0
57	MG	DA	3229	1/1	0.95	0.18	39,39,39,39	0
57	MG	CA	3057	1/1	0.95	0.09	48,48,48,48	0
57	MG	BA	3714	1/1	0.95	0.07	42,42,42,42	0
57	MG	DA	3452	1/1	0.95	0.07	40,40,40,40	0
57	MG	DU	3003	1/1	0.95	0.13	60,60,60,60	0
57	MG	DA	3233	1/1	0.95	0.18	41,41,41,41	0
57	MG	BA	3368	1/1	0.95	0.20	26,26,26,26	0
57	MG	AA	3010	1/1	0.95	0.10	54,54,54,54	0
57	MG	DA	3040	1/1	0.95	0.17	48,48,48,48	0
57	MG	DA	3237	1/1	0.95	0.24	41,41,41,41	0
57	MG	BA	3719	1/1	0.95	0.11	53,53,53,53	0
57	MG	D8	102	1/1	0.95	0.24	63,63,63,63	0
57	MG	BA	3012	1/1	0.95	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	CN	501	1/1	0.95	0.06	101,101,101,101	0
57	MG	BA	3472	1/1	0.95	0.07	39,39,39,39	0
57	MG	BA	3371	1/1	0.95	0.12	53,53,53,53	0
60	K	CX	3001	1/1	0.95	0.07	54,54,54,54	0
57	MG	DA	3023	1/1	0.96	0.09	35,35,35,35	0
57	MG	BA	3321	1/1	0.96	0.09	31,31,31,31	0
57	MG	BA	3122	1/1	0.96	0.12	39,39,39,39	0
57	MG	AA	3072	1/1	0.96	0.27	65,65,65,65	0
57	MG	DA	3031	1/1	0.96	0.05	36,36,36,36	0
57	MG	BQ	3001	1/1	0.96	0.22	51,51,51,51	0
57	MG	BQ	3002	1/1	0.96	0.25	39,39,39,39	0
57	MG	DA	3338	1/1	0.96	0.07	36,36,36,36	0
57	MG	BA	3390	1/1	0.96	0.06	31,31,31,31	0
57	MG	DA	3179	1/1	0.96	0.27	50,50,50,50	0
57	MG	DA	3180	1/1	0.96	0.30	41,41,41,41	0
57	MG	BQ	3004	1/1	0.96	0.13	35,35,35,35	0
57	MG	BQ	3005	1/1	0.96	0.11	39,39,39,39	0
57	MG	DA	3350	1/1	0.96	0.25	44,44,44,44	0
57	MG	BA	3667	1/1	0.96	0.11	31,31,31,31	0
57	MG	BR	202	1/1	0.96	0.16	49,49,49,49	0
57	MG	BA	3206	1/1	0.96	0.05	37,37,37,37	0
57	MG	BA	3092	1/1	0.96	0.06	32,32,32,32	0
57	MG	BA	3476	1/1	0.96	0.07	37,37,37,37	0
57	MG	BA	3394	1/1	0.96	0.09	22,22,22,22	0
57	MG	BA	3578	1/1	0.96	0.06	43,43,43,43	0
57	MG	BV	202	1/1	0.96	0.13	29,29,29,29	0
57	MG	DA	3192	1/1	0.96	0.13	31,31,31,31	0
57	MG	BV	203	1/1	0.96	0.06	31,31,31,31	0
57	MG	DA	3540	1/1	0.96	0.05	43,43,43,43	0
57	MG	DA	3194	1/1	0.96	0.10	43,43,43,43	0
57	MG	DA	3049	1/1	0.96	0.19	46,46,46,46	0
57	MG	DA	3050	1/1	0.96	0.16	48,48,48,48	0
57	MG	DA	3197	1/1	0.96	0.10	35,35,35,35	0
57	MG	BA	3396	1/1	0.96	0.15	20,20,20,20	0
57	MG	DA	3371	1/1	0.96	0.11	47,47,47,47	0
57	MG	DA	3200	1/1	0.96	0.08	38,38,38,38	0
57	MG	BA	3167	1/1	0.96	0.25	51,51,51,51	0
57	MG	BA	3676	1/1	0.96	0.17	44,44,44,44	0
57	MG	BW	204	1/1	0.96	0.12	27,27,27,27	0
57	MG	BA	3582	1/1	0.96	0.09	23,23,23,23	0
57	MG	BX	101	1/1	0.96	0.11	36,36,36,36	0
57	MG	DA	3206	1/1	0.96	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3484	1/1	0.96	0.09	50,50,50,50	0
57	MG	B0	101	1/1	0.96	0.07	33,33,33,33	0
57	MG	BA	3169	1/1	0.96	0.12	40,40,40,40	0
57	MG	BA	3212	1/1	0.96	0.18	24,24,24,24	0
57	MG	DA	3387	1/1	0.96	0.07	29,29,29,29	0
57	MG	BA	3489	1/1	0.96	0.14	36,36,36,36	0
57	MG	BA	3170	1/1	0.96	0.10	41,41,41,41	0
57	MG	DA	3214	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3215	1/1	0.96	0.06	35,35,35,35	0
57	MG	DA	3065	1/1	0.96	0.10	38,38,38,38	0
57	MG	DA	3218	1/1	0.96	0.05	36,36,36,36	0
57	MG	BA	3010	1/1	0.96	0.17	45,45,45,45	0
57	MG	BA	3403	1/1	0.96	0.08	22,22,22,22	0
57	MG	BA	3036	1/1	0.96	0.35	42,42,42,42	0
57	MG	BA	3275	1/1	0.96	0.10	38,38,38,38	0
57	MG	BA	3498	1/1	0.96	0.14	45,45,45,45	0
57	MG	DA	3071	1/1	0.96	0.09	42,42,42,42	0
57	MG	DA	3405	1/1	0.96	0.12	45,45,45,45	0
57	MG	B8	101	1/1	0.96	0.11	34,34,34,34	0
57	MG	DA	3073	1/1	0.96	0.23	49,49,49,49	0
57	MG	B9	502	1/1	0.96	0.07	31,31,31,31	0
57	MG	AA	3135	1/1	0.96	0.10	52,52,52,52	0
57	MG	DA	3231	1/1	0.96	0.12	33,33,33,33	0
57	MG	AA	3136	1/1	0.96	0.08	43,43,43,43	0
57	MG	BA	3218	1/1	0.96	0.34	52,52,52,52	0
57	MG	AA	3037	1/1	0.96	0.07	48,48,48,48	0
57	MG	BA	3176	1/1	0.96	0.10	35,35,35,35	0
57	MG	BA	3044	1/1	0.96	0.06	40,40,40,40	0
57	MG	BA	3345	1/1	0.96	0.09	36,36,36,36	0
57	MG	BA	3414	1/1	0.96	0.17	59,59,59,59	0
57	MG	BA	3071	1/1	0.96	0.19	48,48,48,48	0
57	MG	DA	3421	1/1	0.96	0.07	31,31,31,31	0
57	MG	BA	3348	1/1	0.96	0.05	17,17,17,17	0
57	MG	AA	3096	1/1	0.96	0.11	57,57,57,57	0
57	MG	DA	3243	1/1	0.96	0.26	41,41,41,41	0
57	MG	AA	3074	1/1	0.96	0.16	38,38,38,38	0
57	MG	BA	3289	1/1	0.96	0.12	41,41,41,41	0
57	MG	DA	3597	1/1	0.96	0.06	42,42,42,42	0
57	MG	DA	3598	1/1	0.96	0.12	48,48,48,48	0
57	MG	BA	3352	1/1	0.96	0.11	29,29,29,29	0
57	MG	BA	3290	1/1	0.96	0.06	43,43,43,43	0
57	MG	DA	3092	1/1	0.96	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3354	1/1	0.96	0.06	31,31,31,31	0
57	MG	BA	3518	1/1	0.96	0.12	48,48,48,48	0
57	MG	DA	3096	1/1	0.96	0.11	52,52,52,52	0
57	MG	BA	3355	1/1	0.96	0.06	30,30,30,30	0
57	MG	AA	3185	1/1	0.96	0.07	50,50,50,50	0
57	MG	DA	3100	1/1	0.96	0.21	38,38,38,38	0
57	MG	BA	3106	1/1	0.96	0.16	24,24,24,24	0
57	MG	BA	3142	1/1	0.96	0.11	35,35,35,35	0
57	MG	BA	3524	1/1	0.96	0.09	39,39,39,39	0
57	MG	AA	3128	1/1	0.96	0.23	53,53,53,53	0
57	MG	BA	3432	1/1	0.96	0.15	35,35,35,35	0
57	MG	AA	3022	1/1	0.96	0.09	57,57,57,57	0
57	MG	DA	3108	1/1	0.96	0.10	50,50,50,50	0
57	MG	DA	3616	1/1	0.96	0.06	28,28,28,28	0
57	MG	AK	3001	1/1	0.96	0.12	55,55,55,55	0
57	MG	BB	3003	1/1	0.96	0.16	40,40,40,40	0
57	MG	BA	3365	1/1	0.96	0.09	40,40,40,40	0
57	MG	BA	3436	1/1	0.96	0.09	21,21,21,21	0
57	MG	BB	3006	1/1	0.96	0.15	42,42,42,42	0
57	MG	BA	3236	1/1	0.96	0.10	39,39,39,39	0
57	MG	BA	3439	1/1	0.96	0.07	12,12,12,12	0
57	MG	CA	3142	1/1	0.96	0.16	55,55,55,55	0
57	MG	BA	3440	1/1	0.96	0.13	40,40,40,40	0
57	MG	BA	3367	1/1	0.96	0.06	42,42,42,42	0
57	MG	BB	3013	1/1	0.96	0.16	43,43,43,43	0
57	MG	BA	3237	1/1	0.96	0.10	36,36,36,36	0
57	MG	DA	3459	1/1	0.96	0.31	40,40,40,40	0
57	MG	BA	3001	1/1	0.96	0.33	48,48,48,48	0
57	MG	DA	3281	1/1	0.96	0.07	37,37,37,37	0
57	MG	BA	3239	1/1	0.96	0.08	42,42,42,42	0
57	MG	DA	3463	1/1	0.96	0.07	54,54,54,54	0
57	MG	DA	3465	1/1	0.96	0.13	45,45,45,45	0
57	MG	DA	3124	1/1	0.96	0.12	30,30,30,30	0
57	MG	CA	3040	1/1	0.96	0.24	67,67,67,67	0
57	MG	BA	3194	1/1	0.96	0.21	42,42,42,42	0
57	MG	CA	3151	1/1	0.96	0.07	58,58,58,58	0
57	MG	AA	3083	1/1	0.96	0.26	38,38,38,38	0
57	MG	BA	3242	1/1	0.96	0.17	45,45,45,45	0
57	MG	DD	303	1/1	0.96	0.14	42,42,42,42	0
57	MG	DA	3474	1/1	0.96	0.13	52,52,52,52	0
57	MG	BA	3449	1/1	0.96	0.06	31,31,31,31	0
57	MG	BA	3546	1/1	0.96	0.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BD	309	1/1	0.96	0.15	33,33,33,33	0
57	MG	CA	3047	1/1	0.96	0.14	50,50,50,50	0
57	MG	BA	3058	1/1	0.96	0.11	24,24,24,24	0
57	MG	CA	3049	1/1	0.96	0.09	42,42,42,42	0
57	MG	BA	3083	1/1	0.96	0.15	33,33,33,33	0
57	MG	BA	3376	1/1	0.96	0.11	21,21,21,21	0
57	MG	DF	3002	1/1	0.96	0.11	51,51,51,51	0
57	MG	BA	3453	1/1	0.96	0.09	47,47,47,47	0
57	MG	BE	3003	1/1	0.96	0.09	25,25,25,25	0
57	MG	DA	3305	1/1	0.96	0.07	48,48,48,48	0
57	MG	BE	3004	1/1	0.96	0.07	49,49,49,49	0
57	MG	DA	3489	1/1	0.96	0.07	38,38,38,38	0
57	MG	BA	3552	1/1	0.96	0.10	59,59,59,59	0
57	MG	DA	3147	1/1	0.96	0.06	42,42,42,42	0
57	MG	BF	301	1/1	0.96	0.05	30,30,30,30	0
57	MG	DA	3311	1/1	0.96	0.08	42,42,42,42	0
57	MG	BA	3647	1/1	0.96	0.09	41,41,41,41	0
57	MG	AA	3045	1/1	0.96	0.08	44,44,44,44	0
57	MG	BA	3246	1/1	0.96	0.11	46,46,46,46	0
57	MG	BA	3650	1/1	0.96	0.06	49,49,49,49	0
57	MG	BA	3314	1/1	0.96	0.22	42,42,42,42	0
57	MG	BA	3458	1/1	0.96	0.06	40,40,40,40	0
57	MG	BA	3087	1/1	0.96	0.17	44,44,44,44	0
57	MG	DV	201	1/1	0.96	0.10	49,49,49,49	0
57	MG	BA	3254	1/1	0.96	0.14	30,30,30,30	0
57	MG	BA	3382	1/1	0.96	0.09	31,31,31,31	0
57	MG	DW	202	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3161	1/1	0.96	0.09	35,35,35,35	0
57	MG	AA	3092	1/1	0.96	0.11	36,36,36,36	0
57	MG	DA	3323	1/1	0.96	0.06	39,39,39,39	0
57	MG	BA	3658	1/1	0.96	0.06	16,16,16,16	0
57	MG	DA	3018	1/1	0.96	0.32	51,51,51,51	0
57	MG	BA	3089	1/1	0.96	0.11	30,30,30,30	0
57	MG	AA	3102	1/1	0.96	0.21	52,52,52,52	0
57	MG	BA	3568	1/1	0.96	0.16	43,43,43,43	0
57	MG	DA	3512	1/1	0.96	0.05	24,24,24,24	0
57	MG	DA	3052	1/1	0.97	0.07	33,33,33,33	0
57	MG	BA	3327	1/1	0.97	0.09	32,32,32,32	0
57	MG	BA	3594	1/1	0.97	0.11	34,34,34,34	0
57	MG	BA	3256	1/1	0.97	0.09	36,36,36,36	0
57	MG	BA	3146	1/1	0.97	0.12	47,47,47,47	0
57	MG	DA	3344	1/1	0.97	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3147	1/1	0.97	0.09	34,34,34,34	0
57	MG	AA	3082	1/1	0.97	0.08	55,55,55,55	0
57	MG	CA	3101	1/1	0.97	0.13	41,41,41,41	0
57	MG	DA	3349	1/1	0.97	0.11	35,35,35,35	0
57	MG	AA	3116	1/1	0.97	0.13	41,41,41,41	0
57	MG	BA	3150	1/1	0.97	0.17	40,40,40,40	0
57	MG	DA	3352	1/1	0.97	0.12	25,25,25,25	0
57	MG	BA	3110	1/1	0.97	0.12	40,40,40,40	0
57	MG	DA	3354	1/1	0.97	0.13	25,25,25,25	0
57	MG	DA	3199	1/1	0.97	0.05	41,41,41,41	0
57	MG	B5	103	1/1	0.97	0.06	50,50,50,50	0
57	MG	BA	3202	1/1	0.97	0.19	42,42,42,42	0
57	MG	AM	201	1/1	0.97	0.04	43,43,43,43	0
57	MG	DA	3359	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3701	1/1	0.97	0.12	17,17,17,17	0
57	MG	AA	3103	1/1	0.97	0.15	42,42,42,42	0
57	MG	AA	3070	1/1	0.97	0.22	43,43,43,43	0
57	MG	BA	3268	1/1	0.97	0.07	45,45,45,45	0
57	MG	BA	3269	1/1	0.97	0.09	30,30,30,30	0
57	MG	BA	3418	1/1	0.97	0.11	26,26,26,26	0
57	MG	BA	3270	1/1	0.97	0.23	47,47,47,47	0
57	MG	BA	3022	1/1	0.97	0.20	47,47,47,47	0
57	MG	DA	3211	1/1	0.97	0.05	43,43,43,43	0
57	MG	BA	3023	1/1	0.97	0.07	25,25,25,25	0
57	MG	BA	3423	1/1	0.97	0.10	26,26,26,26	0
57	MG	DA	3373	1/1	0.97	0.12	43,43,43,43	0
57	MG	BA	3208	1/1	0.97	0.04	33,33,33,33	0
57	MG	BA	3274	1/1	0.97	0.17	44,44,44,44	0
57	MG	DA	3216	1/1	0.97	0.17	43,43,43,43	0
57	MG	DA	3377	1/1	0.97	0.07	31,31,31,31	0
57	MG	BA	3209	1/1	0.97	0.16	32,32,32,32	0
57	MG	BA	3716	1/1	0.97	0.10	53,53,53,53	0
57	MG	BA	3159	1/1	0.97	0.10	43,43,43,43	0
57	MG	AA	3167	1/1	0.97	0.05	65,65,65,65	0
57	MG	DA	3382	1/1	0.97	0.09	20,20,20,20	0
57	MG	DA	3221	1/1	0.97	0.09	49,49,49,49	0
57	MG	DA	3556	1/1	0.97	0.08	49,49,49,49	0
57	MG	DA	3222	1/1	0.97	0.09	38,38,38,38	0
57	MG	DA	3083	1/1	0.97	0.07	30,30,30,30	0
57	MG	DA	3386	1/1	0.97	0.12	39,39,39,39	0
57	MG	BA	3117	1/1	0.97	0.11	24,24,24,24	0
57	MG	DA	3085	1/1	0.97	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3163	1/1	0.97	0.16	43,43,43,43	0
57	MG	BA	3522	1/1	0.97	0.06	34,34,34,34	0
57	MG	BA	3025	1/1	0.97	0.09	12,12,12,12	0
57	MG	BA	3056	1/1	0.97	0.10	21,21,21,21	0
57	MG	BA	3026	1/1	0.97	0.18	36,36,36,36	0
57	MG	BA	3624	1/1	0.97	0.09	26,26,26,26	0
57	MG	BB	3007	1/1	0.97	0.05	51,51,51,51	0
57	MG	BA	3285	1/1	0.97	0.10	21,21,21,21	0
57	MG	CA	3024	1/1	0.97	0.09	58,58,58,58	0
57	MG	BA	3527	1/1	0.97	0.14	37,37,37,37	0
57	MG	BA	3121	1/1	0.97	0.16	48,48,48,48	0
57	MG	BA	3361	1/1	0.97	0.08	38,38,38,38	0
57	MG	BA	3438	1/1	0.97	0.09	19,19,19,19	0
57	MG	DA	3101	1/1	0.97	0.16	45,45,45,45	0
57	MG	DA	3240	1/1	0.97	0.18	36,36,36,36	0
57	MG	BA	3362	1/1	0.97	0.06	43,43,43,43	0
57	MG	DA	3580	1/1	0.97	0.05	47,47,47,47	0
57	MG	BA	3168	1/1	0.97	0.04	32,32,32,32	0
57	MG	BB	3017	1/1	0.97	0.05	28,28,28,28	0
57	MG	BA	3288	1/1	0.97	0.05	37,37,37,37	0
57	MG	AA	3081	1/1	0.97	0.10	44,44,44,44	0
57	MG	DA	3414	1/1	0.97	0.08	37,37,37,37	0
57	MG	AW	101	1/1	0.97	0.12	24,24,24,24	0
57	MG	DA	3416	1/1	0.97	0.08	46,46,46,46	0
57	MG	DA	3247	1/1	0.97	0.08	43,43,43,43	0
57	MG	BD	301	1/1	0.97	0.20	37,37,37,37	0
57	MG	BA	3291	1/1	0.97	0.16	44,44,44,44	0
57	MG	BD	303	1/1	0.97	0.26	42,42,42,42	0
57	MG	BD	304	1/1	0.97	0.07	36,36,36,36	0
57	MG	BD	305	1/1	0.97	0.11	41,41,41,41	0
57	MG	DA	3423	1/1	0.97	0.15	33,33,33,33	0
57	MG	BA	3538	1/1	0.97	0.07	25,25,25,25	0
57	MG	BA	3539	1/1	0.97	0.11	18,18,18,18	0
57	MG	BA	3292	1/1	0.97	0.10	26,26,26,26	0
57	MG	DA	3116	1/1	0.97	0.05	36,36,36,36	0
57	MG	DA	3257	1/1	0.97	0.25	46,46,46,46	0
57	MG	DA	3258	1/1	0.97	0.16	32,32,32,32	0
57	MG	BA	3124	1/1	0.97	0.06	31,31,31,31	0
57	MG	AA	3169	1/1	0.97	0.16	48,48,48,48	0
57	MG	BA	3030	1/1	0.97	0.07	44,44,44,44	0
57	MG	DA	3433	1/1	0.97	0.11	27,27,27,27	0
57	MG	BA	3296	1/1	0.97	0.11	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	3112	1/1	0.97	0.09	44,44,44,44	0
57	MG	BA	3095	1/1	0.97	0.13	29,29,29,29	0
57	MG	BA	3008	1/1	0.97	0.06	22,22,22,22	0
57	MG	DA	3438	1/1	0.97	0.12	42,42,42,42	0
57	MG	AA	3095	1/1	0.97	0.14	44,44,44,44	0
57	MG	BA	3067	1/1	0.97	0.21	26,26,26,26	0
57	MG	BF	303	1/1	0.97	0.09	35,35,35,35	0
57	MG	BA	3456	1/1	0.97	0.13	44,44,44,44	0
57	MG	BA	3551	1/1	0.97	0.10	17,17,17,17	0
57	MG	BA	3232	1/1	0.97	0.09	31,31,31,31	0
57	MG	BA	3653	1/1	0.97	0.12	51,51,51,51	0
57	MG	BA	3553	1/1	0.97	0.10	41,41,41,41	0
57	MG	BA	3133	1/1	0.97	0.19	29,29,29,29	0
57	MG	BA	3459	1/1	0.97	0.20	44,44,44,44	0
57	MG	BA	3234	1/1	0.97	0.22	39,39,39,39	0
57	MG	BA	3461	1/1	0.97	0.12	32,32,32,32	0
57	MG	BA	3034	1/1	0.97	0.06	21,21,21,21	0
57	MG	DA	3282	1/1	0.97	0.11	36,36,36,36	0
57	MG	BA	3101	1/1	0.97	0.12	29,29,29,29	0
57	MG	DA	3140	1/1	0.97	0.09	38,38,38,38	0
57	MG	DA	3008	1/1	0.97	0.07	26,26,26,26	0
57	MG	BA	3562	1/1	0.97	0.14	47,47,47,47	0
57	MG	DA	3143	1/1	0.97	0.13	47,47,47,47	0
57	MG	BA	3384	1/1	0.97	0.15	19,19,19,19	0
57	MG	DA	3145	1/1	0.97	0.13	38,38,38,38	0
57	MG	BN	3005	1/1	0.97	0.06	31,31,31,31	0
57	MG	DA	3014	1/1	0.97	0.07	45,45,45,45	0
57	MG	DA	3016	1/1	0.97	0.07	34,34,34,34	0
57	MG	DA	3464	1/1	0.97	0.07	51,51,51,51	0
57	MG	BA	3663	1/1	0.97	0.08	36,36,36,36	0
57	MG	DA	3466	1/1	0.97	0.12	41,41,41,41	0
57	MG	DA	3294	1/1	0.97	0.11	18,18,18,18	0
57	MG	BA	3182	1/1	0.97	0.14	36,36,36,36	0
57	MG	AA	3147	1/1	0.97	0.06	51,51,51,51	0
57	MG	DA	3470	1/1	0.97	0.06	34,34,34,34	0
57	MG	DA	3298	1/1	0.97	0.09	35,35,35,35	0
57	MG	DA	3299	1/1	0.97	0.05	32,32,32,32	0
57	MG	DA	3153	1/1	0.97	0.10	34,34,34,34	0
57	MG	DA	3154	1/1	0.97	0.11	40,40,40,40	0
57	MG	DA	3020	1/1	0.97	0.09	32,32,32,32	0
57	MG	BP	3003	1/1	0.97	0.08	42,42,42,42	0
57	MG	BA	3184	1/1	0.97	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3137	1/1	0.97	0.06	57,57,57,57	0
57	MG	DA	3024	1/1	0.97	0.10	29,29,29,29	0
57	MG	DA	3480	1/1	0.97	0.06	28,28,28,28	0
57	MG	BA	3469	1/1	0.97	0.13	42,42,42,42	0
57	MG	DA	3482	1/1	0.97	0.14	31,31,31,31	0
57	MG	AA	3138	1/1	0.97	0.13	40,40,40,40	0
57	MG	BA	3670	1/1	0.97	0.07	25,25,25,25	0
57	MG	DA	3029	1/1	0.97	0.08	44,44,44,44	0
57	MG	BA	3013	1/1	0.97	0.09	36,36,36,36	0
57	MG	BA	3190	1/1	0.97	0.15	24,24,24,24	0
57	MG	BA	3141	1/1	0.97	0.09	38,38,38,38	0
57	MG	BA	3192	1/1	0.97	0.04	35,35,35,35	0
57	MG	BA	3395	1/1	0.97	0.11	19,19,19,19	0
57	MG	BU	204	1/1	0.97	0.15	38,38,38,38	0
57	MG	BU	205	1/1	0.97	0.07	32,32,32,32	0
57	MG	BA	3481	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3040	1/1	0.97	0.13	28,28,28,28	0
57	MG	DA	3041	1/1	0.97	0.06	36,36,36,36	0
57	MG	DA	3176	1/1	0.97	0.12	42,42,42,42	0
57	MG	AA	3091	1/1	0.97	0.15	35,35,35,35	0
57	MG	DA	3325	1/1	0.97	0.07	43,43,43,43	0
57	MG	BA	3249	1/1	0.97	0.19	44,44,44,44	0
57	MG	DA	3044	1/1	0.97	0.09	38,38,38,38	0
57	MG	BA	3485	1/1	0.97	0.08	40,40,40,40	0
57	MG	BA	3251	1/1	0.97	0.26	48,48,48,48	0
57	MG	BA	3016	1/1	0.97	0.07	35,35,35,35	0
58	SF4	AD	302	8/8	0.97	0.06	59,71,78,78	0
58	SF4	CD	501	8/8	0.97	0.05	59,71,83,91	0
57	MG	BA	3255	1/1	0.97	0.05	37,37,37,37	0
57	MG	BA	3490	1/1	0.97	0.12	17,17,17,17	0
57	MG	DA	3333	1/1	0.97	0.09	41,41,41,41	0
59	ZN	D9	501	1/1	0.97	0.05	75,75,75,75	0
57	MG	BA	3491	1/1	0.97	0.08	33,33,33,33	0
57	MG	BY	201	1/1	0.97	0.08	51,51,51,51	0
57	MG	BA	3563	1/1	0.98	0.04	38,38,38,38	0
57	MG	BA	3248	1/1	0.98	0.15	32,32,32,32	0
57	MG	BA	3157	1/1	0.98	0.04	42,42,42,42	0
57	MG	BA	3250	1/1	0.98	0.06	47,47,47,47	0
57	MG	BA	3473	1/1	0.98	0.07	31,31,31,31	0
57	MG	DA	3150	1/1	0.98	0.27	41,41,41,41	0
57	MG	AX	3004	1/1	0.98	0.07	45,45,45,45	0
57	MG	BU	203	1/1	0.98	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3393	1/1	0.98	0.07	30,30,30,30	0
57	MG	DA	3599	1/1	0.98	0.13	36,36,36,36	0
57	MG	BB	3010	1/1	0.98	0.09	28,28,28,28	0
57	MG	BA	3479	1/1	0.98	0.07	22,22,22,22	0
57	MG	DA	3004	1/1	0.98	0.16	32,32,32,32	0
57	MG	BU	207	1/1	0.98	0.07	23,23,23,23	0
57	MG	DA	3507	1/1	0.98	0.05	33,33,33,33	0
57	MG	BA	3283	1/1	0.98	0.18	22,22,22,22	0
57	MG	BV	201	1/1	0.98	0.10	33,33,33,33	0
57	MG	BA	3252	1/1	0.98	0.19	30,30,30,30	0
57	MG	BA	3528	1/1	0.98	0.10	37,37,37,37	0
57	MG	BV	204	1/1	0.98	0.04	36,36,36,36	0
57	MG	DA	3012	1/1	0.98	0.06	42,42,42,42	0
57	MG	BA	3253	1/1	0.98	0.21	28,28,28,28	0
57	MG	BA	3057	1/1	0.98	0.10	21,21,21,21	0
57	MG	DA	3015	1/1	0.98	0.24	41,41,41,41	0
57	MG	DA	3167	1/1	0.98	0.08	26,26,26,26	0
57	MG	BA	3226	1/1	0.98	0.24	36,36,36,36	0
57	MG	BA	3227	1/1	0.98	0.16	39,39,39,39	0
57	MG	BA	3160	1/1	0.98	0.10	23,23,23,23	0
57	MG	BA	3580	1/1	0.98	0.17	13,13,13,13	0
57	MG	DA	3523	1/1	0.98	0.07	45,45,45,45	0
57	MG	DA	3620	1/1	0.98	0.13	47,47,47,47	0
57	MG	DA	3341	1/1	0.98	0.06	32,32,32,32	0
57	MG	DA	3525	1/1	0.98	0.04	40,40,40,40	0
57	MG	AA	3052	1/1	0.98	0.12	53,53,53,53	0
57	MG	DA	3094	1/1	0.98	0.13	38,38,38,38	0
57	MG	BA	3326	1/1	0.98	0.06	40,40,40,40	0
57	MG	BA	3046	1/1	0.98	0.05	30,30,30,30	0
57	MG	BA	3405	1/1	0.98	0.09	31,31,31,31	0
57	MG	BA	3687	1/1	0.98	0.11	30,30,30,30	0
57	MG	DA	3348	1/1	0.98	0.08	33,33,33,33	0
57	MG	DA	3099	1/1	0.98	0.06	40,40,40,40	0
57	MG	DA	3025	1/1	0.98	0.15	35,35,35,35	0
57	MG	BD	307	1/1	0.98	0.10	40,40,40,40	0
57	MG	BA	3231	1/1	0.98	0.19	42,42,42,42	0
57	MG	DA	3183	1/1	0.98	0.10	31,31,31,31	0
57	MG	DA	3264	1/1	0.98	0.04	33,33,33,33	0
57	MG	B2	3001	1/1	0.98	0.06	43,43,43,43	0
57	MG	BA	3586	1/1	0.98	0.04	33,33,33,33	0
57	MG	DA	3541	1/1	0.98	0.07	40,40,40,40	0
57	MG	DA	3030	1/1	0.98	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3037	1/1	0.98	0.08	38,38,38,38	0
57	MG	DA	3451	1/1	0.98	0.14	39,39,39,39	0
57	MG	BA	3330	1/1	0.98	0.08	14,14,14,14	0
57	MG	DA	3033	1/1	0.98	0.11	46,46,46,46	0
57	MG	AA	3181	1/1	0.98	0.07	82,82,82,82	0
57	MG	BA	3591	1/1	0.98	0.04	42,42,42,42	0
57	MG	BA	3593	1/1	0.98	0.07	36,36,36,36	0
57	MG	DA	3275	1/1	0.98	0.10	36,36,36,36	0
57	MG	BA	3695	1/1	0.98	0.10	19,19,19,19	0
57	MG	BA	3187	1/1	0.98	0.06	35,35,35,35	0
57	MG	BE	3007	1/1	0.98	0.09	31,31,31,31	0
57	MG	BA	3039	1/1	0.98	0.04	27,27,27,27	0
57	MG	BA	3699	1/1	0.98	0.04	33,33,33,33	0
57	MG	BA	3646	1/1	0.98	0.06	43,43,43,43	0
57	MG	DA	3557	1/1	0.98	0.07	54,54,54,54	0
57	MG	BA	3145	1/1	0.98	0.14	41,41,41,41	0
57	MG	BA	3014	1/1	0.98	0.15	46,46,46,46	0
57	MG	CA	3072	1/1	0.98	0.31	38,38,38,38	0
57	MG	BA	3128	1/1	0.98	0.07	33,33,33,33	0
57	MG	BA	3096	1/1	0.98	0.11	39,39,39,39	0
57	MG	BA	3051	1/1	0.98	0.10	36,36,36,36	0
57	MG	BA	3706	1/1	0.98	0.19	27,27,27,27	0
57	MG	BA	3065	1/1	0.98	0.18	43,43,43,43	0
57	MG	BA	3708	1/1	0.98	0.13	38,38,38,38	0
57	MG	DA	3127	1/1	0.98	0.22	40,40,40,40	0
57	MG	BA	3341	1/1	0.98	0.04	52,52,52,52	0
57	MG	BA	3041	1/1	0.98	0.10	39,39,39,39	0
57	MG	BA	3053	1/1	0.98	0.06	33,33,33,33	0
57	MG	DA	3131	1/1	0.98	0.12	34,34,34,34	0
57	MG	BA	3305	1/1	0.98	0.10	45,45,45,45	0
57	MG	BA	3554	1/1	0.98	0.05	44,44,44,44	0
57	MG	DA	3057	1/1	0.98	0.13	22,22,22,22	0
57	MG	BA	3346	1/1	0.98	0.12	29,29,29,29	0
57	MG	AA	3149	1/1	0.98	0.08	48,48,48,48	0
57	MG	DA	3302	1/1	0.98	0.11	30,30,30,30	0
57	MG	D5	101	1/1	0.98	0.09	42,42,42,42	0
57	MG	BA	3557	1/1	0.98	0.10	35,35,35,35	0
57	MG	BA	3154	1/1	0.98	0.12	36,36,36,36	0
57	MG	DA	3395	1/1	0.98	0.03	31,31,31,31	0
57	MG	BP	3002	1/1	0.98	0.16	32,32,32,32	0
59	ZN	AN	501	1/1	0.98	0.05	71,71,71,71	0
59	ZN	B4	501	1/1	0.98	0.04	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3718	1/1	0.98	0.05	36,36,36,36	0
57	MG	BA	3276	1/1	0.98	0.13	19,19,19,19	0
57	MG	BA	3427	1/1	0.98	0.08	23,23,23,23	0
57	MG	DA	3403	1/1	0.98	0.09	31,31,31,31	0
57	MG	BA	3085	1/1	0.98	0.07	18,18,18,18	0
57	MG	BA	3004	1/1	0.98	0.06	26,26,26,26	0
57	MG	BA	3475	1/1	0.99	0.04	31,31,31,31	0
57	MG	DA	3175	1/1	0.99	0.08	42,42,42,42	0
57	MG	BA	3572	1/1	0.99	0.09	27,27,27,27	0
57	MG	BA	3319	1/1	0.99	0.06	37,37,37,37	0
57	MG	BA	3477	1/1	0.99	0.04	19,19,19,19	0
57	MG	BA	3332	1/1	0.99	0.08	29,29,29,29	0
57	MG	BA	3081	1/1	0.99	0.07	26,26,26,26	0
57	MG	BA	3503	1/1	0.99	0.05	50,50,50,50	0
57	MG	BA	3186	1/1	0.99	0.14	42,42,42,42	0
57	MG	CA	3108	1/1	0.99	0.06	51,51,51,51	0
57	MG	BA	3505	1/1	0.99	0.09	16,16,16,16	0
57	MG	DA	3009	1/1	0.99	0.06	39,39,39,39	0
57	MG	DA	3295	1/1	0.99	0.05	58,58,58,58	0
57	MG	BA	3363	1/1	0.99	0.05	31,31,31,31	0
57	MG	BA	3444	1/1	0.99	0.09	32,32,32,32	0
57	MG	AA	3182	1/1	0.99	0.04	40,40,40,40	0
57	MG	DA	3516	1/1	0.99	0.03	43,43,43,43	0
57	MG	BA	3311	1/1	0.99	0.05	42,42,42,42	0
57	MG	DA	3339	1/1	0.99	0.05	23,23,23,23	0
57	MG	BA	3637	1/1	0.99	0.07	40,40,40,40	0
57	MG	BA	3077	1/1	0.99	0.09	33,33,33,33	0
57	MG	BA	3140	1/1	0.99	0.16	26,26,26,26	0
57	MG	BP	3004	1/1	0.99	0.06	41,41,41,41	0
57	MG	BA	3488	1/1	0.99	0.03	34,34,34,34	0
57	MG	BA	3009	1/1	0.99	0.03	34,34,34,34	0
57	MG	DA	3306	1/1	0.99	0.06	31,31,31,31	0
57	MG	BA	3588	1/1	0.99	0.06	19,19,19,19	0
57	MG	BA	3697	1/1	0.99	0.06	23,23,23,23	0
57	MG	AA	3159	1/1	0.99	0.04	31,31,31,31	0
57	MG	CA	3156	1/1	0.99	0.06	57,57,57,57	0
57	MG	DA	3272	1/1	0.99	0.04	29,29,29,29	0
57	MG	BE	3005	1/1	0.99	0.06	15,15,15,15	0
57	MG	BA	3400	1/1	0.99	0.09	33,33,33,33	0
57	MG	B7	101	1/1	0.99	0.07	48,48,48,48	0
57	MG	BA	3086	1/1	0.99	0.08	15,15,15,15	0
57	MG	DA	3399	1/1	0.99	0.06	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3400	1/1	0.99	0.03	33,33,33,33	0
57	MG	DA	3401	1/1	0.99	0.03	36,36,36,36	0
57	MG	BA	3493	1/1	0.99	0.07	39,39,39,39	0
57	MG	BA	3265	1/1	0.99	0.05	30,30,30,30	0
59	ZN	BY	202	1/1	0.99	0.04	70,70,70,70	0
57	MG	BA	3343	1/1	0.99	0.07	18,18,18,18	0
59	ZN	B5	102	1/1	0.99	0.03	41,41,41,41	0
59	ZN	B6	501	1/1	0.99	0.03	43,43,43,43	0
57	MG	DA	3588	1/1	0.99	0.04	21,21,21,21	0
57	MG	BA	3420	1/1	0.99	0.04	23,23,23,23	0
59	ZN	DY	501	1/1	0.99	0.04	88,88,88,88	0
57	MG	DA	3361	1/1	0.99	0.06	32,32,32,32	0
59	ZN	D5	102	1/1	0.99	0.06	58,58,58,58	0
59	ZN	D6	501	1/1	0.99	0.06	64,64,64,64	0
57	MG	AA	3161	1/1	0.99	0.07	28,28,28,28	0
57	MG	DA	3363	1/1	0.99	0.10	35,35,35,35	0
57	MG	BB	3014	1/1	0.99	0.02	41,41,41,41	0
57	MG	BA	3512	1/1	1.00	0.04	32,32,32,32	0
57	MG	BA	3478	1/1	1.00	0.05	22,22,22,22	0
57	MG	DA	3570	1/1	1.00	0.04	28,28,28,28	0
57	MG	DA	3340	1/1	1.00	0.07	38,38,38,38	0
57	MG	BA	3592	1/1	1.00	0.05	14,14,14,14	0
57	MG	BA	3309	1/1	1.00	0.05	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.