



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 08:50 pm BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

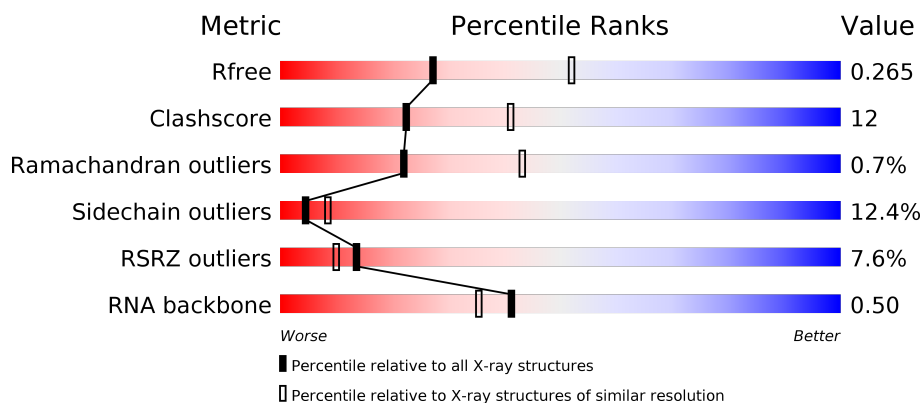
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>11%</div> <div> <div>49%</div> <div>38%</div> <div>11%</div> <div>..</div> </div> </div>
1	CA	1521	<div> <div>4%</div> <div> <div>43%</div> <div>40%</div> <div>14%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>11%</div> <div> <div>45%</div> <div>37%</div> <div>8%</div> <div>10%</div> </div> </div>
2	CB	256	<div> <div>33%</div> <div> <div>36%</div> <div>44%</div> <div>10%</div> <div>10%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	CW	76	
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	

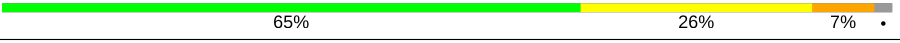





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Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	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
25	PSU	CY	39	-	-	X	-
25	5MU	CY	54	-	-	-	X
25	PSU	CY	55	-	-	-	X
57	MG	BA	3710	-	-	-	X
57	MG	DA	3024	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3624	-	-	-	X
57	MG	DA	3657	-	-	-	X
57	MG	DQ	3003	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1544	970	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
			1678	1052	333	286	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
			812	514	146	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	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
			986	626	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		
			833	519	156	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		
			966	598	200	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	84	Total	C	N	O	S	0	0	0
			661	423	122	114	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
			731	449	156	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	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1599	722	287	515	73	2			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1552	697	280	502	72	1			

- 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
			1635	731	296	530	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	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- 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
			2142	1352	426	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
			1073	688	188	196	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
			1139	709	231	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
			558	352	102	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
			517	331	102	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	814	Total	Mg	0	0
			814	814		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	3	Total	Mg	0	0
			3	3		
57	D3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AB	1	Total 1	Mg 1	0	0
57	DF	5	Total 5	Mg 5	0	0
57	B8	2	Total 2	Mg 2	0	0
57	BE	6	Total 6	Mg 6	0	0
57	AW	2	Total 2	Mg 2	0	0
57	DU	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	2	Total 2	Mg 2	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	169	Total 169	Mg 169	0	0
57	B5	3	Total 3	Mg 3	0	0
57	BB	23	Total 23	Mg 23	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0
57	CF	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	11	Total 11	Mg 11	0	0
57	BX	1	Total 1	Mg 1	0	0
57	B2	1	Total 1	Mg 1	0	0

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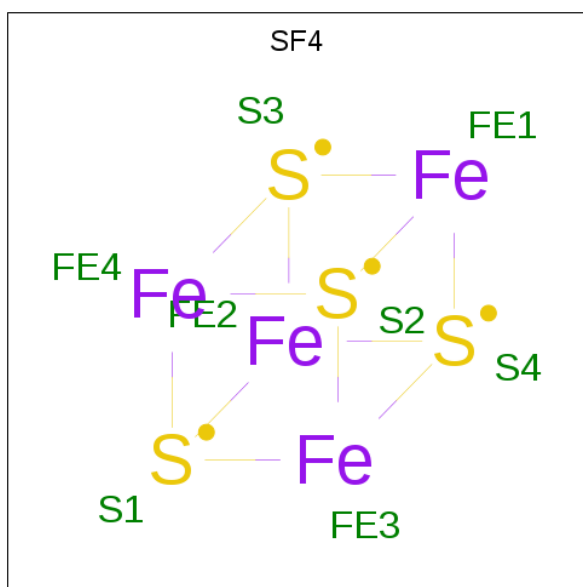
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	216	Total 216	Mg 216	0	0
57	BQ	2	Total 2	Mg 2	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DV	1	Total 1	Mg 1	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	2	Total 2	Mg 2	0	0
57	BU	4	Total 4	Mg 4	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	3	Total 3	Mg 3	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	7	Total 7	Mg 7	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	664	Total 664	Mg 664	0	0
57	AU	1	Total 1	Mg 1	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	5	Total 5	Mg 5	0	0
57	AL	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BV	5	Total 5	Mg 5	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DO	2	Total 2	Mg 2	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BZ	2	Total 2	Mg 2	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	DG	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	10	Total 10	Mg 10	0	0
57	AT	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	4	Total 4	Mg 4	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	BH	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

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

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

- Molecule 61 is water.

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

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

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

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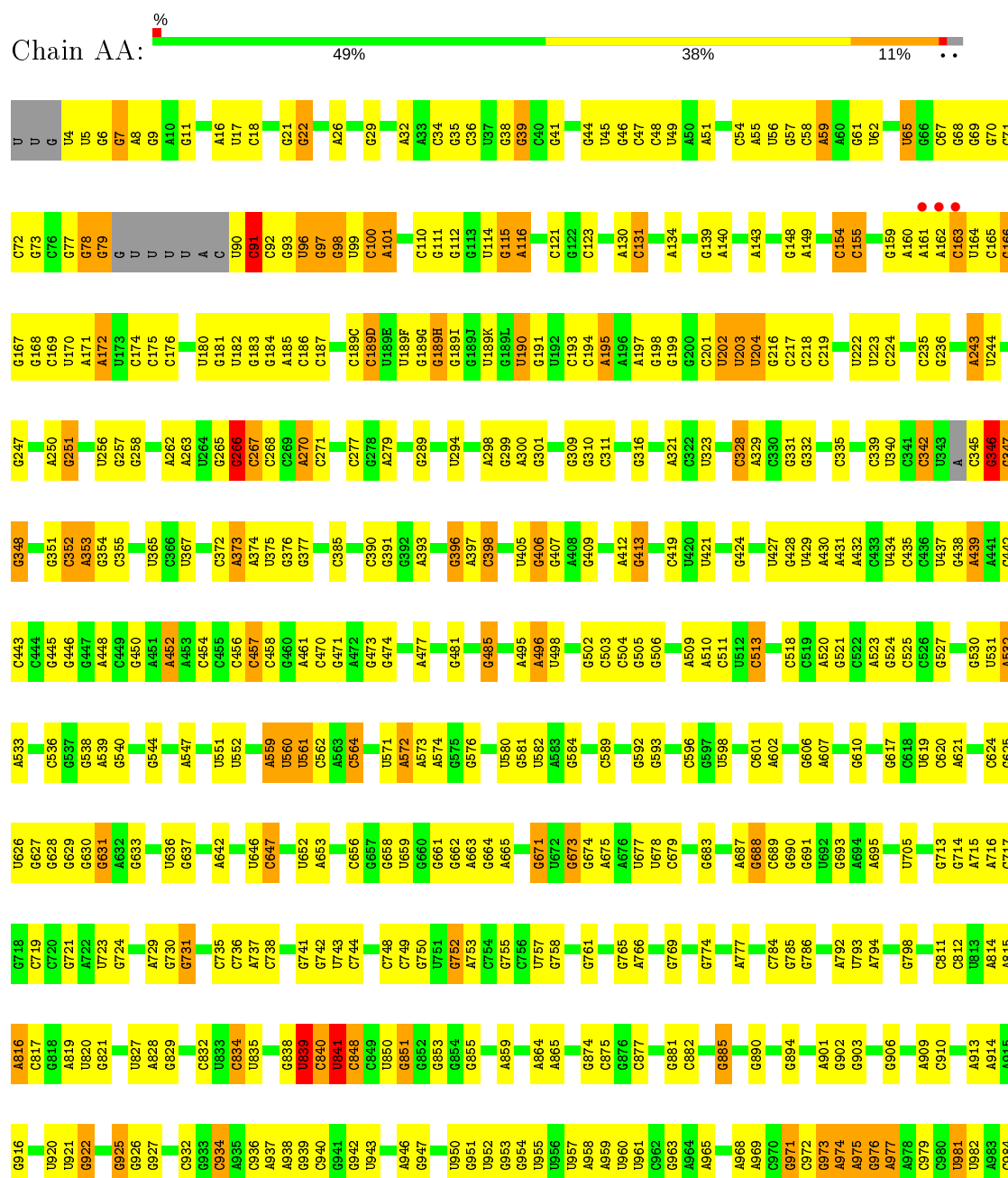
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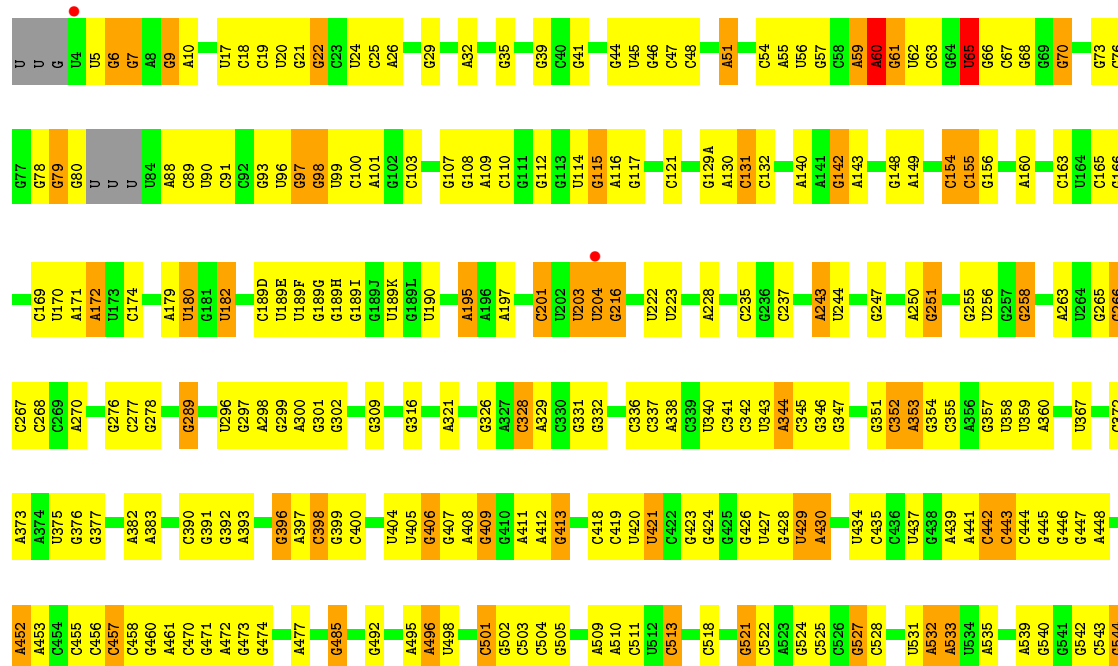
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			4	4		
61	DU	1	Total	O	0	0
			1	1		
61	DV	1	Total	O	0	0
			1	1		
61	DW	1	Total	O	0	0
			1	1		
61	DX	2	Total	O	0	0
			2	2		
61	DY	1	Total	O	0	0
			1	1		
61	D0	4	Total	O	0	0
			4	4		
61	D1	1	Total	O	0	0
		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

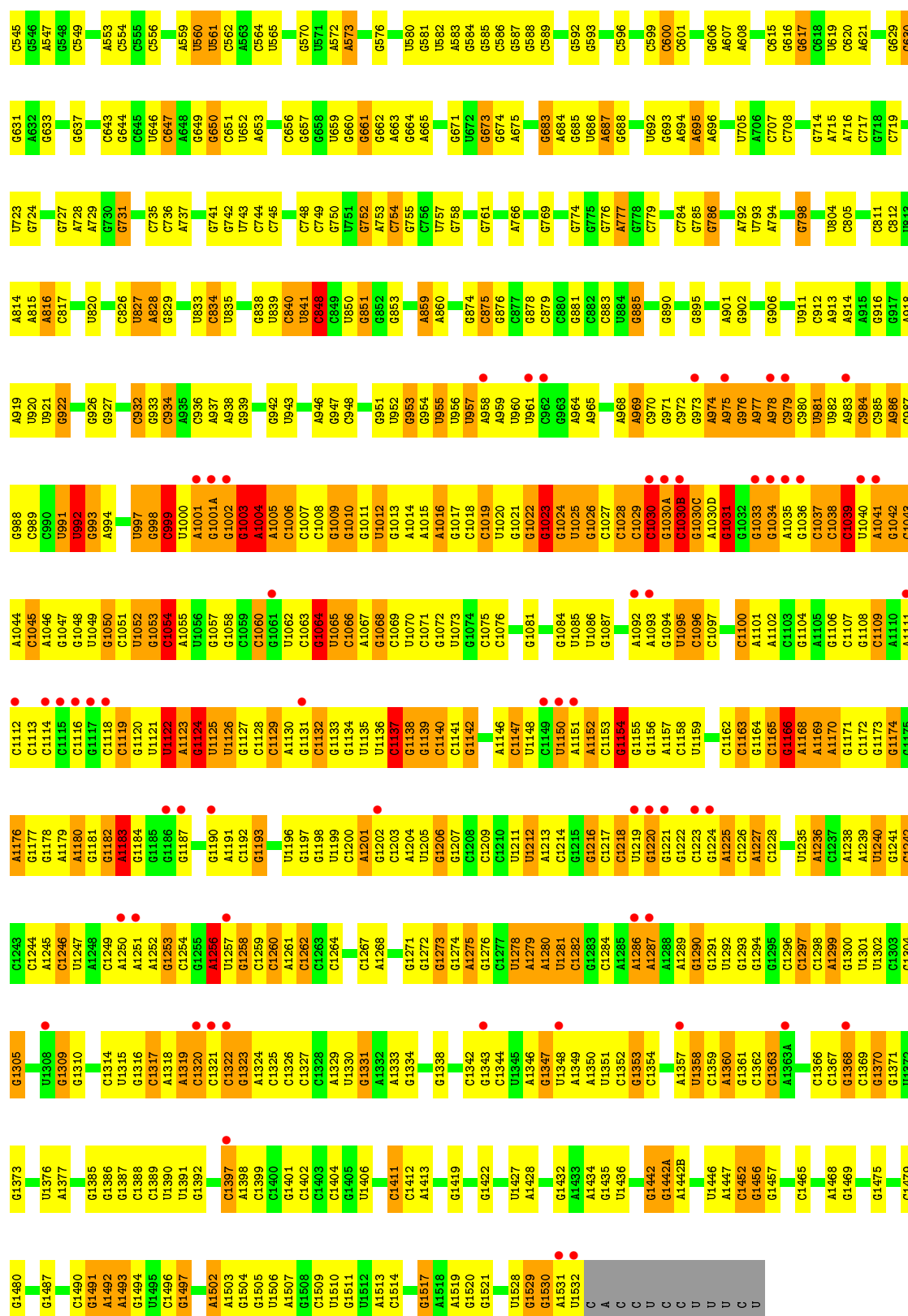
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

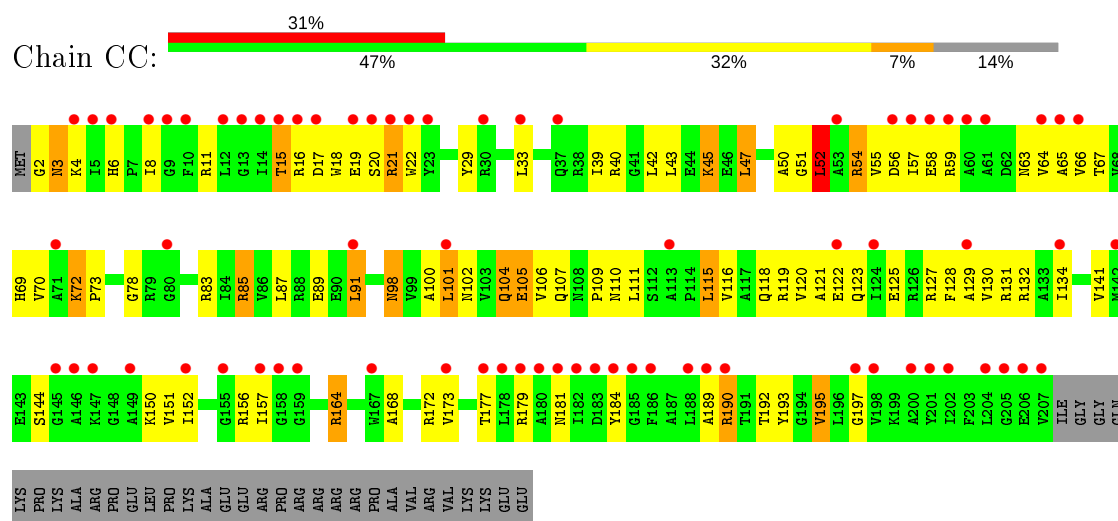
#### • Molecule 1: 16S Ribosomal RNA



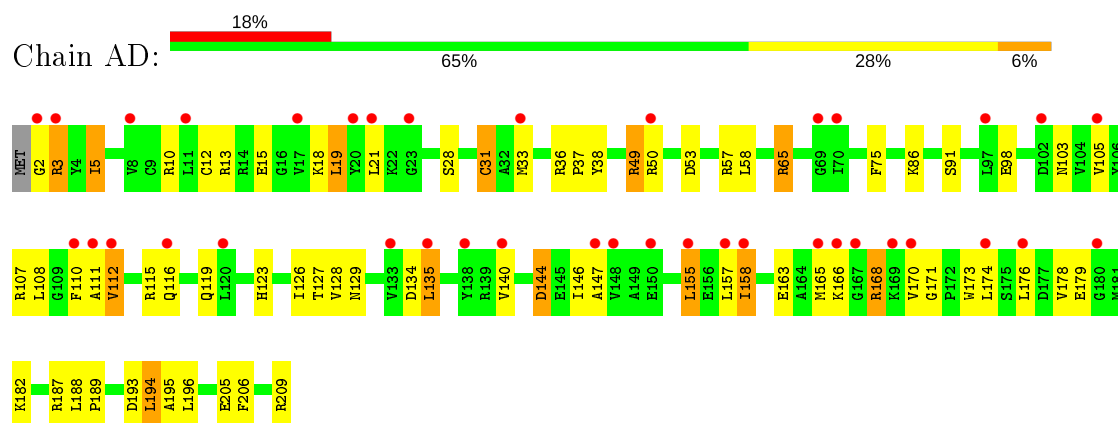




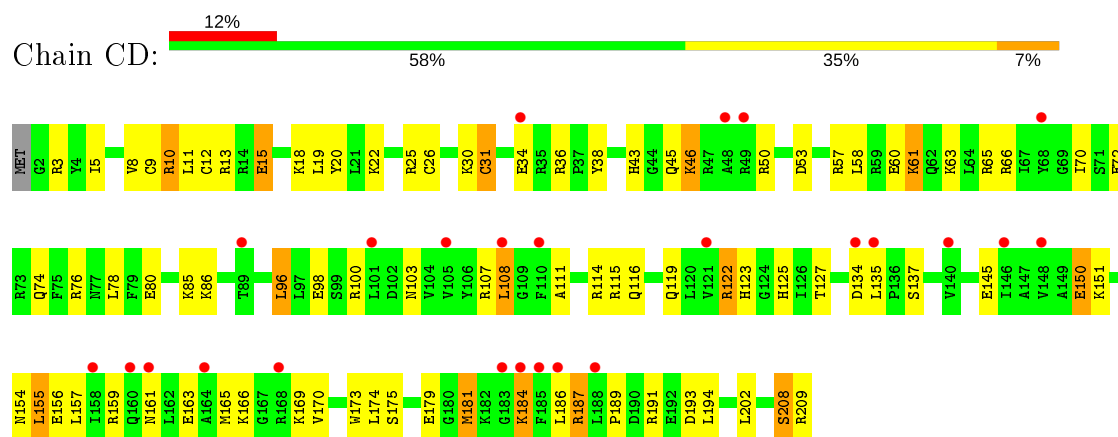




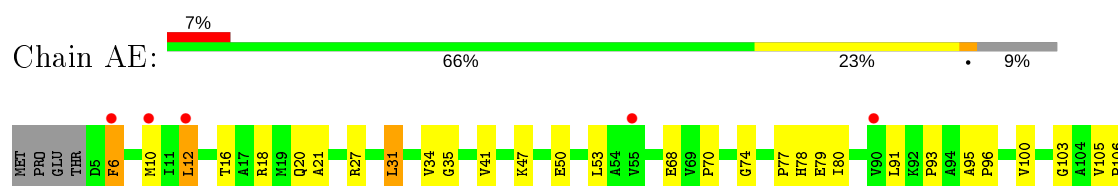
• Molecule 4: 30S ribosomal protein S4

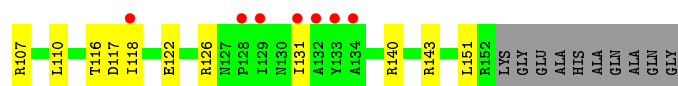


• Molecule 4: 30S ribosomal protein S4

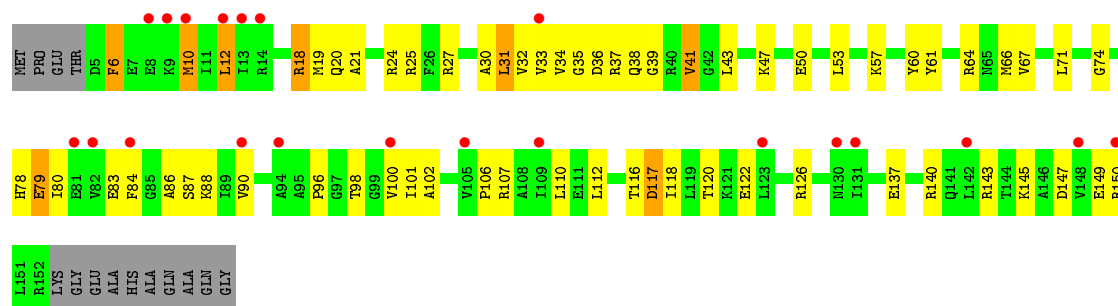


• Molecule 5: 30S ribosomal protein S5

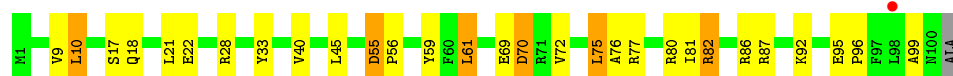




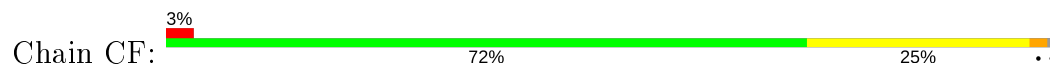
- Molecule 5: 30S ribosomal protein S5



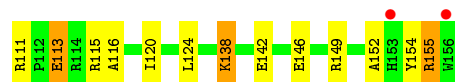
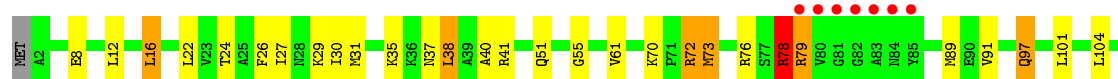
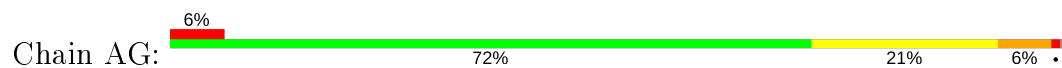
- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



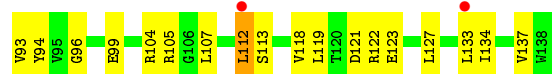
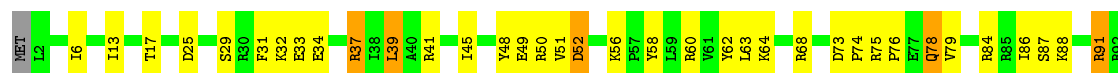
- Molecule 7: 30S ribosomal protein S7



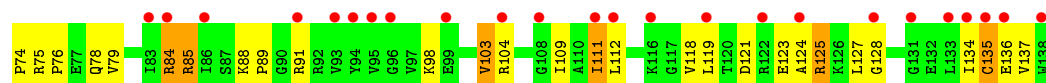




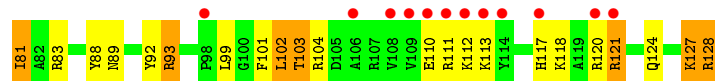
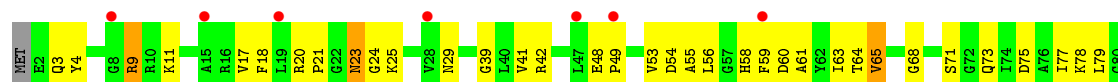
- Molecule 8: 30S ribosomal protein S8



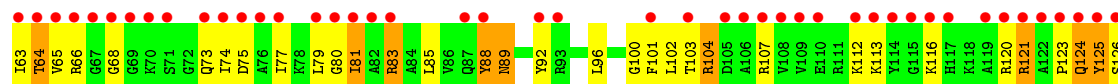
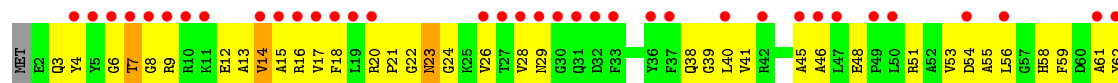
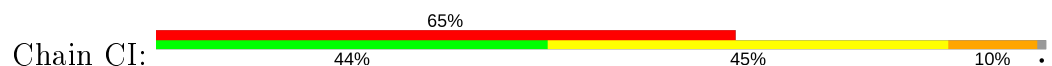
- Molecule 8: 30S ribosomal protein S8



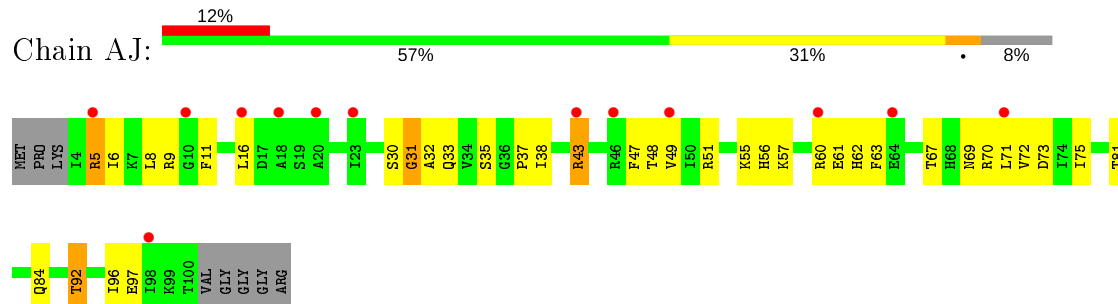
- Molecule 9: 30S ribosomal protein S9



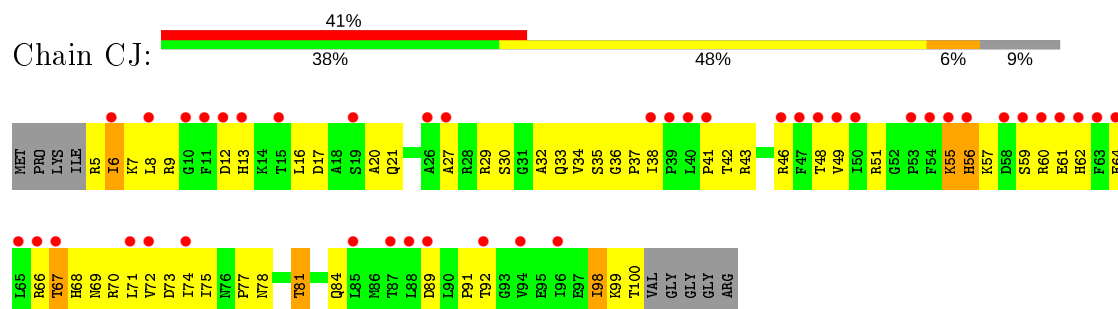
- Molecule 9: 30S ribosomal protein S9



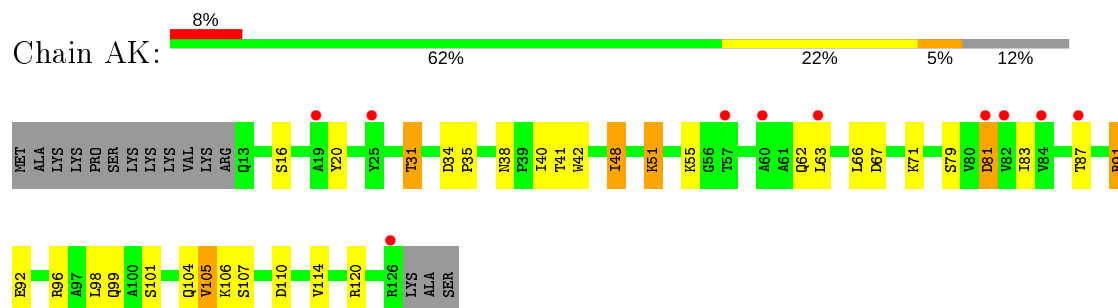
- Molecule 10: 30S ribosomal protein S10



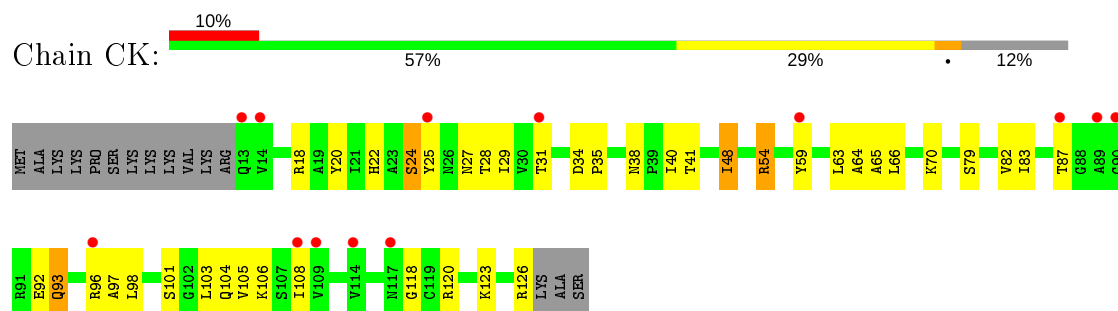
- Molecule 10: 30S ribosomal protein S10



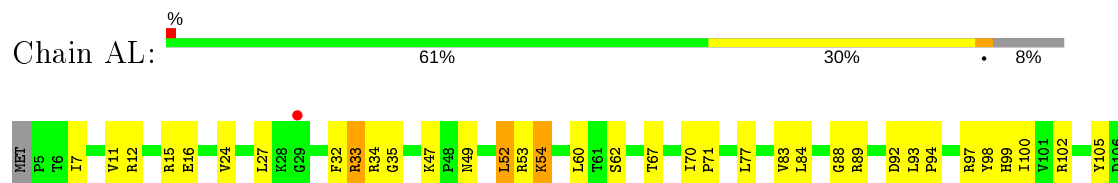
- Molecule 11: 30S ribosomal protein S11

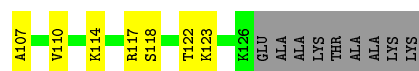


- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

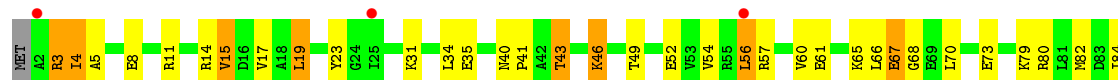




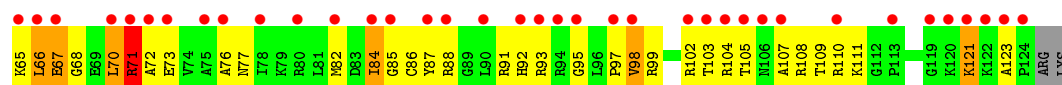
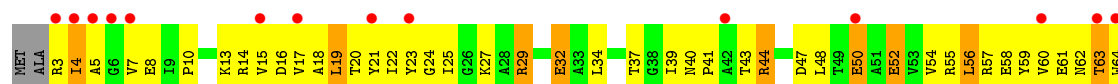
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



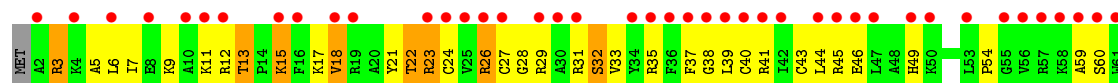
- Molecule 13: 30S ribosomal protein S13



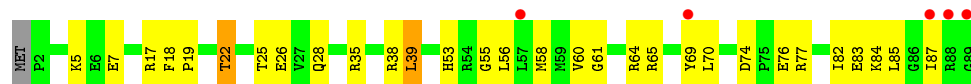
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



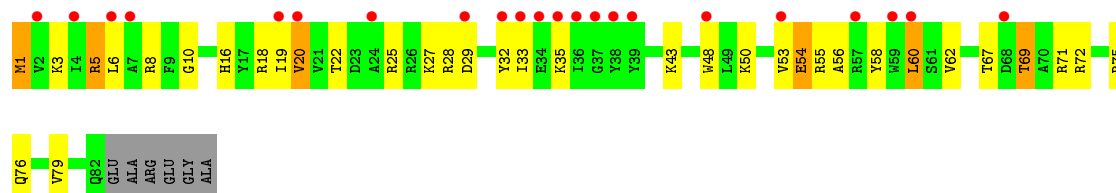
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



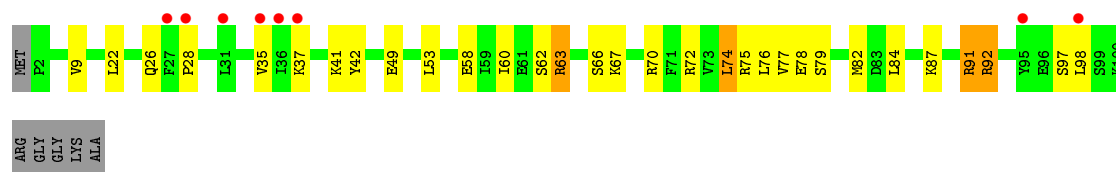
- Molecule 16: 30S ribosomal protein S16



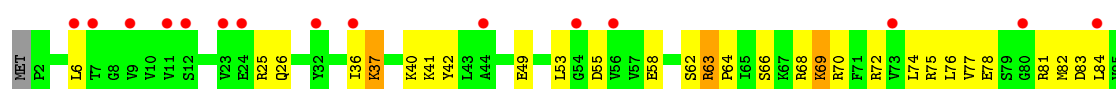
- Molecule 16: 30S ribosomal protein S16

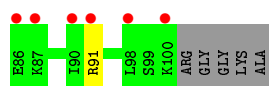


- Molecule 17: 30S ribosomal protein S17

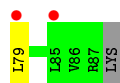
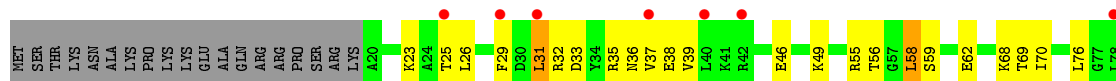


- Molecule 17: 30S ribosomal protein S17

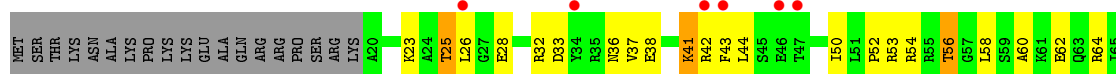
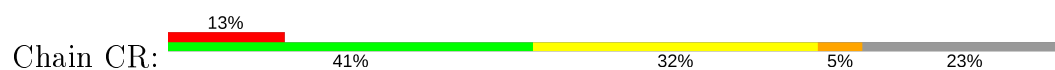




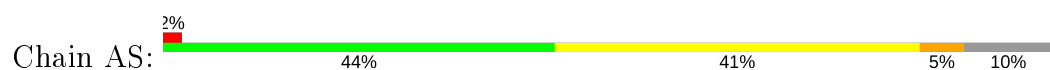
- Molecule 18: 30S ribosomal protein S18



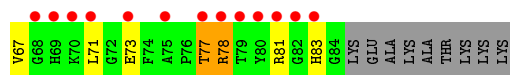
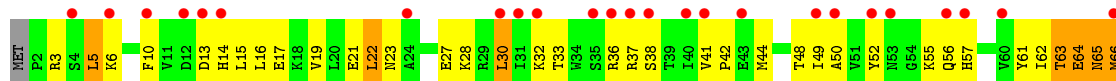
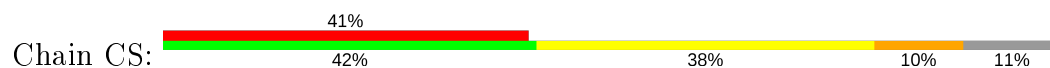
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

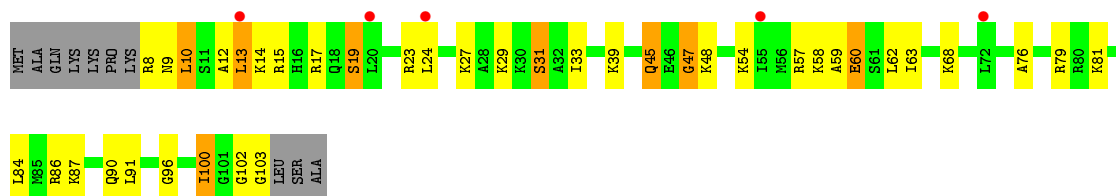


- Molecule 19: 30S ribosomal protein S19

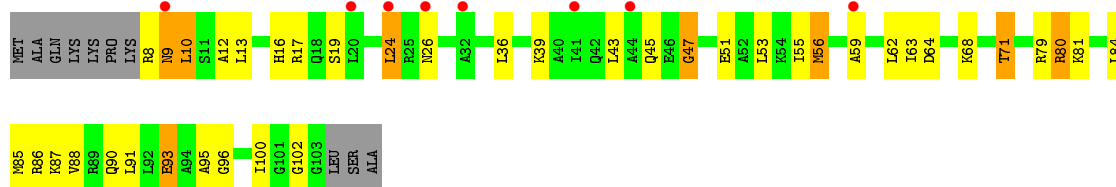


- Molecule 20: 30S ribosomal protein S20

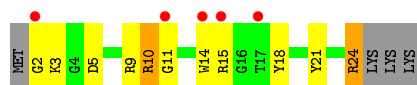




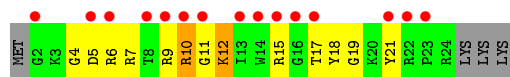
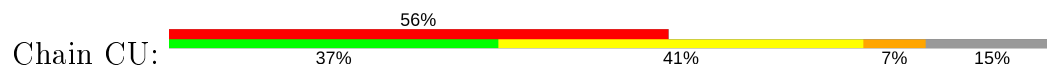
- Molecule 20: 30S ribosomal protein S20



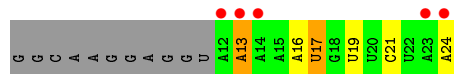
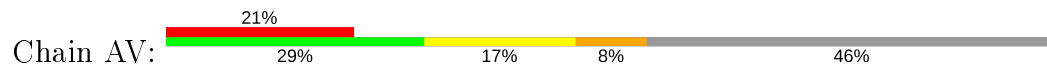
- Molecule 21: 30S ribosomal protein Thx



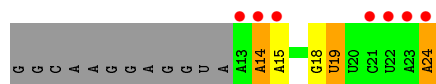
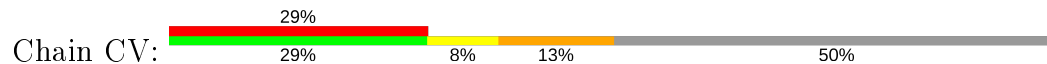
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA

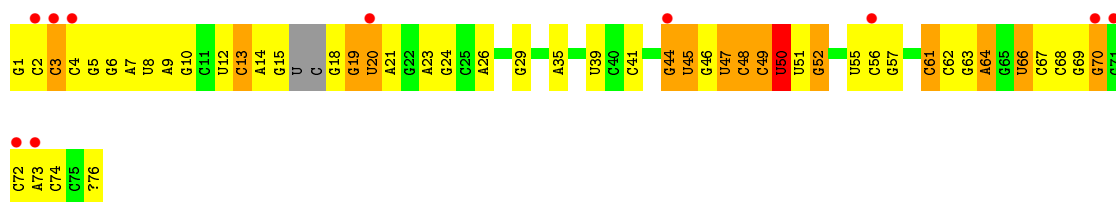


- Molecule 22: mRNA

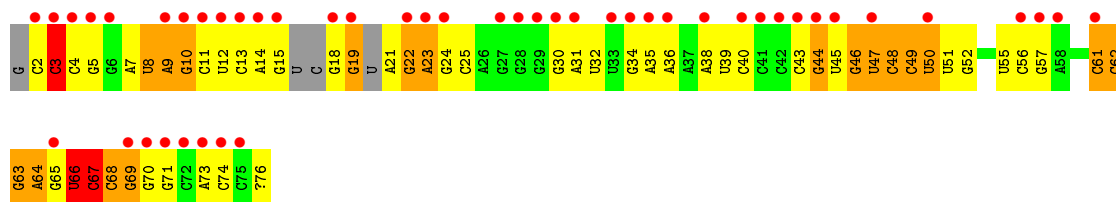
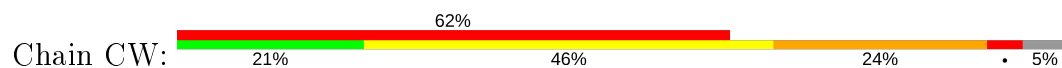


- Molecule 23: A-site tRNA

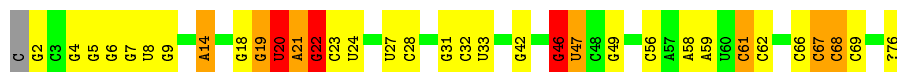




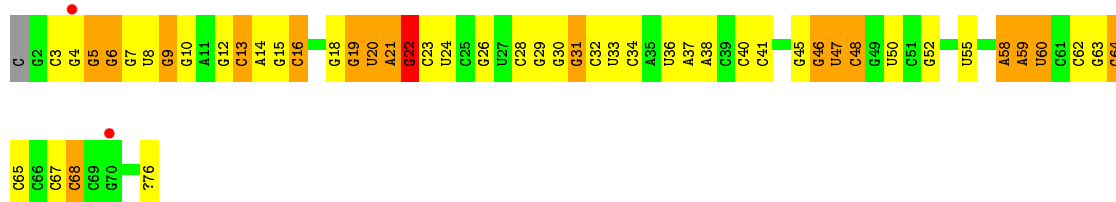
• Molecule 23: A-site tRNA



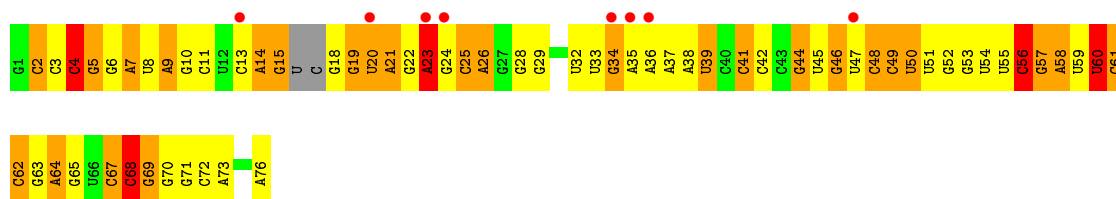
• Molecule 24: P-site tRNA



• Molecule 24: P-site tRNA

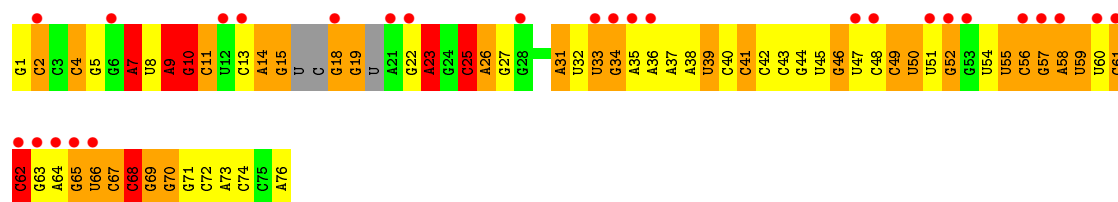


• Molecule 25: E-site tRNA

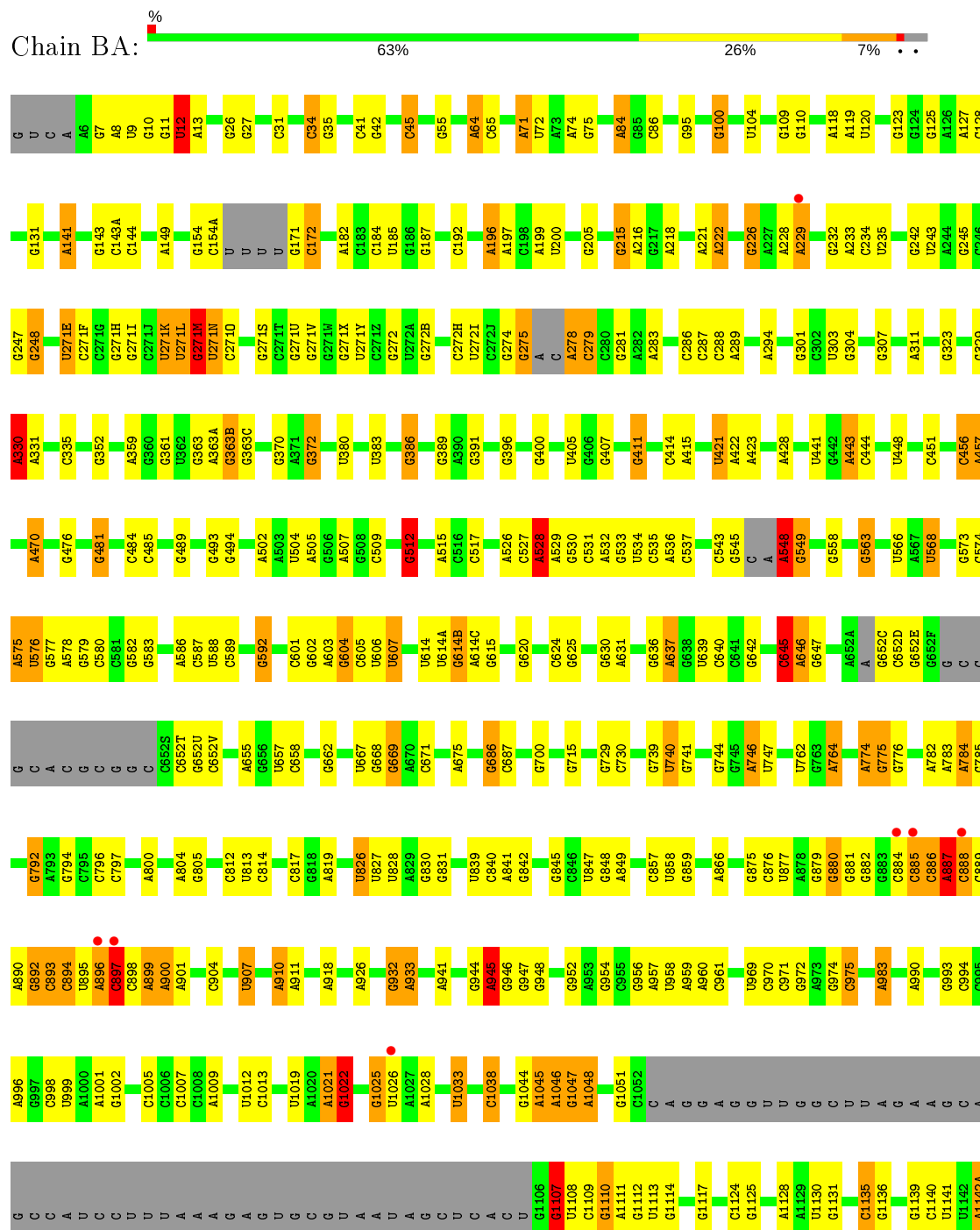


• Molecule 25: E-site tRNA



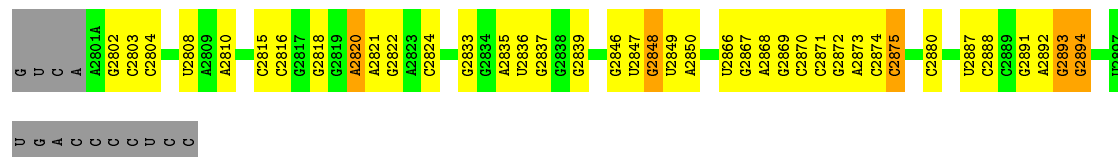


• Molecule 26: 23S Ribosomal RNA

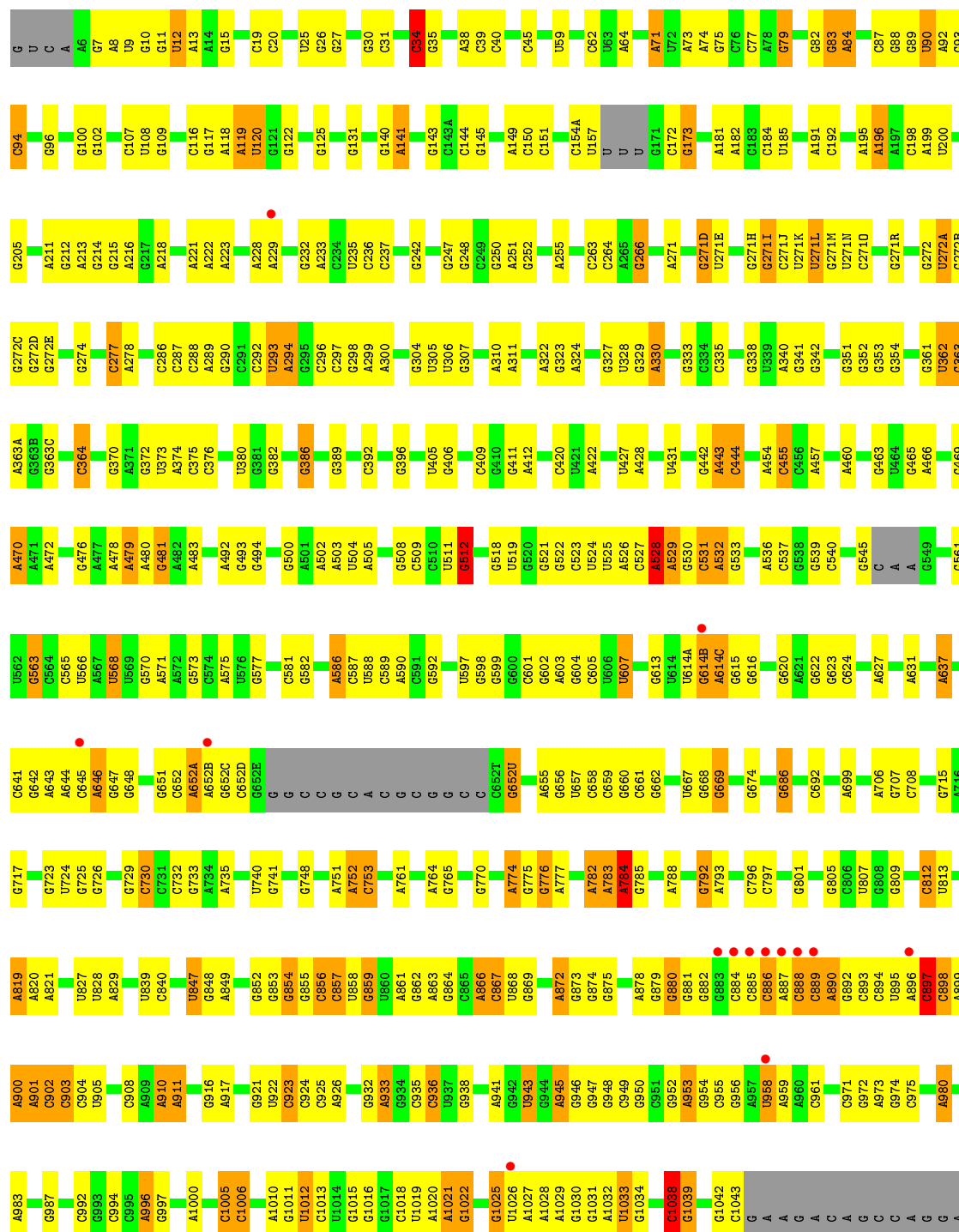




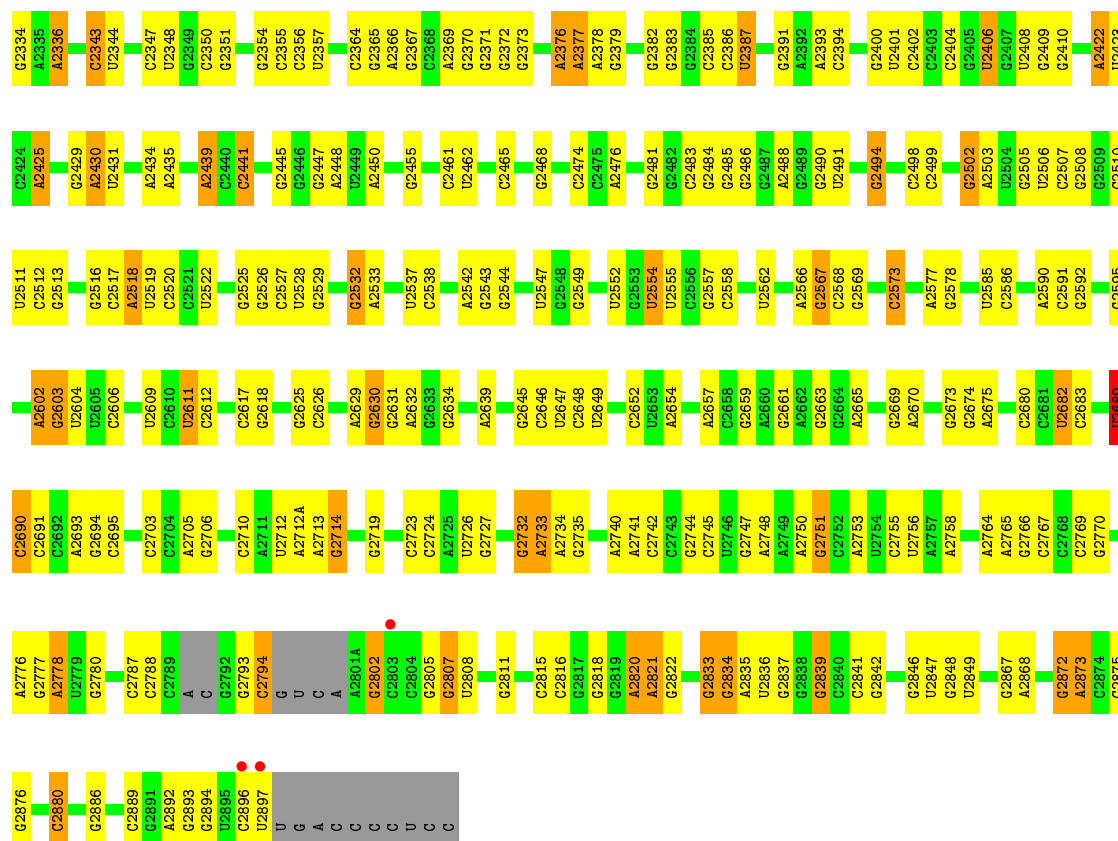
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C2690	G2550	C2297	C2297	U2189	C2128	U2041	A1919	A1785	A1674	A	G1422	A1278	C1153
C2691	G2554	C2404	A2298	G2190	C2129	A2042	A1919	A1786	A1674	C	G1537	A1292	A1155
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C2694	G2557	U2406	A2305	C2192	U2131	G2049	A1928	U1794	C1684	G1539	C1429	C1293	U1164
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C2703	U2562	C2313	C2313	C2200	C2136	G2056	G1930	C1797	U1688	A1542	A1434	U1300	A1177
G2706	U2563	A2418	A2305	G2206	C2137	A2059	A1937	U1798	A1689	C1543	A1441	A1301	G1170
U2709	A2564	U2419	G2319	G2207	C2138	A2060	U1939	G1799	U1689	A1564	G1442	A1302	G1171
C2710	A2565	A2422	A2320	A2208	C2139	A2062	U1939	C1800	U1689	C1557	A1445	G1303	A1173
A2711	A2566	A2422	G2325	U2218	C2140	A2062	G1948	A1803	G1696	A1566	A1445	G1310	A1174
U2712	C2567	G2425	G2326	U2218	C2141	G2067	A1952	G1814	G1697	A1567	A1447	U1313	G1175
A2714	C2568	A2425	A2327	A2225	C2143	U2068	A1953	G1815	G1699	A1568	G1448	C1314	A1177
U2715	C2573	A2428	A2328	U2233	U2144	G2069	G1954	G1816	G1700	A1569	A1449	C1315	C1178
A2716	G2582	A2430	G2329	G2234	C2145	G2070	U1955	G1817	A1701	U1578	G1450	A1342	C1180
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A2764	G2640	C2478	C2358	A2273	U2167	C2108	U2011	C1866	A1762	A1632	C1505	A1395	A1253
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U2788	A2654	U2506	A2366	G2280	C2172	A2114	C2021	C1882	U1768	U1639	C1509	C1409	A1269
C2788	A2657	A2518	G2367	C2283	C2175	G2115	U2022	G1883	G1769	C1648	G1515	G1416	C1270
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U2791	G2659	A2378	A2378	C2285	C2177	U2117	U2028	G1899	U1776	G1650	G1517	C1408	A1272
G2792	C2683	G2522	G2383	A2287	C2178	A2119	G2029	A1900	G1776	G1651	U1518	C1409	G1418
U2793	U2687	G2529	G2384	A2288	U2180	G2120	A2030	A1900	U1777	G1652	G1519	C1409	G1418
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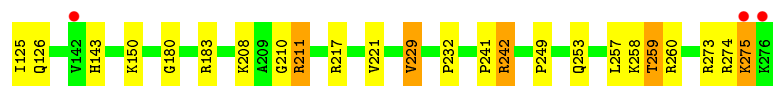


• Molecule 26: 23S Ribosomal RNA

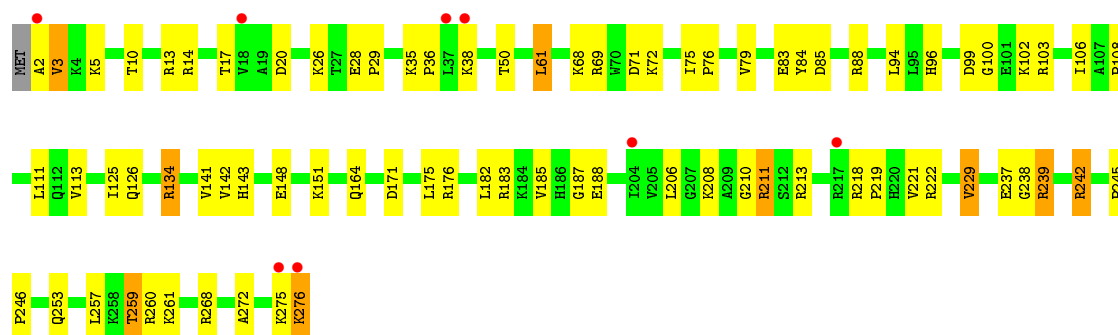
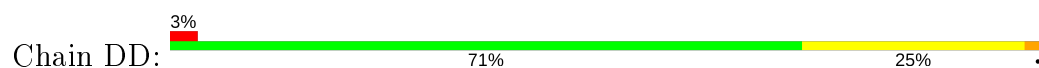




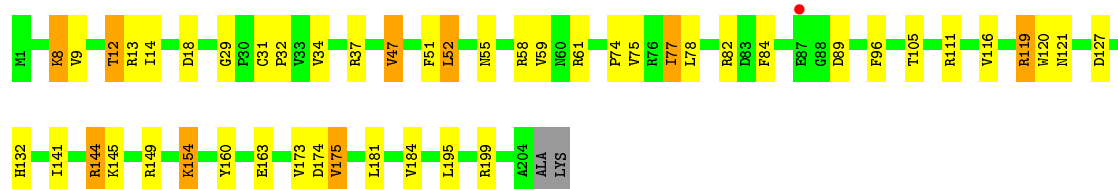
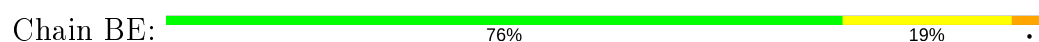




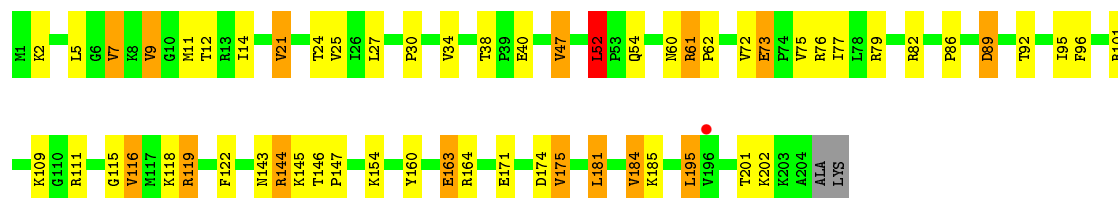
- Molecule 28: 50S ribosomal protein L2



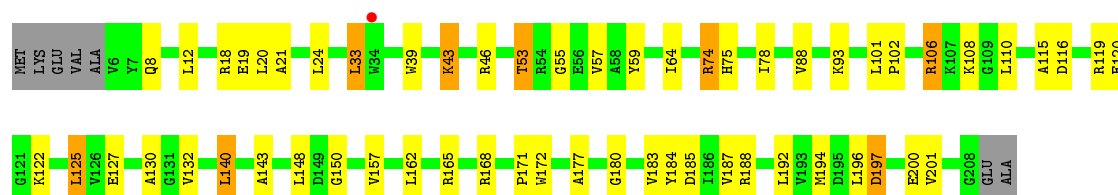
- Molecule 29: 50S ribosomal protein L3



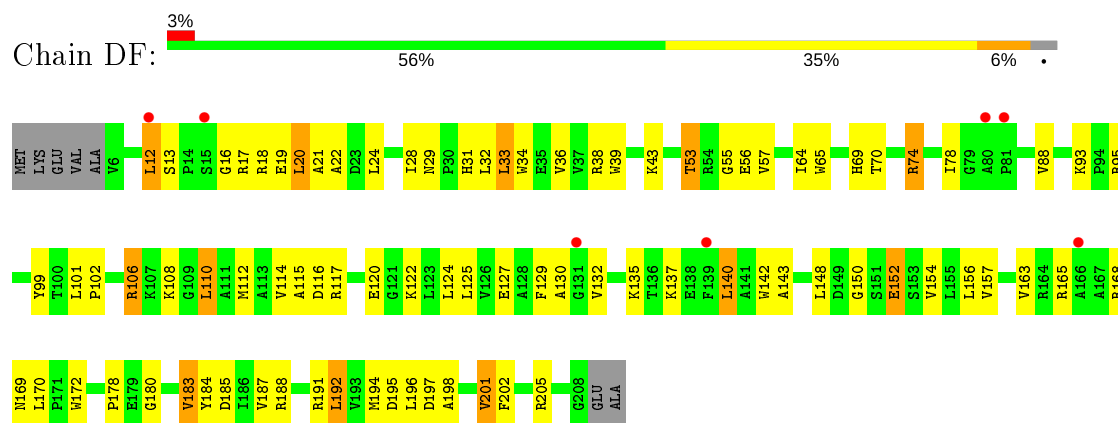
- Molecule 29: 50S ribosomal protein L3



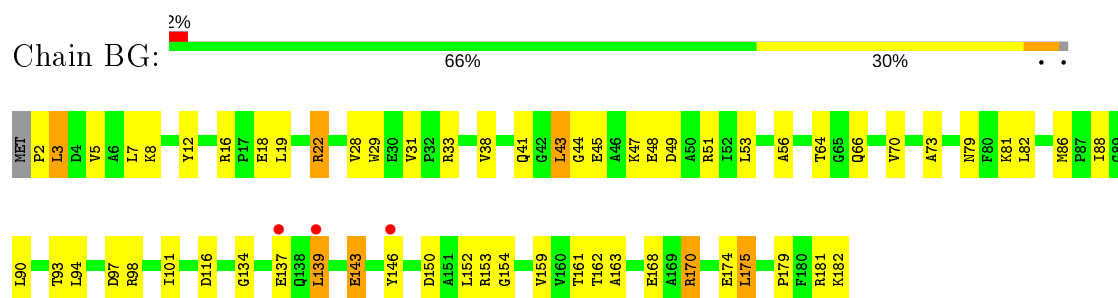
- Molecule 30: 50S ribosomal protein L4

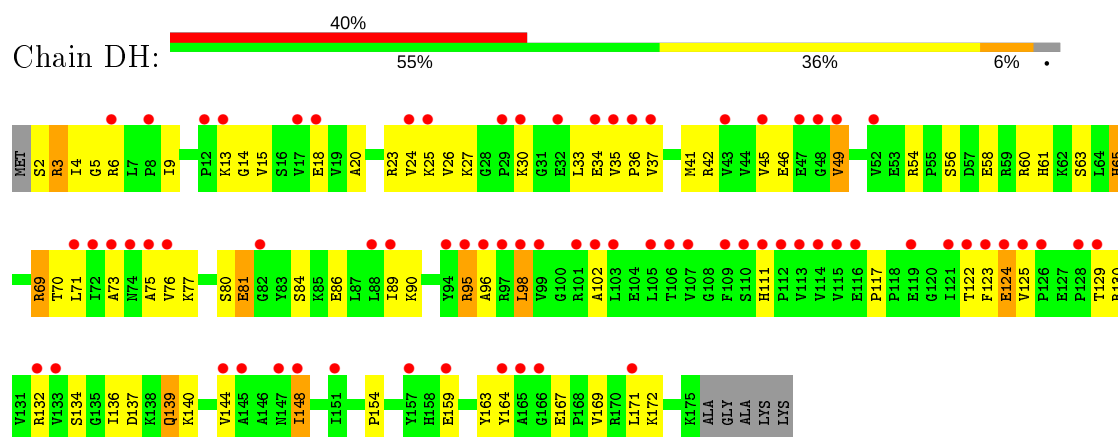


- Molecule 30: 50S ribosomal protein L4

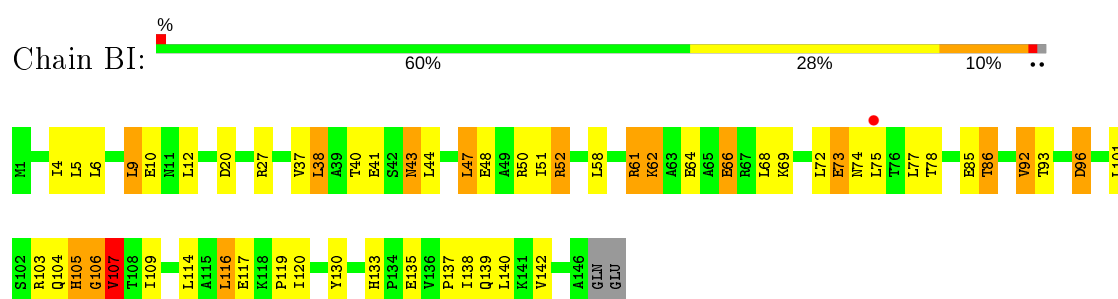


- Molecule 31: 50S ribosomal protein L5

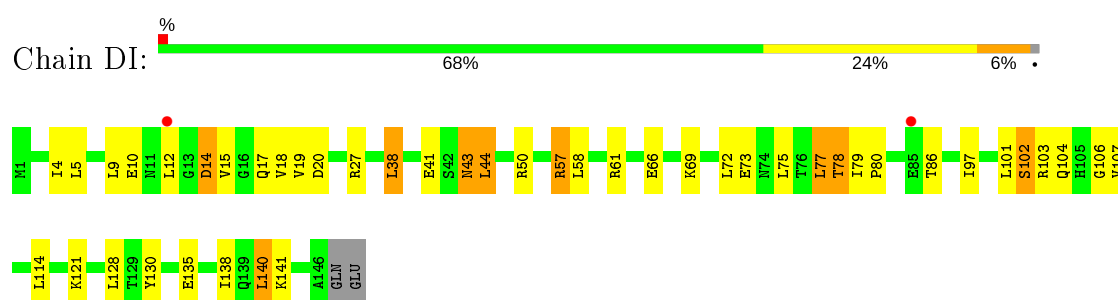




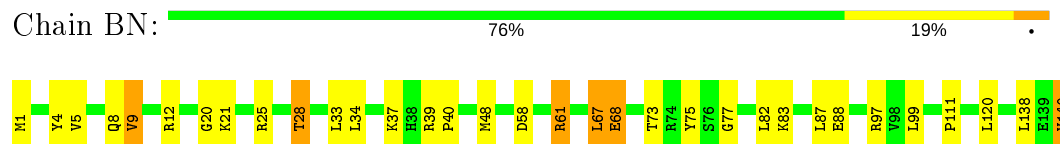
• Molecule 33: 50S ribosomal protein L9



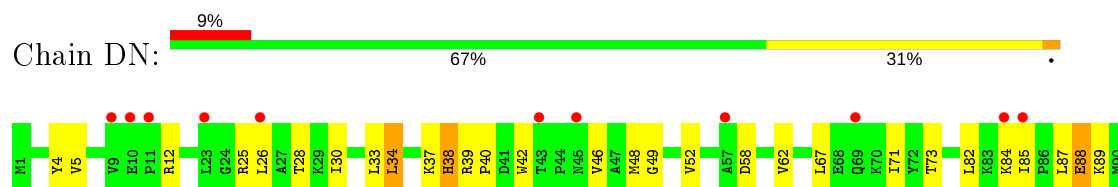
• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

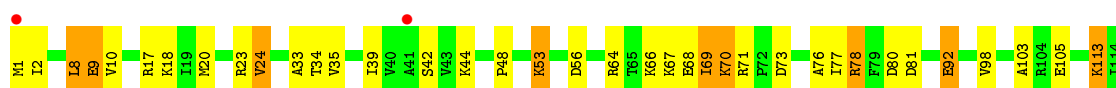




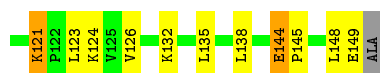
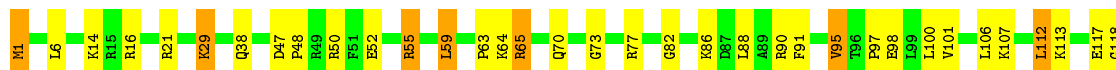
- Molecule 35: 50S ribosomal protein L14



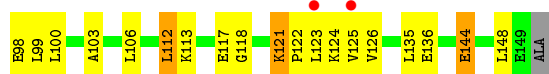
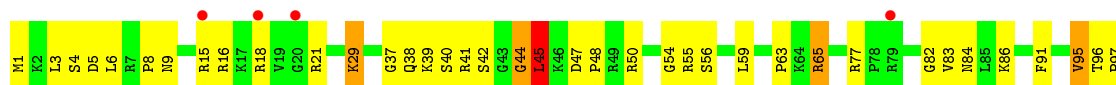
- Molecule 35: 50S ribosomal protein L14



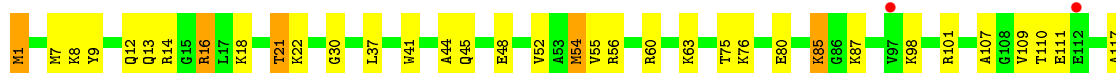
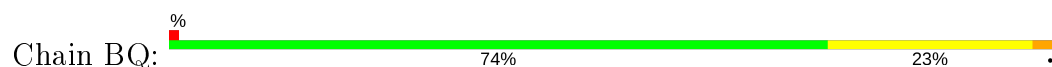
- Molecule 36: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L15



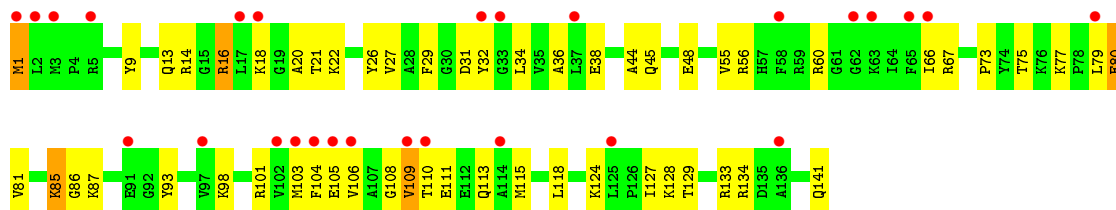
- Molecule 37: 50S ribosomal protein L16



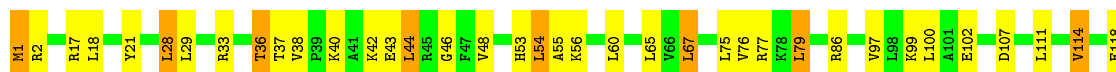




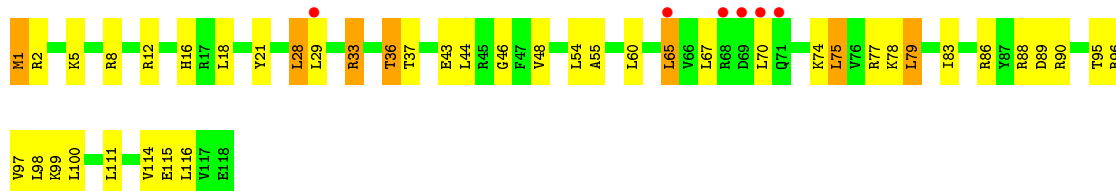
• Molecule 37: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L17



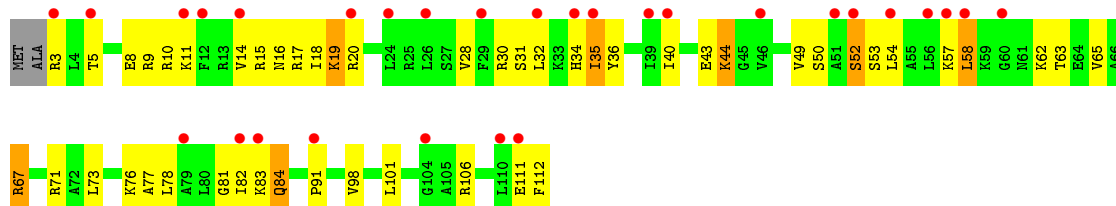
• Molecule 38: 50S ribosomal protein L17



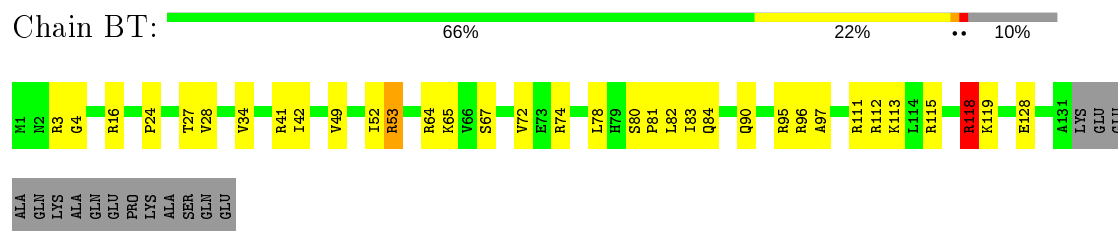
• Molecule 39: 50S ribosomal protein L18



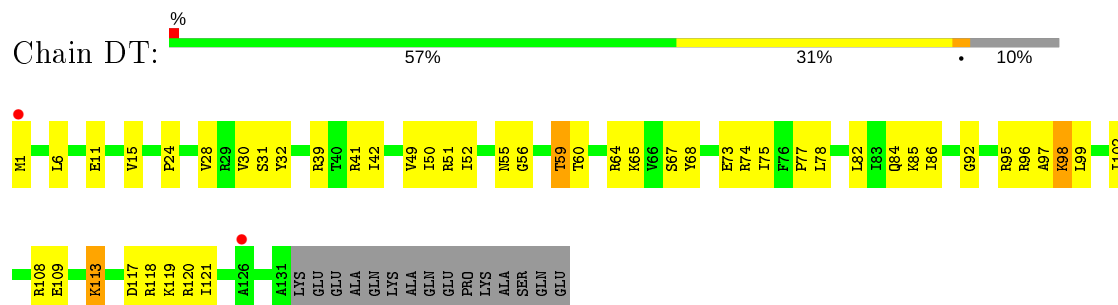
• Molecule 39: 50S ribosomal protein L18



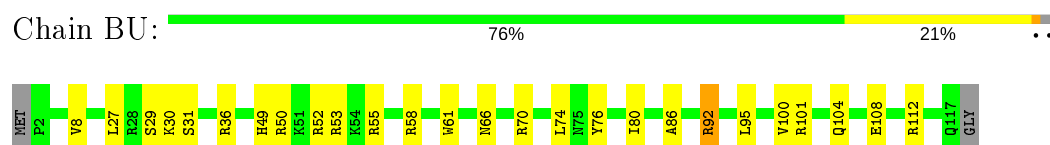
- Molecule 40: 50S ribosomal protein L19



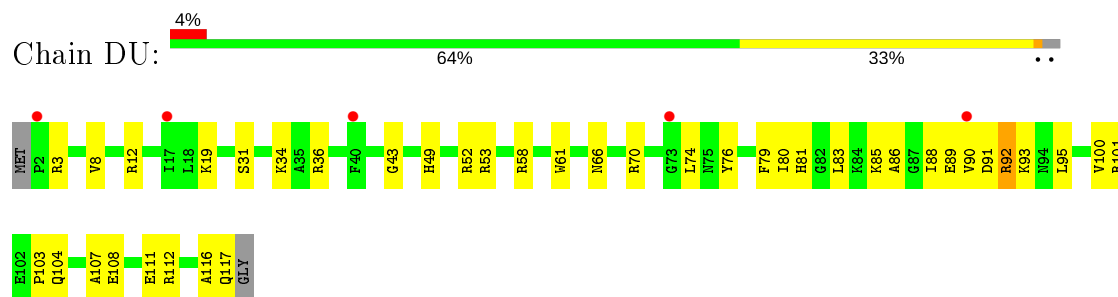
- Molecule 40: 50S ribosomal protein L19



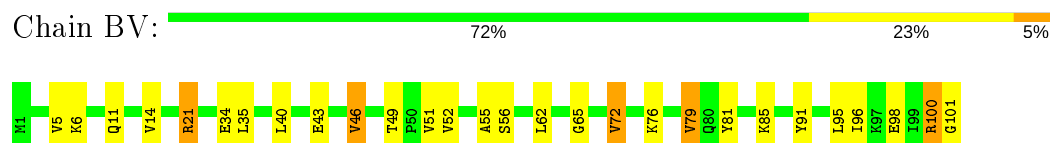
- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20

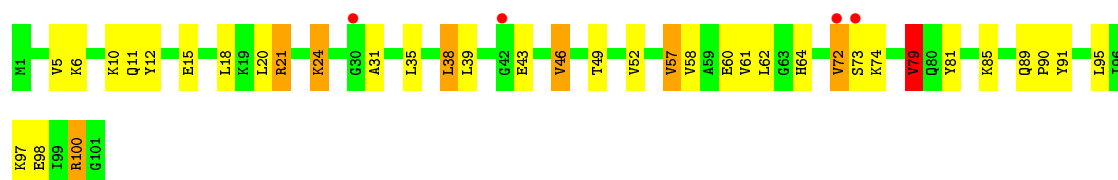


- Molecule 42: 50S ribosomal protein L21



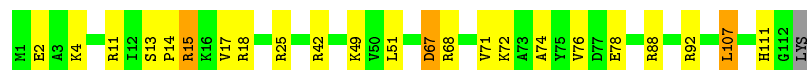
- Molecule 42: 50S ribosomal protein L21





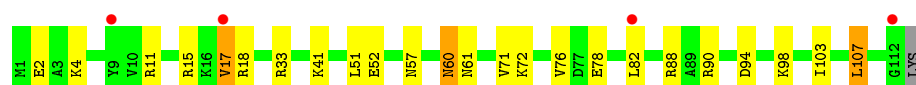
- Molecule 43: 50S ribosomal protein L22

Chain BW: 79% 18% ..



- Molecule 43: 50S ribosomal protein L22

Chain DW: 4% 78% 19% ..



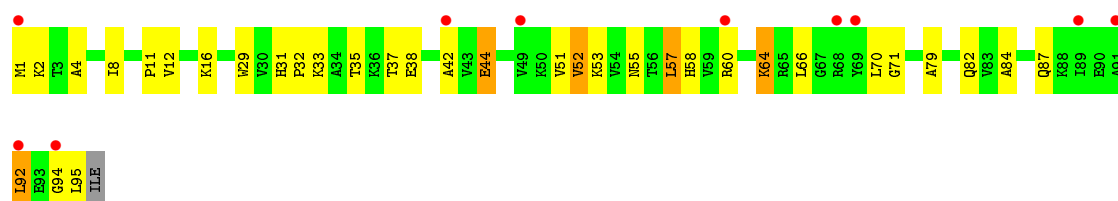
- Molecule 44: 50S ribosomal protein L23

Chain BX: 75% 20% ..



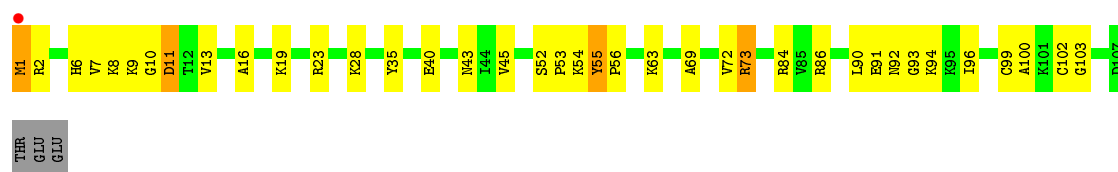
- Molecule 44: 50S ribosomal protein L23

Chain DX: 10% 64% 30% 5% .



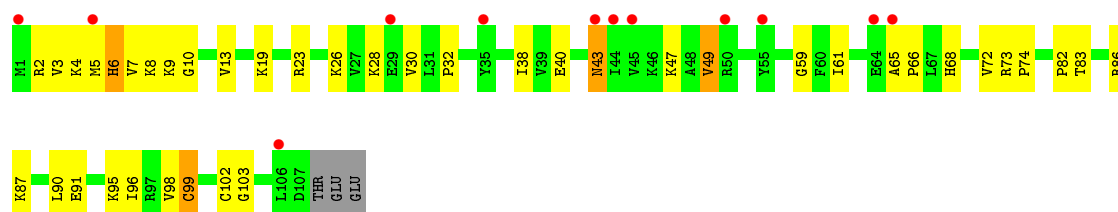
- Molecule 45: 50S ribosomal protein L24

Chain BY: 63% 31% ..



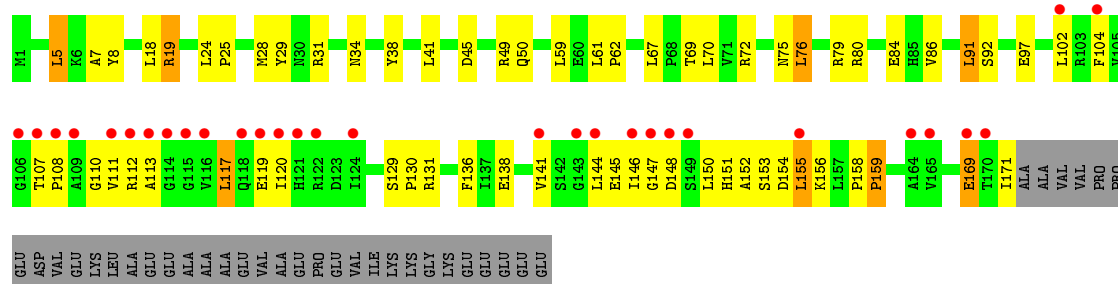
- Molecule 45: 50S ribosomal protein L24

Chain DY:



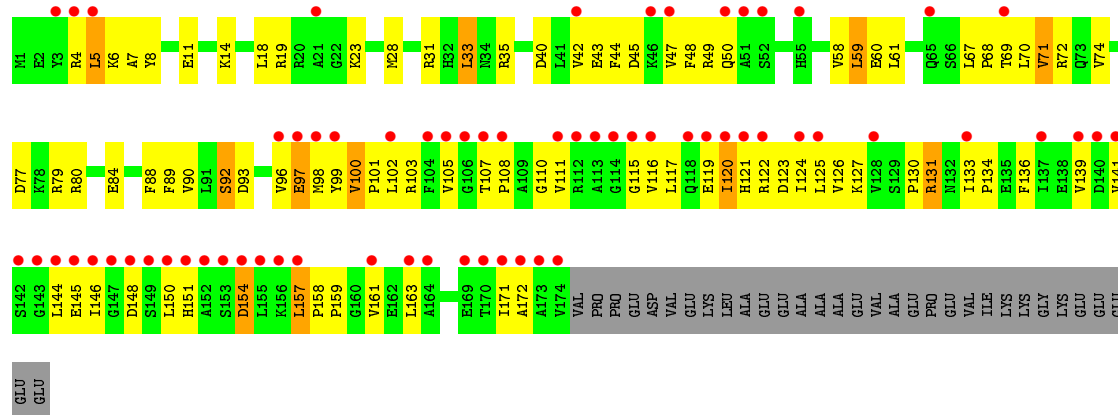
- Molecule 46: 50S ribosomal protein L25

Chain BZ:



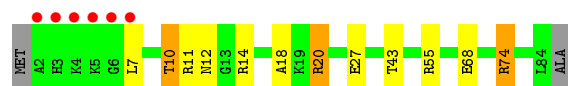
- Molecule 46: 50S ribosomal protein L25

Chain DZ:



- Molecule 47: 50S ribosomal protein L27

Chain B0:

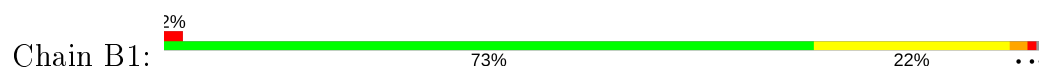


- Molecule 47: 50S ribosomal protein L27

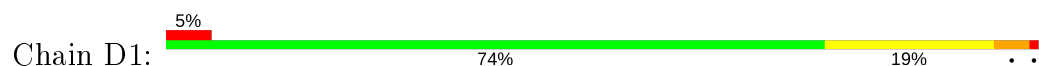
Chain D0:



- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28



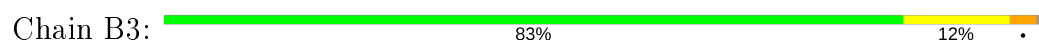
- Molecule 49: 50S ribosomal protein L29



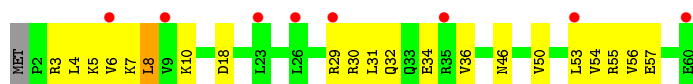
- Molecule 49: 50S ribosomal protein L29



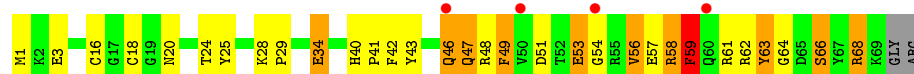
- Molecule 50: 50S ribosomal protein L30



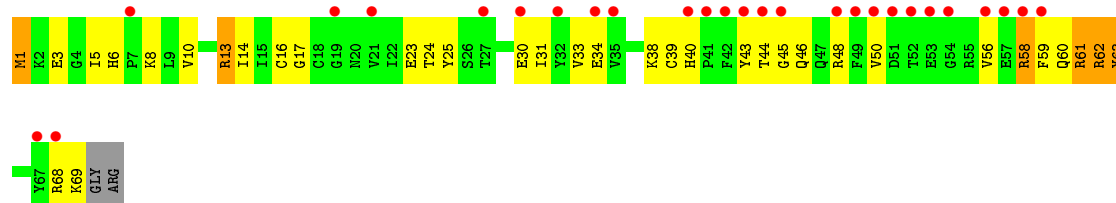
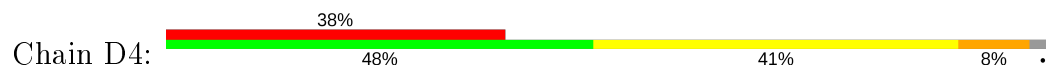
- Molecule 50: 50S ribosomal protein L30



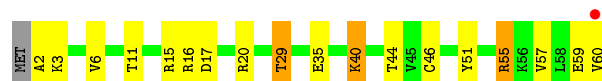
- Molecule 51: 50S ribosomal protein L31



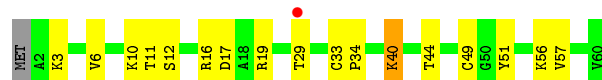
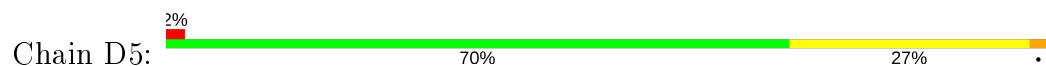
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



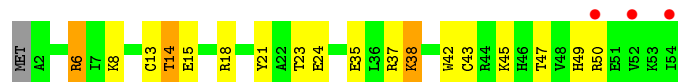
- Molecule 52: 50S ribosomal protein L32



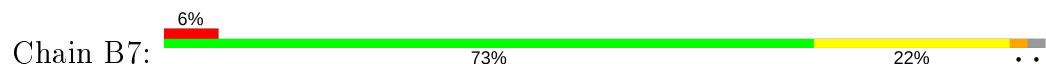
- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33

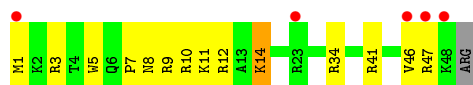


- Molecule 54: 50S ribosomal protein L34





- Molecule 54: 50S ribosomal protein L34



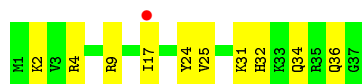
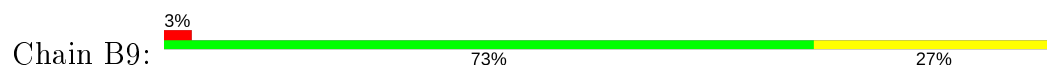
- Molecule 55: 50S ribosomal protein L35



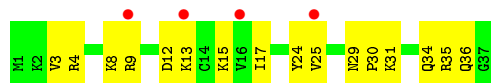
- Molecule 55: 50S ribosomal protein L35



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

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

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	2
2	CB	0	1
7	AG	0	2
20	CT	0	1
33	BI	0	1
35	BO	0	1
39	BS	0	1
51	B4	0	1
All	All	0	10

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

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

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

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

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide
7	AG	79	ARG	Peptide
33	BI	9	LEU	Peptide

## 5.2 Too-close contacts

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	9	0
22	AV	277	0	140	3	0
22	CV	252	0	130	6	0
23	AW	1599	0	830	42	0
23	CW	1552	0	794	51	0
24	AX	1635	0	839	23	0
24	CX	1635	0	839	36	0
25	AY	1581	0	805	82	0
25	CY	1561	0	796	94	0
26	BA	60729	0	30622	666	0
26	DA	60311	0	30412	876	0
27	BB	2573	0	1306	20	0
27	DB	2573	0	1306	76	0
28	BD	2136	0	2218	42	0
28	DD	2142	0	2229	58	0
29	BE	1559	0	1618	25	0
29	DE	1559	0	1618	39	0
30	BF	1584	0	1625	39	0
30	DF	1580	0	1619	60	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	90	0
32	BH	1330	0	1407	34	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	37	0
33	DI	1073	0	1106	22	0
34	BN	1117	0	1184	23	0
34	DN	1117	0	1184	26	0
35	BO	933	0	996	25	0
35	DO	933	0	996	32	0
36	BP	1139	0	1223	41	0
36	DP	1135	0	1212	52	0
37	BQ	1122	0	1179	28	0
37	DQ	1122	0	1179	40	0
38	BR	968	0	1033	22	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	20	0
39	DS	870	0	923	33	0
40	BT	1091	0	1151	26	0
40	DT	1083	0	1136	37	0
41	BU	959	0	1019	18	0
41	DU	959	0	1018	30	0
42	BV	771	0	830	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DV	771	0	830	24	0
43	BW	886	0	940	17	0
43	DW	886	0	940	13	0
44	BX	750	0	814	15	0
44	DX	750	0	814	27	0
45	BY	806	0	881	27	0
45	DY	806	0	881	30	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	70	0
47	B0	653	0	674	13	0
47	D0	653	0	674	22	0
48	B1	755	0	826	16	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	14	0
50	B3	469	0	518	6	0
50	D3	464	0	514	13	0
51	B4	558	0	544	37	0
51	D4	532	0	503	25	0
52	B5	455	0	465	14	0
52	D5	455	0	465	13	0
53	B6	453	0	473	13	0
53	D6	449	0	469	12	0
54	B7	418	0	467	10	0
54	D7	418	0	467	13	0
55	B8	517	0	582	17	0
55	D8	517	0	582	15	0
56	B9	307	0	335	7	0
56	D9	307	0	335	11	0
57	AA	216	0	0	0	0
57	AB	1	0	0	0	0
57	AE	1	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	2	0	0	0	0
57	AN	2	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0
57	AW	2	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	2	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
57	DW	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
61	AA	210	0	0	13	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	1	0
61	AM	2	0	0	0	0
61	AV	2	0	0	0	0
61	AW	4	0	0	0	0
61	AX	4	0	0	0	0
61	AY	1	0	0	0	0
61	B0	6	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	4	0	0	0	0
61	B6	2	0	0	0	0
61	B7	3	0	0	2	0

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5502 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2139:C:N4	26:DA:2152:G:H1	1.46	1.14
1:CA:999:C:N4	1:CA:1042:G:H1	1.48	1.12
25:AY:49:C:N4	25:AY:65:G:H1	1.51	1.09
1:CA:985:C:N4	1:CA:1220:G:H1	1.50	1.09
1:CA:998:G:H1	1:CA:1043:C:N4	1.51	1.09

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	229/256 (90%)	208 (91%)	13 (6%)	8 (4%)	<b>3</b> <b>5</b>
2	CB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	<b>4</b> <b>6</b>

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
40	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	32
42	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	32
43	BW	110/113 (97%)	110 (100%)	0	0	100	100
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	30
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	25	47
46	DZ	172/206 (84%)	159 (92%)	13 (8%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	13	27
48	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
48	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
51	D4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	3
52	B5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	12
55	B8	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11410/12128 (94%)	10945 (96%)	381 (3%)	84 (1%)	22	43

5 of 84 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	155 (81%)	37 (19%)	1	2
2	CB	187/220 (85%)	151 (81%)	36 (19%)	1	2
3	AC	143/188 (76%)	127 (89%)	16 (11%)	6	10
3	CC	141/188 (75%)	116 (82%)	25 (18%)	2	3
4	AD	170/181 (94%)	147 (86%)	23 (14%)	4	6
4	CD	174/181 (96%)	147 (84%)	27 (16%)	2	4
5	AE	113/123 (92%)	106 (94%)	7 (6%)	18	37
5	CE	114/123 (93%)	99 (87%)	15 (13%)	4	7
6	AF	84/90 (93%)	74 (88%)	10 (12%)	5	9
6	CF	86/90 (96%)	79 (92%)	7 (8%)	11	23
7	AG	119/127 (94%)	99 (83%)	20 (17%)	2	3
7	CG	120/127 (94%)	106 (88%)	14 (12%)	5	10
8	AH	114/119 (96%)	101 (89%)	13 (11%)	5	10

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

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

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

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

Mol	Chain	Res	Type
51	B4	3	GLU
5	CE	79	GLU
43	DW	4	LYS
53	B6	28	ARG
3	CC	21	ARG

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

Mol	Chain	Res	Type
51	B4	46	GLN
4	CD	77	ASN
42	DV	64	HIS
2	CB	16	HIS
3	CC	3	ASN

### 5.3.3 RNA ⓘ

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

5 of 1960 RNA backbone outliers are listed below:

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

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2181	G
1	CA	266	G
26	DA	1653	G

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Mol	Chain	Res	Type
26	BA	2183	C
26	BA	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
23	PSU	AW	32	57,23	17,21,22	1.51	2 (11%)	20,30,33	3.11	6 (30%)
23	MIA	AW	37	23	24,31,32	2.20	4 (16%)	26,44,47	2.40	9 (34%)
23	MIA	CW	37	23	18,24,32	1.12	2 (11%)	18,35,47	1.23	2 (11%)
24	31H	AX	76	24,57	28,34,35	1.20	4 (14%)	23,47,50	1.61	4 (17%)
23	7MG	AW	46	23	22,26,27	1.79	4 (18%)	28,39,42	2.72	9 (32%)
25	7MG	AY	46	25	22,26,27	1.70	4 (18%)	28,39,42	3.20	12 (42%)
24	4SU	CX	8	24	14,21,22	1.24	2 (14%)	15,30,33	2.35	2 (13%)
25	PSU	CY	32	25	17,21,22	1.47	3 (17%)	20,30,33	3.26	7 (35%)
23	PSU	CW	32	23	17,21,22	1.53	2 (11%)	20,30,33	3.20	6 (30%)
23	PSU	AW	55	23	17,21,22	1.59	2 (11%)	20,30,33	3.39	6 (30%)
25	PSU	CY	55	25	17,21,22	1.39	3 (17%)	20,30,33	3.23	6 (30%)
25	PSU	AY	55	25	17,21,22	1.63	3 (17%)	20,30,33	3.02	6 (30%)
23	5MU	AW	54	23	15,22,23	1.06	1 (6%)	16,32,35	1.99	1 (6%)
24	5MC	AX	32	24	15,22,23	1.33	1 (6%)	19,32,35	1.30	3 (15%)
23	4SU	AW	8	23	14,21,22	1.31	1 (7%)	15,30,33	1.54	2 (13%)
23	PSU	AW	39	23	17,21,22	1.53	2 (11%)	20,30,33	3.15	6 (30%)
25	MIA	AY	37	25	18,24,32	1.15	2 (11%)	18,35,47	1.24	2 (11%)
24	5MU	CX	54	24	15,22,23	1.10	1 (6%)	16,32,35	1.74	2 (12%)
24	5MC	CX	32	24	15,22,23	1.23	1 (6%)	19,32,35	1.39	2 (10%)
23	F3N	CW	76	23	30,36,37	1.50	6 (20%)	29,51,54	1.19	1 (3%)
25	PSU	AY	32	25	17,21,22	1.45	2 (11%)	20,30,33	3.18	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	CX	55	24	17,21,22	1.58	2 (11%)	20,30,33	3.10	6 (30%)
23	5MU	CW	54	23	15,22,23	1.10	1 (6%)	16,32,35	2.11	1 (6%)
23	PSU	CW	55	23	17,21,22	1.50	2 (11%)	20,30,33	3.19	6 (30%)
25	4SU	CY	8	25	14,21,22	1.38	1 (7%)	15,30,33	1.44	2 (13%)
23	F3N	AW	76	23	30,36,37	1.49	5 (16%)	29,51,54	1.21	1 (3%)
24	PSU	AX	55	24	17,21,22	1.78	3 (17%)	20,30,33	3.16	7 (35%)
25	4SU	AY	8	25	14,21,22	1.31	1 (7%)	15,30,33	1.40	2 (13%)
25	5MU	CY	54	25	15,22,23	1.05	1 (6%)	16,32,35	1.86	2 (12%)
23	4SU	CW	8	23	14,21,22	1.27	1 (7%)	15,30,33	1.30	2 (13%)
25	PSU	CY	39	25	17,21,22	1.85	4 (23%)	20,30,33	2.88	7 (35%)
25	MIA	CY	37	25	18,24,32	1.17	2 (11%)	18,35,47	1.27	2 (11%)
25	5MU	AY	54	25	15,22,23	1.12	1 (6%)	16,32,35	1.99	2 (12%)
24	4SU	AX	8	24	14,21,22	1.46	2 (14%)	15,30,33	2.69	2 (13%)
23	7MG	CW	46	23	22,26,27	1.84	4 (18%)	28,39,42	2.56	10 (35%)
25	7MG	CY	46	25	22,26,27	1.80	4 (18%)	28,39,42	2.81	12 (42%)
23	PSU	CW	39	23	17,21,22	1.55	2 (11%)	20,30,33	3.51	6 (30%)
24	5MU	AX	54	24,57	15,22,23	1.08	1 (6%)	16,32,35	1.88	2 (12%)
25	PSU	AY	39	25	17,21,22	1.51	2 (11%)	20,30,33	3.30	7 (35%)
24	31H	CX	76	24,57	28,34,35	1.21	3 (10%)	23,47,50	1.51	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	57,23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
24	31H	AX	76	24,57	-	7/18/40/41	0/3/3/3
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
25	7MG	AY	46	25	-	4/7/37/38	0/3/3/3
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
25	PSU	CY	32	25	-	3/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	PSU	CY	55	25	-	6/7/25/26	0/2/2/2

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

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.34	1.53	1.32
23	AW	37	MIA	C2-S10	-6.22	1.70	1.75
23	CW	46	7MG	C6-C5	5.71	1.49	1.41
24	AX	55	PSU	C5-C1'	-5.39	1.47	1.52
25	CY	39	PSU	C5-C1'	-5.30	1.47	1.52

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	46	7MG	N3-C4-N9	11.30	141.42	126.91
23	CW	39	PSU	N1-C2-N3	-9.66	120.75	128.43
25	CY	55	PSU	N1-C2-N3	-9.28	121.06	128.43
24	AX	8	4SU	C2-N3-C4	9.19	128.48	115.15
25	AY	39	PSU	N1-C2-N3	-9.08	121.21	128.43

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
24	AX	76	31H	OCN-CN-N-CA
25	AY	46	7MG	C4'-C5'-O5'-P
25	CY	55	PSU	C2'-C1'-C5-C4
25	CY	55	PSU	C2'-C1'-C5-C6

There are no ring outliers.

26 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	76	31H	1	0
25	AY	46	7MG	3	0
24	CX	8	4SU	3	0
23	CW	32	PSU	1	0
23	AW	55	PSU	1	0
25	CY	55	PSU	2	0
25	AY	55	PSU	1	0
24	AX	32	5MC	2	0
23	AW	39	PSU	1	0
25	AY	37	MIA	1	0
24	CX	32	5MC	1	0
23	CW	76	F3N	3	0
24	CX	55	PSU	1	0
23	CW	55	PSU	1	0
25	CY	8	4SU	2	0
23	AW	76	F3N	1	0
25	AY	8	4SU	1	0
23	CW	8	4SU	2	0
25	CY	39	PSU	8	0
25	CY	37	MIA	3	0
24	AX	8	4SU	1	0
23	CW	46	7MG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	CY	46	7MG	4	0
23	CW	39	PSU	1	0
25	AY	39	PSU	2	0
24	CX	76	31H	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2063 ligands modelled in this entry, 2061 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	CD	501	4	0,12,12	0.00	-	-		
58	SF4	AD	501	4	0,12,12	0.00	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 2 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1497/1521 (98%)	0.04	16 (1%) 80 78	41, 72, 93, 106	0
1	CA	1503/1521 (98%)	0.06	62 (4%) 37 30	43, 75, 94, 106	0
2	AB	231/256 (90%)	0.69	29 (12%) 3 2	68, 82, 89, 95	0
2	CB	231/256 (90%)	1.72	85 (36%) 0 0	68, 83, 90, 96	0
3	AC	206/239 (86%)	0.79	24 (11%) 4 3	69, 79, 87, 94	0
3	CC	206/239 (86%)	1.62	73 (35%) 0 0	70, 82, 90, 94	0
4	AD	208/209 (99%)	1.04	38 (18%) 1 0	57, 72, 81, 87	0
4	CD	208/209 (99%)	0.96	25 (12%) 4 2	60, 72, 81, 89	0
5	AE	148/162 (91%)	0.74	12 (8%) 12 8	58, 71, 81, 85	0
5	CE	148/162 (91%)	1.07	21 (14%) 2 1	60, 74, 83, 86	0
6	AF	100/101 (99%)	0.41	1 (1%) 82 80	52, 67, 75, 85	0
6	CF	100/101 (99%)	0.38	3 (3%) 50 43	57, 71, 81, 85	0
7	AG	155/156 (99%)	0.42	9 (5%) 23 17	66, 76, 85, 96	0
7	CG	155/156 (99%)	1.29	47 (30%) 0 0	68, 77, 86, 97	0
8	AH	137/138 (99%)	0.32	2 (1%) 73 70	62, 72, 79, 83	0
8	CH	137/138 (99%)	1.22	35 (25%) 0 0	64, 74, 80, 85	0
9	AI	127/128 (99%)	0.99	19 (14%) 2 1	62, 80, 87, 89	0
9	CI	127/128 (99%)	2.96	83 (65%) 0 0	69, 82, 89, 91	0
10	AJ	97/105 (92%)	0.82	13 (13%) 3 2	66, 83, 91, 92	0
10	CJ	96/105 (91%)	2.14	43 (44%) 0 0	68, 84, 91, 93	0
11	AK	114/129 (88%)	0.86	10 (8%) 10 7	51, 70, 80, 84	0
11	CK	114/129 (88%)	0.93	13 (11%) 5 3	52, 72, 81, 85	0
12	AL	122/132 (92%)	0.24	1 (0%) 86 84	41, 56, 71, 75	0
12	CL	122/132 (92%)	0.85	23 (18%) 1 0	58, 73, 82, 87	0

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

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

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

The worst 5 of 1598 RSRZ outliers are listed below:

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

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

## 6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
25	7MG	CY	46	24/25	0.71	0.25	87,101,108,135	0
23	7MG	CW	46	24/25	0.73	0.33	81,97,101,125	0
25	5MU	CY	54	21/22	0.74	0.49	89,99,105,136	0
25	PSU	CY	55	20/21	0.75	0.41	86,100,107,118	0
23	4SU	CW	8	20/21	0.77	0.29	85,96,117,121	0
25	4SU	CY	8	20/21	0.79	0.16	88,102,112,128	0
25	MIA	CY	37	22/30	0.79	0.30	79,95,102,124	0
24	4SU	CX	8	20/21	0.80	0.13	84,92,105,111	0
23	7MG	AW	46	24/25	0.80	0.21	80,97,112,135	0
25	PSU	CY	39	20/21	0.81	0.27	86,91,104,110	0
25	PSU	AY	55	20/21	0.81	0.20	85,96,106,117	0
25	7MG	AY	46	24/25	0.82	0.18	80,99,107,116	0
25	PSU	CY	32	20/21	0.83	0.26	77,91,109,114	0
25	4SU	AY	8	20/21	0.83	0.13	83,95,104,129	0
23	PSU	AW	55	20/21	0.83	0.27	76,88,103,105	0
25	PSU	AY	32	20/21	0.83	0.26	76,92,107,110	0
23	4SU	AW	8	20/21	0.84	0.17	83,89,107,110	0
23	PSU	CW	55	20/21	0.84	0.34	76,90,103,106	0
25	5MU	AY	54	21/22	0.85	0.20	81,89,99,128	0
23	PSU	AW	32	20/21	0.86	0.26	77,84,98,106	0
23	5MU	CW	54	21/22	0.86	0.23	76,87,97,99	0
25	MIA	AY	37	22/30	0.86	0.22	79,89,101,116	0
25	PSU	AY	39	20/21	0.86	0.25	84,90,102,107	0
23	MIA	CW	37	22/30	0.87	0.30	72,86,92,96	0
23	PSU	CW	32	20/21	0.87	0.48	77,86,95,106	0
23	PSU	CW	39	20/21	0.89	0.43	76,85,92,95	0
24	31H	CX	76	32/33	0.90	0.35	48,68,88,99	0
23	5MU	AW	54	21/22	0.91	0.21	66,80,87,93	0
24	PSU	CX	55	20/21	0.92	0.15	81,87,92,97	0
23	PSU	AW	39	20/21	0.93	0.24	71,82,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MIA	AW	37	29/30	0.93	0.25	56,65,80,82	0
24	4SU	AX	8	20/21	0.93	0.17	59,69,79,85	0
23	F3N	CW	76	33/34	0.93	0.44	53,69,79,80	0
24	31H	AX	76	32/33	0.94	0.33	31,57,76,77	10
24	5MU	CX	54	21/22	0.94	0.21	71,85,94,104	0
23	F3N	AW	76	33/34	0.94	0.38	44,58,72,77	0
24	PSU	AX	55	20/21	0.94	0.16	52,69,77,77	0
24	5MC	CX	32	21/22	0.95	0.18	63,77,85,87	0
24	5MU	AX	54	21/22	0.96	0.16	46,72,77,86	0
24	5MC	AX	32	21/22	0.97	0.20	50,57,69,76	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
57	MG	CE	202	1/1	0.26	0.19	95,95,95,95	0
59	ZN	D4	501	1/1	0.33	0.12	162,162,162,162	0
57	MG	AA	1784	1/1	0.34	0.29	72,72,72,72	0
57	MG	DA	3254	1/1	0.43	0.15	68,68,68,68	0
57	MG	BA	3327	1/1	0.47	0.17	39,39,39,39	0
57	MG	CA	3086	1/1	0.48	0.13	93,93,93,93	0
57	MG	BA	3702	1/1	0.49	0.12	39,39,39,39	0
57	MG	DA	3135	1/1	0.49	0.18	63,63,63,63	0
57	MG	AA	1618	1/1	0.55	0.18	68,68,68,68	0
57	MG	DA	3628	1/1	0.57	0.19	77,77,77,77	0
57	MG	BA	3734	1/1	0.57	0.14	65,65,65,65	0
57	MG	CA	3115	1/1	0.58	0.34	82,82,82,82	0
57	MG	DA	3070	1/1	0.59	0.19	65,65,65,65	0
57	MG	DA	3033	1/1	0.60	0.49	68,68,68,68	0
57	MG	DA	3463	1/1	0.60	0.19	44,44,44,44	0
57	MG	DA	3204	1/1	0.60	0.21	68,68,68,68	0
57	MG	BA	3439	1/1	0.61	0.18	36,36,36,36	0
57	MG	DA	3318	1/1	0.62	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3057	1/1	0.63	0.20	44,44,44,44	0
57	MG	AX	3007	1/1	0.63	0.30	68,68,68,68	0
57	MG	BA	3154	1/1	0.63	0.21	52,52,52,52	0
57	MG	BA	3693	1/1	0.64	0.16	77,77,77,77	0
57	MG	CA	3003	1/1	0.64	0.16	58,58,58,58	0
57	MG	DA	3516	1/1	0.65	0.21	67,67,67,67	0
57	MG	BA	3272	1/1	0.66	0.26	64,64,64,64	0
57	MG	BA	3710	1/1	0.66	0.79	65,65,65,65	0
57	MG	DA	3116	1/1	0.67	0.16	53,53,53,53	0
57	MG	AA	1743	1/1	0.67	0.17	66,66,66,66	0
57	MG	DA	3099	1/1	0.68	0.18	63,63,63,63	0
57	MG	DA	3487	1/1	0.68	0.12	55,55,55,55	0
57	MG	BA	3655	1/1	0.69	0.13	55,55,55,55	0
57	MG	BA	3569	1/1	0.69	0.22	56,56,56,56	0
57	MG	DA	3122	1/1	0.69	0.19	60,60,60,60	0
57	MG	AA	1713	1/1	0.69	0.11	67,67,67,67	0
57	MG	BA	3652	1/1	0.69	0.09	58,58,58,58	0
57	MG	DA	3199	1/1	0.69	0.25	62,62,62,62	0
57	MG	AA	1679	1/1	0.69	0.19	51,51,51,51	0
57	MG	DA	3313	1/1	0.70	0.11	39,39,39,39	0
57	MG	DA	3545	1/1	0.70	0.12	62,62,62,62	0
57	MG	BA	3288	1/1	0.70	0.18	44,44,44,44	0
57	MG	BA	3041	1/1	0.71	0.29	63,63,63,63	0
57	MG	BA	3068	1/1	0.71	0.17	49,49,49,49	0
57	MG	BA	3712	1/1	0.71	0.22	51,51,51,51	0
57	MG	BA	3727	1/1	0.71	0.24	53,53,53,53	0
57	MG	CA	3006	1/1	0.71	0.11	68,68,68,68	0
57	MG	AA	1669	1/1	0.72	0.18	69,69,69,69	0
57	MG	AL	201	1/1	0.72	0.13	63,63,63,63	0
57	MG	CA	3058	1/1	0.72	0.19	66,66,66,66	0
57	MG	BA	3667	1/1	0.72	0.24	58,58,58,58	0
57	MG	AA	1701	1/1	0.72	0.27	73,73,73,73	0
57	MG	BA	3688	1/1	0.72	0.27	61,61,61,61	0
57	MG	DQ	3003	1/1	0.73	0.64	62,62,62,62	0
57	MG	BA	3176	1/1	0.73	0.26	55,55,55,55	0
57	MG	DA	3071	1/1	0.73	0.23	47,47,47,47	0
57	MG	BA	3680	1/1	0.73	0.32	42,42,42,42	0
57	MG	DA	3634	1/1	0.73	0.14	68,68,68,68	0
57	MG	DA	3332	1/1	0.73	0.18	46,46,46,46	0
57	MG	CA	3059	1/1	0.73	0.16	75,75,75,75	0
57	MG	DA	3596	1/1	0.73	0.19	69,69,69,69	0
57	MG	BA	3538	1/1	0.74	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3487	1/1	0.74	0.14	54,54,54,54	0
57	MG	DA	3376	1/1	0.74	0.11	51,51,51,51	0
57	MG	BB	3004	1/1	0.74	0.21	69,69,69,69	0
57	MG	BA	3265	1/1	0.74	0.29	72,72,72,72	0
57	MG	DA	3097	1/1	0.74	0.15	47,47,47,47	0
57	MG	BB	3020	1/1	0.75	0.16	65,65,65,65	0
57	MG	BA	3016	1/1	0.75	0.28	67,67,67,67	0
57	MG	AA	1684	1/1	0.75	0.13	54,54,54,54	0
57	MG	CA	3130	1/1	0.75	0.28	64,64,64,64	0
57	MG	DA	3502	1/1	0.75	0.24	48,48,48,48	0
57	MG	DA	3624	1/1	0.75	0.48	59,59,59,59	0
57	MG	AA	1686	1/1	0.75	0.14	61,61,61,61	0
57	MG	DA	3253	1/1	0.75	0.13	54,54,54,54	0
57	MG	BA	3340	1/1	0.75	0.18	27,27,27,27	0
57	MG	BA	3121	1/1	0.75	0.29	42,42,42,42	0
57	MG	DA	3086	1/1	0.76	0.11	47,47,47,47	0
57	MG	DA	3279	1/1	0.76	0.14	36,36,36,36	0
57	MG	DA	3032	1/1	0.76	0.21	57,57,57,57	0
57	MG	BA	3579	1/1	0.76	0.11	63,63,63,63	0
57	MG	CA	3005	1/1	0.76	0.20	73,73,73,73	0
57	MG	CA	3014	1/1	0.76	0.15	62,62,62,62	0
57	MG	CA	3122	1/1	0.76	0.13	69,69,69,69	0
57	MG	DA	3061	1/1	0.76	0.21	60,60,60,60	0
57	MG	CA	3154	1/1	0.76	0.18	68,68,68,68	0
57	MG	DA	3174	1/1	0.76	0.19	52,52,52,52	0
57	MG	DA	3400	1/1	0.76	0.14	62,62,62,62	0
57	MG	AA	1689	1/1	0.77	0.29	71,71,71,71	0
57	MG	BA	3224	1/1	0.77	0.30	59,59,59,59	0
57	MG	DA	3108	1/1	0.77	0.12	50,50,50,50	0
57	MG	CA	3032	1/1	0.77	0.16	53,53,53,53	0
57	MG	DA	3066	1/1	0.77	0.10	58,58,58,58	0
57	MG	BA	3015	1/1	0.77	0.18	47,47,47,47	0
57	MG	BA	3164	1/1	0.77	0.22	46,46,46,46	0
57	MG	BA	3637	1/1	0.77	0.14	38,38,38,38	0
57	MG	DA	3015	1/1	0.77	0.23	60,60,60,60	0
57	MG	DA	3079	1/1	0.77	0.11	72,72,72,72	0
57	MG	BG	202	1/1	0.78	0.15	52,52,52,52	0
57	MG	AA	1620	1/1	0.78	0.14	59,59,59,59	0
57	MG	BA	3074	1/1	0.78	0.23	69,69,69,69	0
57	MG	AA	1631	1/1	0.78	0.14	64,64,64,64	0
57	MG	BA	3676	1/1	0.78	0.17	70,70,70,70	0
57	MG	DA	3016	1/1	0.78	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3730	1/1	0.78	0.17	68,68,68,68	0
57	MG	BA	3369	1/1	0.78	0.28	62,62,62,62	0
57	MG	DA	3114	1/1	0.78	0.12	51,51,51,51	0
57	MG	BA	3611	1/1	0.78	0.18	59,59,59,59	0
57	MG	DA	3284	1/1	0.78	0.14	58,58,58,58	0
57	MG	BA	3026	1/1	0.78	0.15	60,60,60,60	0
57	MG	DA	3314	1/1	0.78	0.12	43,43,43,43	0
57	MG	DA	3041	1/1	0.78	0.18	60,60,60,60	0
57	MG	DA	3520	1/1	0.79	0.11	57,57,57,57	0
57	MG	BA	3715	1/1	0.79	0.17	52,52,52,52	0
57	MG	BA	3229	1/1	0.79	0.24	52,52,52,52	0
57	MG	BA	3498	1/1	0.79	0.21	45,45,45,45	0
57	MG	DA	3320	1/1	0.79	0.09	49,49,49,49	0
57	MG	AA	1625	1/1	0.79	0.17	73,73,73,73	0
57	MG	DA	3024	1/1	0.79	0.41	61,61,61,61	0
57	MG	DA	3191	1/1	0.79	0.30	54,54,54,54	0
57	MG	DA	3052	1/1	0.79	0.10	49,49,49,49	0
57	MG	AA	1655	1/1	0.79	0.12	53,53,53,53	0
57	MG	DA	3542	1/1	0.79	0.17	60,60,60,60	0
57	MG	DB	3007	1/1	0.79	0.12	67,67,67,67	0
57	MG	DA	3657	1/1	0.79	0.45	54,54,54,54	0
57	MG	DA	3002	1/1	0.79	0.14	64,64,64,64	0
57	MG	CA	3019	1/1	0.79	0.16	68,68,68,68	0
57	MG	AA	1610	1/1	0.79	0.18	81,81,81,81	0
57	MG	BA	3759	1/1	0.79	0.13	70,70,70,70	0
57	MG	AA	1711	1/1	0.79	0.13	51,51,51,51	0
57	MG	BA	3160	1/1	0.79	0.20	49,49,49,49	0
57	MG	BA	3006	1/1	0.79	0.24	54,54,54,54	0
57	MG	BA	3231	1/1	0.79	0.17	57,57,57,57	0
57	MG	DA	3420	1/1	0.80	0.11	49,49,49,49	0
57	MG	CA	3013	1/1	0.80	0.14	67,67,67,67	0
57	MG	BA	3696	1/1	0.80	0.10	46,46,46,46	0
57	MG	DA	3612	1/1	0.80	0.08	58,58,58,58	0
57	MG	CA	3091	1/1	0.80	0.15	69,69,69,69	0
57	MG	AA	1604	1/1	0.80	0.12	58,58,58,58	0
57	MG	BA	3700	1/1	0.80	0.24	36,36,36,36	0
57	MG	CA	3061	1/1	0.80	0.21	66,66,66,66	0
57	MG	DA	3356	1/1	0.80	0.16	39,39,39,39	0
57	MG	BA	3713	1/1	0.80	0.28	33,33,33,33	0
57	MG	DA	3089	1/1	0.80	0.18	52,52,52,52	0
57	MG	BA	3721	1/1	0.80	0.10	47,47,47,47	0
57	MG	BA	3557	1/1	0.80	0.18	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	3678	1/1	0.80	0.10	67,67,67,67	0
57	MG	AA	1622	1/1	0.80	0.21	69,69,69,69	0
57	MG	DA	3650	1/1	0.80	0.14	61,61,61,61	0
57	MG	DA	3649	1/1	0.80	0.13	71,71,71,71	0
57	MG	DA	3056	1/1	0.80	0.12	49,49,49,49	0
57	MG	BA	3257	1/1	0.81	0.18	43,43,43,43	0
57	MG	DA	3648	1/1	0.81	0.07	62,62,62,62	0
57	MG	BA	3281	1/1	0.81	0.28	50,50,50,50	0
57	MG	BA	3458	1/1	0.81	0.20	59,59,59,59	0
57	MG	AA	1697	1/1	0.81	0.11	65,65,65,65	0
57	MG	BA	3411	1/1	0.81	0.24	50,50,50,50	0
57	MG	AA	1741	1/1	0.81	0.12	86,86,86,86	0
57	MG	DA	3351	1/1	0.81	0.08	56,56,56,56	0
57	MG	BA	3644	1/1	0.81	0.18	64,64,64,64	0
57	MG	CA	3049	1/1	0.81	0.21	65,65,65,65	0
57	MG	BA	3453	1/1	0.81	0.28	50,50,50,50	0
57	MG	BA	3670	1/1	0.81	0.18	54,54,54,54	0
57	MG	DA	3513	1/1	0.81	0.14	69,69,69,69	0
57	MG	AA	1710	1/1	0.81	0.15	64,64,64,64	0
57	MG	BA	3442	1/1	0.81	0.19	65,65,65,65	0
57	MG	DA	3395	1/1	0.81	0.17	58,58,58,58	0
57	MG	BA	3270	1/1	0.81	0.22	56,56,56,56	0
57	MG	DA	3625	1/1	0.81	0.10	60,60,60,60	0
57	MG	BA	3197	1/1	0.81	0.24	58,58,58,58	0
57	MG	AA	1623	1/1	0.81	0.24	65,65,65,65	0
57	MG	DA	3301	1/1	0.81	0.11	63,63,63,63	0
57	MG	CA	3094	1/1	0.81	0.08	61,61,61,61	0
57	MG	BA	3475	1/1	0.81	0.09	49,49,49,49	0
57	MG	DA	3591	1/1	0.81	0.06	66,66,66,66	0
57	MG	DA	3205	1/1	0.82	0.16	62,62,62,62	0
57	MG	AA	1616	1/1	0.82	0.09	73,73,73,73	0
57	MG	BB	3001	1/1	0.82	0.29	68,68,68,68	0
57	MG	DA	3233	1/1	0.82	0.13	65,65,65,65	0
57	MG	DA	3101	1/1	0.82	0.13	56,56,56,56	0
57	MG	BN	3002	1/1	0.82	0.20	51,51,51,51	0
57	MG	BA	3755	1/1	0.82	0.24	43,43,43,43	0
57	MG	BA	3183	1/1	0.82	0.48	49,49,49,49	0
57	MG	BE	301	1/1	0.82	0.20	31,31,31,31	0
57	MG	AA	1810	1/1	0.82	0.09	86,86,86,86	0
57	MG	CA	3102	1/1	0.82	0.16	71,71,71,71	0
57	MG	AA	1644	1/1	0.82	0.12	56,56,56,56	0
57	MG	BA	3343	1/1	0.82	0.18	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	3257	1/1	0.82	0.20	44,44,44,44	0
57	MG	BA	3058	1/1	0.82	0.19	54,54,54,54	0
57	MG	DA	3514	1/1	0.82	0.14	47,47,47,47	0
57	MG	DA	3468	1/1	0.82	0.14	62,62,62,62	0
57	MG	BF	310	1/1	0.82	0.23	56,56,56,56	0
57	MG	DA	3497	1/1	0.82	0.19	58,58,58,58	0
57	MG	CA	3162	1/1	0.82	0.07	79,79,79,79	0
57	MG	DB	3003	1/1	0.82	0.10	78,78,78,78	0
57	MG	BA	3347	1/1	0.82	0.19	38,38,38,38	0
57	MG	DA	3619	1/1	0.82	0.15	40,40,40,40	0
57	MG	DA	3530	1/1	0.82	0.14	55,55,55,55	0
57	MG	BZ	301	1/1	0.82	0.18	49,49,49,49	0
57	MG	DA	3627	1/1	0.82	0.14	57,57,57,57	0
57	MG	CA	3146	1/1	0.82	0.18	72,72,72,72	0
57	MG	DA	3592	1/1	0.82	0.14	67,67,67,67	0
57	MG	DA	3035	1/1	0.82	0.12	37,37,37,37	0
57	MG	AA	1660	1/1	0.82	0.24	51,51,51,51	0
57	MG	AX	3016	1/1	0.82	0.61	86,86,86,86	0
57	MG	DA	3143	1/1	0.82	0.14	62,62,62,62	0
57	MG	DA	3560	1/1	0.82	0.15	60,60,60,60	0
57	MG	BA	3717	1/1	0.82	0.15	72,72,72,72	0
57	MG	DA	3607	1/1	0.82	0.14	64,64,64,64	0
57	MG	CA	3050	1/1	0.82	0.19	73,73,73,73	0
57	MG	DA	3549	1/1	0.82	0.20	49,49,49,49	0
57	MG	BA	3807	1/1	0.82	0.24	66,66,66,66	0
57	MG	BA	3200	1/1	0.83	0.25	48,48,48,48	0
57	MG	CA	3004	1/1	0.83	0.09	69,69,69,69	0
57	MG	DA	3397	1/1	0.83	0.15	42,42,42,42	0
57	MG	BA	3060	1/1	0.83	0.22	51,51,51,51	0
57	MG	DA	3394	1/1	0.83	0.05	60,60,60,60	0
57	MG	BA	3423	1/1	0.83	0.16	69,69,69,69	0
57	MG	BA	3233	1/1	0.83	0.28	40,40,40,40	0
57	MG	CA	3143	1/1	0.83	0.20	74,74,74,74	0
57	MG	BA	3593	1/1	0.83	0.20	55,55,55,55	0
57	MG	AA	1766	1/1	0.83	0.19	71,71,71,71	0
57	MG	BA	3235	1/1	0.83	0.20	44,44,44,44	0
57	MG	CE	201	1/1	0.83	0.18	65,65,65,65	0
57	MG	DA	3618	1/1	0.83	0.10	46,46,46,46	0
57	MG	AW	3001	1/1	0.83	0.11	59,59,59,59	0
57	MG	DB	3001	1/1	0.83	0.17	63,63,63,63	0
57	MG	AA	1664	1/1	0.83	0.22	62,62,62,62	0
57	MG	CA	3002	1/1	0.83	0.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3238	1/1	0.83	0.15	48,48,48,48	0
57	MG	BA	3111	1/1	0.83	0.32	53,53,53,53	0
57	MG	BA	3600	1/1	0.83	0.28	44,44,44,44	0
57	MG	BA	3608	1/1	0.83	0.29	58,58,58,58	0
57	MG	AA	1650	1/1	0.83	0.15	74,74,74,74	0
57	MG	CA	3070	1/1	0.83	0.15	69,69,69,69	0
57	MG	BB	3019	1/1	0.83	0.20	70,70,70,70	0
57	MG	DA	3606	1/1	0.83	0.20	74,74,74,74	0
57	MG	DA	3369	1/1	0.83	0.12	55,55,55,55	0
57	MG	CA	3031	1/1	0.83	0.14	58,58,58,58	0
57	MG	DA	3227	1/1	0.83	0.20	56,56,56,56	0
57	MG	BA	3240	1/1	0.83	0.18	53,53,53,53	0
57	MG	BA	3738	1/1	0.83	0.13	41,41,41,41	0
57	MG	CA	3090	1/1	0.83	0.17	76,76,76,76	0
57	MG	CA	3017	1/1	0.83	0.15	54,54,54,54	0
57	MG	CA	3012	1/1	0.83	0.32	64,64,64,64	0
57	MG	BA	3002	1/1	0.83	0.28	53,53,53,53	0
57	MG	CA	3016	1/1	0.83	0.13	48,48,48,48	0
57	MG	DB	3010	1/1	0.83	0.13	75,75,75,75	0
57	MG	AX	3005	1/1	0.84	0.11	65,65,65,65	0
57	MG	DA	3140	1/1	0.84	0.10	64,64,64,64	0
57	MG	AA	1696	1/1	0.84	0.10	83,83,83,83	0
57	MG	CA	3112	1/1	0.84	0.10	72,72,72,72	0
57	MG	DA	3568	1/1	0.84	0.14	43,43,43,43	0
57	MG	DA	3411	1/1	0.84	0.18	37,37,37,37	0
57	MG	DA	3426	1/1	0.84	0.12	49,49,49,49	0
57	MG	BA	3598	1/1	0.84	0.15	33,33,33,33	0
57	MG	B7	104	1/1	0.84	0.27	62,62,62,62	0
57	MG	DF	303	1/1	0.84	0.15	42,42,42,42	0
57	MG	CA	3039	1/1	0.84	0.16	64,64,64,64	0
57	MG	DA	3379	1/1	0.84	0.09	46,46,46,46	0
57	MG	CA	3108	1/1	0.84	0.11	72,72,72,72	0
57	MG	DA	3065	1/1	0.84	0.10	56,56,56,56	0
57	MG	BA	3155	1/1	0.84	0.19	40,40,40,40	0
57	MG	DA	3087	1/1	0.84	0.18	55,55,55,55	0
57	MG	DA	3456	1/1	0.84	0.21	38,38,38,38	0
57	MG	AA	1695	1/1	0.84	0.20	59,59,59,59	0
57	MG	AA	1723	1/1	0.84	0.15	63,63,63,63	0
57	MG	DA	3123	1/1	0.84	0.16	54,54,54,54	0
57	MG	BA	3049	1/1	0.84	0.19	46,46,46,46	0
57	MG	BA	3687	1/1	0.84	0.18	64,64,64,64	0
57	MG	DA	3604	1/1	0.84	0.15	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	BA	3145	1/1	0.84	0.25	48,48,48,48	0
57	MG	DF	302	1/1	0.84	0.14	53,53,53,53	0
57	MG	BA	3778	1/1	0.84	0.08	40,40,40,40	0
57	MG	CA	3009	1/1	0.84	0.12	73,73,73,73	0
57	MG	CA	3001	1/1	0.84	0.14	59,59,59,59	0
57	MG	BA	3809	1/1	0.84	0.37	61,61,61,61	0
57	MG	AA	1613	1/1	0.84	0.18	75,75,75,75	0
57	MG	BA	3505	1/1	0.84	0.22	53,53,53,53	0
57	MG	AA	1789	1/1	0.85	0.15	60,60,60,60	0
57	MG	DA	3234	1/1	0.85	0.15	54,54,54,54	0
57	MG	CA	3164	1/1	0.85	0.33	76,76,76,76	0
57	MG	DA	3111	1/1	0.85	0.13	56,56,56,56	0
57	MG	DA	3281	1/1	0.85	0.11	36,36,36,36	0
57	MG	DA	3491	1/1	0.85	0.25	43,43,43,43	0
57	MG	AA	1663	1/1	0.85	0.12	50,50,50,50	0
57	MG	DA	3196	1/1	0.85	0.16	54,54,54,54	0
57	MG	BA	3571	1/1	0.85	0.24	28,28,28,28	0
57	MG	DA	3092	1/1	0.85	0.16	57,57,57,57	0
57	MG	AA	1612	1/1	0.85	0.16	63,63,63,63	0
57	MG	BA	3477	1/1	0.85	0.16	68,68,68,68	0
57	MG	DA	3620	1/1	0.85	0.12	53,53,53,53	0
57	MG	BA	3078	1/1	0.85	0.32	54,54,54,54	0
57	MG	DA	3637	1/1	0.85	0.14	72,72,72,72	0
57	MG	BA	3656	1/1	0.85	0.17	45,45,45,45	0
57	MG	CA	3139	1/1	0.85	0.36	81,81,81,81	0
57	MG	AA	1699	1/1	0.85	0.32	58,58,58,58	0
57	MG	AX	3012	1/1	0.85	0.18	52,52,52,52	0
57	MG	AX	3013	1/1	0.85	0.20	70,70,70,70	0
57	MG	DA	3317	1/1	0.85	0.10	54,54,54,54	0
57	MG	DA	3636	1/1	0.85	0.16	62,62,62,62	0
57	MG	BA	3175	1/1	0.85	0.29	57,57,57,57	0
57	MG	DA	3574	1/1	0.85	0.07	61,61,61,61	0
57	MG	AA	1682	1/1	0.85	0.26	59,59,59,59	0
57	MG	BA	3225	1/1	0.85	0.13	46,46,46,46	0
57	MG	CA	3161	1/1	0.85	0.13	76,76,76,76	0
57	MG	BA	3570	1/1	0.85	0.21	31,31,31,31	0
57	MG	BA	3056	1/1	0.85	0.31	46,46,46,46	0
57	MG	CA	3068	1/1	0.85	0.16	58,58,58,58	0
57	MG	AA	1764	1/1	0.85	0.10	66,66,66,66	0
57	MG	AA	1667	1/1	0.85	0.19	55,55,55,55	0
57	MG	CA	3125	1/1	0.85	0.21	64,64,64,64	0
57	MG	BA	3632	1/1	0.85	0.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3107	1/1	0.85	0.12	68,68,68,68	0
57	MG	CA	3041	1/1	0.85	0.11	57,57,57,57	0
57	MG	BA	3283	1/1	0.85	0.40	57,57,57,57	0
57	MG	DA	3173	1/1	0.85	0.15	62,62,62,62	0
57	MG	DA	3046	1/1	0.85	0.14	56,56,56,56	0
57	MG	DA	3280	1/1	0.85	0.09	48,48,48,48	0
57	MG	AA	1601	1/1	0.85	0.12	81,81,81,81	0
57	MG	AA	1787	1/1	0.85	0.15	49,49,49,49	0
57	MG	DA	3462	1/1	0.85	0.22	50,50,50,50	0
57	MG	BA	3062	1/1	0.85	0.30	59,59,59,59	0
57	MG	D8	5001	1/1	0.85	0.22	44,44,44,44	0
57	MG	BA	3103	1/1	0.85	0.35	63,63,63,63	0
57	MG	CA	3011	1/1	0.85	0.25	66,66,66,66	0
57	MG	BA	3057	1/1	0.85	0.18	48,48,48,48	0
57	MG	BA	3485	1/1	0.85	0.24	26,26,26,26	0
57	MG	BA	3263	1/1	0.85	0.28	60,60,60,60	0
57	MG	AA	1602	1/1	0.85	0.10	68,68,68,68	0
57	MG	DA	3008	1/1	0.85	0.12	45,45,45,45	0
57	MG	DA	3488	1/1	0.86	0.10	53,53,53,53	0
57	MG	BA	3456	1/1	0.86	0.30	37,37,37,37	0
57	MG	BA	3338	1/1	0.86	0.18	55,55,55,55	0
57	MG	DA	3415	1/1	0.86	0.18	43,43,43,43	0
57	MG	AA	1738	1/1	0.86	0.22	68,68,68,68	0
57	MG	AA	1777	1/1	0.86	0.09	71,71,71,71	0
57	MG	BA	3318	1/1	0.86	0.16	54,54,54,54	0
57	MG	B8	5002	1/1	0.86	0.31	53,53,53,53	0
57	MG	CA	3109	1/1	0.86	0.15	74,74,74,74	0
57	MG	DA	3170	1/1	0.86	0.10	35,35,35,35	0
57	MG	CA	3052	1/1	0.86	0.12	71,71,71,71	0
57	MG	DA	3136	1/1	0.86	0.18	48,48,48,48	0
57	MG	DA	3617	1/1	0.86	0.25	51,51,51,51	0
57	MG	BA	3102	1/1	0.86	0.31	57,57,57,57	0
57	MG	DA	3088	1/1	0.86	0.26	50,50,50,50	0
57	MG	BA	3029	1/1	0.86	0.27	36,36,36,36	0
57	MG	BA	3525	1/1	0.86	0.16	43,43,43,43	0
57	MG	BA	3052	1/1	0.86	0.27	50,50,50,50	0
57	MG	DA	3418	1/1	0.86	0.07	47,47,47,47	0
57	MG	BA	3346	1/1	0.86	0.10	39,39,39,39	0
57	MG	BA	3232	1/1	0.86	0.24	49,49,49,49	0
57	MG	AA	1606	1/1	0.86	0.14	54,54,54,54	0
57	MG	DA	3417	1/1	0.86	0.13	52,52,52,52	0
57	MG	DA	3161	1/1	0.86	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3253	1/1	0.86	0.20	31,31,31,31	0
57	MG	BA	3099	1/1	0.86	0.24	61,61,61,61	0
57	MG	BA	3018	1/1	0.86	0.40	39,39,39,39	0
57	MG	BA	3243	1/1	0.86	0.67	44,44,44,44	0
57	MG	AX	3003	1/1	0.86	0.23	56,56,56,56	0
57	MG	BA	3250	1/1	0.86	0.21	68,68,68,68	0
57	MG	DA	3118	1/1	0.86	0.16	39,39,39,39	0
57	MG	BA	3107	1/1	0.86	0.33	57,57,57,57	0
57	MG	BA	3005	1/1	0.86	0.19	44,44,44,44	0
57	MG	DA	3130	1/1	0.86	0.15	52,52,52,52	0
57	MG	DA	3172	1/1	0.86	0.21	61,61,61,61	0
57	MG	AA	1763	1/1	0.86	0.07	79,79,79,79	0
57	MG	DA	3390	1/1	0.86	0.10	58,58,58,58	0
57	MG	BW	3001	1/1	0.86	0.35	44,44,44,44	0
57	MG	BA	3094	1/1	0.86	0.19	52,52,52,52	0
57	MG	BA	3726	1/1	0.86	0.20	31,31,31,31	0
57	MG	DA	3538	1/1	0.86	0.12	60,60,60,60	0
57	MG	BA	3577	1/1	0.86	0.17	58,58,58,58	0
57	MG	DA	3112	1/1	0.86	0.13	56,56,56,56	0
57	MG	DA	3275	1/1	0.86	0.14	65,65,65,65	0
57	MG	DA	3330	1/1	0.86	0.17	36,36,36,36	0
57	MG	DA	3333	1/1	0.86	0.17	47,47,47,47	0
57	MG	BA	3723	1/1	0.86	0.18	30,30,30,30	0
57	MG	AA	1658	1/1	0.86	0.14	64,64,64,64	0
57	MG	BA	3416	1/1	0.86	0.26	60,60,60,60	0
57	MG	DA	3424	1/1	0.86	0.18	41,41,41,41	0
57	MG	BA	3633	1/1	0.86	0.18	57,57,57,57	0
57	MG	DA	3435	1/1	0.86	0.12	44,44,44,44	0
57	MG	DG	3001	1/1	0.86	0.14	66,66,66,66	0
57	MG	BA	3530	1/1	0.86	0.25	33,33,33,33	0
57	MG	DA	3519	1/1	0.86	0.14	58,58,58,58	0
57	MG	BA	3365	1/1	0.86	0.13	51,51,51,51	0
57	MG	DA	3286	1/1	0.86	0.09	55,55,55,55	0
57	MG	BA	3592	1/1	0.86	0.09	65,65,65,65	0
57	MG	DA	3611	1/1	0.86	0.10	53,53,53,53	0
57	MG	DA	3141	1/1	0.86	0.13	51,51,51,51	0
57	MG	DA	3512	1/1	0.86	0.12	37,37,37,37	0
57	MG	DA	3153	1/1	0.86	0.15	44,44,44,44	0
57	MG	CA	3157	1/1	0.86	0.12	60,60,60,60	0
57	MG	BA	3681	1/1	0.86	0.23	61,61,61,61	0
57	MG	BA	3271	1/1	0.86	0.18	60,60,60,60	0
57	MG	DA	3235	1/1	0.86	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3109	1/1	0.86	0.13	56,56,56,56	0
57	MG	BA	3523	1/1	0.86	0.21	41,41,41,41	0
57	MG	AA	1628	1/1	0.86	0.10	65,65,65,65	0
57	MG	BA	3668	1/1	0.86	0.15	75,75,75,75	0
57	MG	BA	3360	1/1	0.86	0.23	37,37,37,37	0
57	MG	BA	3747	1/1	0.86	0.24	55,55,55,55	0
57	MG	BA	3377	1/1	0.86	0.21	51,51,51,51	0
57	MG	BA	3286	1/1	0.86	0.17	44,44,44,44	0
57	MG	DA	3653	1/1	0.86	0.17	33,33,33,33	0
57	MG	AA	1812	1/1	0.86	0.13	63,63,63,63	0
57	MG	BA	3614	1/1	0.86	0.17	53,53,53,53	0
60	K	AX	3001	1/1	0.87	0.13	77,77,77,77	0
57	MG	BA	3732	1/1	0.87	0.24	33,33,33,33	0
57	MG	DP	201	1/1	0.87	0.21	69,69,69,69	0
57	MG	BA	3504	1/1	0.87	0.20	56,56,56,56	0
57	MG	BA	3484	1/1	0.87	0.13	40,40,40,40	0
57	MG	DA	3452	1/1	0.87	0.11	45,45,45,45	0
57	MG	DA	3192	1/1	0.87	0.32	34,34,34,34	0
57	MG	BA	3604	1/1	0.87	0.20	43,43,43,43	0
57	MG	BA	3745	1/1	0.87	0.24	61,61,61,61	0
57	MG	CA	3110	1/1	0.87	0.12	63,63,63,63	0
57	MG	BA	3230	1/1	0.87	0.33	58,58,58,58	0
57	MG	BA	3149	1/1	0.87	0.19	42,42,42,42	0
57	MG	AA	1632	1/1	0.87	0.11	48,48,48,48	0
57	MG	DA	3442	1/1	0.87	0.15	64,64,64,64	0
57	MG	DA	3493	1/1	0.87	0.08	51,51,51,51	0
57	MG	DA	3600	1/1	0.87	0.13	72,72,72,72	0
57	MG	CA	3051	1/1	0.87	0.11	77,77,77,77	0
57	MG	BA	3588	1/1	0.87	0.09	43,43,43,43	0
57	MG	BA	3106	1/1	0.87	0.25	52,52,52,52	0
57	MG	DA	3023	1/1	0.87	0.14	58,58,58,58	0
57	MG	BA	3597	1/1	0.87	0.20	55,55,55,55	0
57	MG	BA	3127	1/1	0.87	0.30	45,45,45,45	0
57	MG	AA	1614	1/1	0.87	0.19	75,75,75,75	0
57	MG	B2	3001	1/1	0.87	0.25	53,53,53,53	0
57	MG	DA	3042	1/1	0.87	0.29	49,49,49,49	0
57	MG	DA	3338	1/1	0.87	0.07	44,44,44,44	0
57	MG	BA	3805	1/1	0.87	0.13	48,48,48,48	0
57	MG	BA	3653	1/1	0.87	0.21	57,57,57,57	0
57	MG	BA	3564	1/1	0.87	0.09	44,44,44,44	0
57	MG	BA	3792	1/1	0.87	0.19	52,52,52,52	0
57	MG	AA	1788	1/1	0.87	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3441	1/1	0.87	0.20	39,39,39,39	0
57	MG	DA	3623	1/1	0.87	0.10	45,45,45,45	0
57	MG	AA	1634	1/1	0.87	0.15	64,64,64,64	0
57	MG	AA	1630	1/1	0.87	0.14	53,53,53,53	0
57	MG	DA	3603	1/1	0.87	0.06	65,65,65,65	0
57	MG	DA	3190	1/1	0.87	0.20	63,63,63,63	0
57	MG	AA	1651	1/1	0.87	0.25	58,58,58,58	0
57	MG	DA	3106	1/1	0.87	0.14	50,50,50,50	0
57	MG	DA	3010	1/1	0.87	0.10	41,41,41,41	0
57	MG	DA	3150	1/1	0.87	0.16	50,50,50,50	0
57	MG	BA	3549	1/1	0.87	0.11	66,66,66,66	0
57	MG	AA	1771	1/1	0.87	0.15	75,75,75,75	0
57	MG	AA	1755	1/1	0.87	0.09	80,80,80,80	0
57	MG	DA	3067	1/1	0.87	0.14	63,63,63,63	0
57	MG	CA	3045	1/1	0.87	0.22	62,62,62,62	0
57	MG	BA	3561	1/1	0.87	0.26	34,34,34,34	0
57	MG	DD	302	1/1	0.87	0.14	49,49,49,49	0
57	MG	BA	3239	1/1	0.87	0.22	47,47,47,47	0
57	MG	AA	1680	1/1	0.87	0.17	51,51,51,51	0
57	MG	BA	3510	1/1	0.87	0.16	45,45,45,45	0
57	MG	CA	3087	1/1	0.87	0.07	57,57,57,57	0
57	MG	BA	3660	1/1	0.87	0.19	60,60,60,60	0
57	MG	CA	3111	1/1	0.87	0.15	72,72,72,72	0
57	MG	AA	1666	1/1	0.87	0.33	63,63,63,63	0
57	MG	BA	3140	1/1	0.87	0.12	58,58,58,58	0
57	MG	BA	3024	1/1	0.87	0.23	58,58,58,58	0
57	MG	BA	3212	1/1	0.87	0.21	57,57,57,57	0
57	MG	DA	3626	1/1	0.87	0.11	81,81,81,81	0
57	MG	BA	3245	1/1	0.87	0.32	59,59,59,59	0
57	MG	DA	3500	1/1	0.87	0.35	55,55,55,55	0
57	MG	AA	1629	1/1	0.87	0.35	68,68,68,68	0
57	MG	DA	3508	1/1	0.88	0.18	57,57,57,57	0
57	MG	CA	3007	1/1	0.88	0.12	51,51,51,51	0
57	MG	DA	3201	1/1	0.88	0.10	52,52,52,52	0
57	MG	DA	3017	1/1	0.88	0.12	59,59,59,59	0
57	MG	CA	3030	1/1	0.88	0.07	74,74,74,74	0
57	MG	DA	3577	1/1	0.88	0.07	60,60,60,60	0
57	MG	BA	3418	1/1	0.88	0.21	38,38,38,38	0
57	MG	CA	3022	1/1	0.88	0.23	76,76,76,76	0
57	MG	BA	3254	1/1	0.88	0.16	33,33,33,33	0
57	MG	DA	3445	1/1	0.88	0.13	52,52,52,52	0
57	MG	BA	3088	1/1	0.88	0.17	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	BA	3139	1/1	0.88	0.22	44,44,44,44	0
57	MG	DA	3541	1/1	0.88	0.10	59,59,59,59	0
57	MG	CA	3153	1/1	0.88	0.11	69,69,69,69	0
57	MG	DA	3051	1/1	0.88	0.13	44,44,44,44	0
57	MG	BA	3508	1/1	0.88	0.21	20,20,20,20	0
57	MG	AA	1633	1/1	0.88	0.27	59,59,59,59	0
57	MG	BA	3129	1/1	0.88	0.16	54,54,54,54	0
57	MG	AA	1747	1/1	0.88	0.15	55,55,55,55	0
57	MG	DA	3324	1/1	0.88	0.10	54,54,54,54	0
57	MG	DA	3633	1/1	0.88	0.10	58,58,58,58	0
57	MG	DA	3200	1/1	0.88	0.16	41,41,41,41	0
57	MG	DA	3347	1/1	0.88	0.14	35,35,35,35	0
57	MG	DA	3494	1/1	0.88	0.12	45,45,45,45	0
57	MG	BA	3275	1/1	0.88	0.16	66,66,66,66	0
57	MG	BB	3006	1/1	0.88	0.14	62,62,62,62	0
57	MG	DA	3663	1/1	0.88	0.15	73,73,73,73	0
57	MG	AX	3010	1/1	0.88	0.40	68,68,68,68	0
57	MG	BA	3794	1/1	0.88	0.13	37,37,37,37	0
57	MG	AA	1640	1/1	0.88	0.22	54,54,54,54	0
57	MG	B0	3002	1/1	0.88	0.21	63,63,63,63	0
57	MG	DA	3311	1/1	0.88	0.14	46,46,46,46	0
57	MG	DA	3250	1/1	0.88	0.08	50,50,50,50	0
57	MG	DA	3341	1/1	0.88	0.12	55,55,55,55	0
57	MG	BA	3313	1/1	0.88	0.19	38,38,38,38	0
57	MG	BA	3381	1/1	0.88	0.11	49,49,49,49	0
57	MG	BA	3642	1/1	0.88	0.18	64,64,64,64	0
57	MG	DA	3375	1/1	0.88	0.10	57,57,57,57	0
57	MG	DB	3005	1/1	0.88	0.12	68,68,68,68	0
57	MG	AN	503	1/1	0.88	0.18	52,52,52,52	0
57	MG	DA	3271	1/1	0.88	0.16	30,30,30,30	0
57	MG	DA	3187	1/1	0.88	0.20	47,47,47,47	0
57	MG	AA	1707	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3506	1/1	0.88	0.22	61,61,61,61	0
57	MG	BA	3131	1/1	0.88	0.19	44,44,44,44	0
57	MG	DA	3444	1/1	0.88	0.21	44,44,44,44	0
57	MG	CA	3020	1/1	0.88	0.20	45,45,45,45	0
57	MG	BA	3065	1/1	0.88	0.31	50,50,50,50	0
57	MG	DA	3289	1/1	0.88	0.16	52,52,52,52	0
57	MG	BA	3014	1/1	0.88	0.14	35,35,35,35	0
57	MG	BA	3073	1/1	0.88	0.16	32,32,32,32	0
57	MG	AA	1603	1/1	0.88	0.15	64,64,64,64	0
57	MG	BA	3383	1/1	0.88	0.16	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	3515	1/1	0.88	0.17	27,27,27,27	0
57	MG	DA	3427	1/1	0.88	0.15	47,47,47,47	0
57	MG	DA	3578	1/1	0.88	0.14	43,43,43,43	0
57	MG	BA	3767	1/1	0.88	0.23	45,45,45,45	0
57	MG	DA	3208	1/1	0.88	0.16	54,54,54,54	0
57	MG	DA	3194	1/1	0.88	0.16	48,48,48,48	0
57	MG	AA	1621	1/1	0.88	0.14	44,44,44,44	0
57	MG	BA	3203	1/1	0.88	0.34	61,61,61,61	0
57	MG	BA	3255	1/1	0.88	0.21	55,55,55,55	0
57	MG	AX	3008	1/1	0.88	0.15	76,76,76,76	0
57	MG	BA	3763	1/1	0.88	0.15	44,44,44,44	0
57	MG	CA	3129	1/1	0.88	0.13	69,69,69,69	0
57	MG	DA	3384	1/1	0.88	0.10	38,38,38,38	0
57	MG	AA	1605	1/1	0.88	0.15	50,50,50,50	0
57	MG	BA	3638	1/1	0.88	0.17	65,65,65,65	0
57	MG	AF	3001	1/1	0.88	0.18	50,50,50,50	0
57	MG	BA	3594	1/1	0.88	0.14	45,45,45,45	0
57	MG	DA	3306	1/1	0.88	0.28	65,65,65,65	0
57	MG	DV	201	1/1	0.88	0.51	58,58,58,58	0
57	MG	BA	3666	1/1	0.88	0.26	74,74,74,74	0
57	MG	DA	3522	1/1	0.88	0.11	51,51,51,51	0
57	MG	DA	3455	1/1	0.88	0.09	64,64,64,64	0
57	MG	AY	3001	1/1	0.88	0.32	63,63,63,63	0
57	MG	AA	1704	1/1	0.88	0.13	57,57,57,57	0
57	MG	BA	3359	1/1	0.88	0.06	60,60,60,60	0
57	MG	DB	3012	1/1	0.88	0.24	66,66,66,66	0
57	MG	DU	201	1/1	0.88	0.57	58,58,58,58	0
57	MG	DA	3580	1/1	0.88	0.21	62,62,62,62	0
57	MG	DA	3218	1/1	0.88	0.17	52,52,52,52	0
57	MG	DA	3125	1/1	0.89	0.14	56,56,56,56	0
57	MG	AA	1693	1/1	0.89	0.20	76,76,76,76	0
57	MG	BA	3389	1/1	0.89	0.21	37,37,37,37	0
57	MG	BA	3379	1/1	0.89	0.18	35,35,35,35	0
57	MG	DA	3132	1/1	0.89	0.13	43,43,43,43	0
57	MG	DA	3129	1/1	0.89	0.20	56,56,56,56	0
57	MG	DA	3515	1/1	0.89	0.13	55,55,55,55	0
57	MG	DA	3064	1/1	0.89	0.11	46,46,46,46	0
57	MG	BA	3266	1/1	0.89	0.10	44,44,44,44	0
57	MG	BA	3529	1/1	0.89	0.25	24,24,24,24	0
57	MG	BA	3705	1/1	0.89	0.14	59,59,59,59	0
57	MG	AA	1626	1/1	0.89	0.21	59,59,59,59	0
57	MG	DA	3021	1/1	0.89	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3491	1/1	0.89	0.22	56,56,56,56	0
57	MG	AA	1739	1/1	0.89	0.22	72,72,72,72	0
57	MG	DA	3212	1/1	0.89	0.23	62,62,62,62	0
57	MG	DB	3011	1/1	0.89	0.26	67,67,67,67	0
57	MG	BA	3222	1/1	0.89	0.14	42,42,42,42	0
57	MG	DA	3645	1/1	0.89	0.11	64,64,64,64	0
57	MG	AY	3003	1/1	0.89	0.15	79,79,79,79	0
57	MG	DA	3486	1/1	0.89	0.13	57,57,57,57	0
57	MG	BA	3689	1/1	0.89	0.19	59,59,59,59	0
57	MG	AA	1708	1/1	0.89	0.19	60,60,60,60	0
57	MG	DA	3237	1/1	0.89	0.12	59,59,59,59	0
57	MG	DA	3422	1/1	0.89	0.24	62,62,62,62	0
57	MG	DA	3068	1/1	0.89	0.19	53,53,53,53	0
57	MG	DA	3471	1/1	0.89	0.31	54,54,54,54	0
57	MG	DA	3480	1/1	0.89	0.12	58,58,58,58	0
57	MG	AA	1671	1/1	0.89	0.10	60,60,60,60	0
57	MG	BP	3002	1/1	0.89	0.14	60,60,60,60	0
57	MG	BA	3646	1/1	0.89	0.17	50,50,50,50	0
57	MG	BA	3248	1/1	0.89	0.15	67,67,67,67	0
57	MG	BA	3443	1/1	0.89	0.18	59,59,59,59	0
57	MG	DA	3358	1/1	0.89	0.19	50,50,50,50	0
57	MG	DA	3239	1/1	0.89	0.14	49,49,49,49	0
57	MG	BA	3329	1/1	0.89	0.10	60,60,60,60	0
57	MG	BA	3125	1/1	0.89	0.25	38,38,38,38	0
57	MG	BA	3558	1/1	0.89	0.13	51,51,51,51	0
57	MG	BA	3513	1/1	0.89	0.34	50,50,50,50	0
57	MG	CW	3001	1/1	0.89	0.19	66,66,66,66	0
57	MG	AA	1662	1/1	0.89	0.20	58,58,58,58	0
57	MG	CA	3008	1/1	0.89	0.32	47,47,47,47	0
57	MG	CA	3023	1/1	0.89	0.10	39,39,39,39	0
57	MG	BA	3299	1/1	0.89	0.21	60,60,60,60	0
57	MG	BA	3609	1/1	0.89	0.20	56,56,56,56	0
57	MG	DA	3558	1/1	0.89	0.11	48,48,48,48	0
57	MG	BA	3274	1/1	0.89	0.27	66,66,66,66	0
57	MG	BA	3554	1/1	0.89	0.09	51,51,51,51	0
57	MG	BA	3766	1/1	0.89	0.16	47,47,47,47	0
57	MG	BA	3622	1/1	0.89	0.21	43,43,43,43	0
57	MG	DA	3291	1/1	0.89	0.16	36,36,36,36	0
57	MG	DA	3232	1/1	0.89	0.20	56,56,56,56	0
57	MG	AA	1759	1/1	0.89	0.15	55,55,55,55	0
57	MG	CA	3065	1/1	0.89	0.14	59,59,59,59	0
57	MG	AA	1652	1/1	0.89	0.23	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	AA	1712	1/1	0.89	0.21	69,69,69,69	0
57	MG	AX	3015	1/1	0.89	0.29	51,51,51,51	0
57	MG	BA	3295	1/1	0.89	0.22	23,23,23,23	0
57	MG	BA	3536	1/1	0.89	0.14	32,32,32,32	0
57	MG	BA	3194	1/1	0.89	0.25	39,39,39,39	0
57	MG	DA	3601	1/1	0.89	0.10	55,55,55,55	0
57	MG	BA	3390	1/1	0.89	0.10	31,31,31,31	0
57	MG	BA	3735	1/1	0.89	0.23	50,50,50,50	0
57	MG	CA	3077	1/1	0.89	0.21	60,60,60,60	0
57	MG	CA	3119	1/1	0.89	0.12	59,59,59,59	0
57	MG	BA	3325	1/1	0.89	0.15	45,45,45,45	0
57	MG	DA	3219	1/1	0.89	0.16	50,50,50,50	0
57	MG	BA	3407	1/1	0.89	0.17	32,32,32,32	0
57	MG	CA	3029	1/1	0.89	0.11	50,50,50,50	0
57	MG	BA	3522	1/1	0.89	0.16	44,44,44,44	0
57	MG	AM	3002	1/1	0.89	0.12	68,68,68,68	0
57	MG	CA	3137	1/1	0.89	0.15	78,78,78,78	0
57	MG	DA	3552	1/1	0.89	0.13	34,34,34,34	0
57	MG	DA	3451	1/1	0.89	0.08	55,55,55,55	0
57	MG	CA	3148	1/1	0.89	0.15	68,68,68,68	0
57	MG	CA	3063	1/1	0.89	0.23	65,65,65,65	0
57	MG	BA	3367	1/1	0.89	0.22	52,52,52,52	0
57	MG	BA	3138	1/1	0.89	0.16	43,43,43,43	0
57	MG	BA	3406	1/1	0.89	0.10	56,56,56,56	0
57	MG	BA	3079	1/1	0.89	0.37	58,58,58,58	0
57	MG	CA	3034	1/1	0.89	0.23	66,66,66,66	0
57	MG	BA	3574	1/1	0.89	0.15	42,42,42,42	0
57	MG	BA	3501	1/1	0.89	0.14	42,42,42,42	0
57	MG	DA	3393	1/1	0.89	0.16	37,37,37,37	0
57	MG	DA	3095	1/1	0.89	0.16	60,60,60,60	0
57	MG	DA	3377	1/1	0.89	0.11	50,50,50,50	0
57	MG	DP	202	1/1	0.89	0.09	49,49,49,49	0
57	MG	BB	3009	1/1	0.90	0.09	57,57,57,57	0
57	MG	BA	3546	1/1	0.90	0.14	68,68,68,68	0
57	MG	DA	3063	1/1	0.90	0.11	47,47,47,47	0
57	MG	DA	3476	1/1	0.90	0.08	45,45,45,45	0
57	MG	BA	3694	1/1	0.90	0.19	53,53,53,53	0
57	MG	BA	3658	1/1	0.90	0.12	61,61,61,61	0
57	MG	DQ	3002	1/1	0.90	0.16	47,47,47,47	0
57	MG	DA	3651	1/1	0.90	0.12	48,48,48,48	0
57	MG	BA	3117	1/1	0.90	0.64	38,38,38,38	0
57	MG	BA	3087	1/1	0.90	0.38	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	BA	3273	1/1	0.90	0.21	45,45,45,45	0
57	MG	DA	3532	1/1	0.90	0.13	48,48,48,48	0
57	MG	BA	3631	1/1	0.90	0.26	46,46,46,46	0
57	MG	BA	3171	1/1	0.90	0.32	35,35,35,35	0
57	MG	BA	3765	1/1	0.90	0.24	49,49,49,49	0
57	MG	AA	1635	1/1	0.90	0.15	65,65,65,65	0
57	MG	BB	3016	1/1	0.90	0.14	34,34,34,34	0
57	MG	BA	3761	1/1	0.90	0.10	36,36,36,36	0
57	MG	BA	3115	1/1	0.90	0.23	33,33,33,33	0
57	MG	BA	3110	1/1	0.90	0.18	36,36,36,36	0
57	MG	DA	3399	1/1	0.90	0.15	59,59,59,59	0
57	MG	BA	3372	1/1	0.90	0.12	40,40,40,40	0
57	MG	BA	3404	1/1	0.90	0.34	59,59,59,59	0
57	MG	CA	3135	1/1	0.90	0.06	59,59,59,59	0
57	MG	DA	3590	1/1	0.90	0.22	51,51,51,51	0
57	MG	DA	3505	1/1	0.90	0.08	51,51,51,51	0
57	MG	BA	3333	1/1	0.90	0.14	57,57,57,57	0
57	MG	DA	3406	1/1	0.90	0.17	70,70,70,70	0
57	MG	BA	3264	1/1	0.90	0.23	51,51,51,51	0
57	MG	BA	3573	1/1	0.90	0.19	41,41,41,41	0
57	MG	CA	3099	1/1	0.90	0.09	64,64,64,64	0
57	MG	DA	3572	1/1	0.90	0.19	65,65,65,65	0
57	MG	BA	3166	1/1	0.90	0.19	33,33,33,33	0
57	MG	DA	3211	1/1	0.90	0.21	51,51,51,51	0
57	MG	BA	3518	1/1	0.90	0.20	46,46,46,46	0
57	MG	BA	3217	1/1	0.90	0.11	50,50,50,50	0
57	MG	DA	3055	1/1	0.90	0.14	53,53,53,53	0
57	MG	BA	3619	1/1	0.90	0.14	28,28,28,28	0
57	MG	BV	204	1/1	0.90	0.26	39,39,39,39	0
57	MG	DA	3091	1/1	0.90	0.20	54,54,54,54	0
57	MG	BA	3636	1/1	0.90	0.19	66,66,66,66	0
57	MG	DA	3485	1/1	0.90	0.09	56,56,56,56	0
57	MG	DA	3158	1/1	0.90	0.39	56,56,56,56	0
57	MG	CA	3131	1/1	0.90	0.24	69,69,69,69	0
57	MG	DA	3439	1/1	0.90	0.12	40,40,40,40	0
57	MG	BA	3063	1/1	0.90	0.33	47,47,47,47	0
57	MG	DA	3244	1/1	0.90	0.27	55,55,55,55	0
57	MG	DA	3413	1/1	0.90	0.20	62,62,62,62	0
57	MG	DA	3459	1/1	0.90	0.14	49,49,49,49	0
57	MG	BA	3704	1/1	0.90	0.18	26,26,26,26	0
57	MG	BA	3625	1/1	0.90	0.14	33,33,33,33	0
57	MG	AA	1674	1/1	0.90	0.20	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	DA	3658	1/1	0.90	0.49	62,62,62,62	0
57	MG	AA	1768	1/1	0.90	0.11	53,53,53,53	0
57	MG	DA	3336	1/1	0.90	0.09	49,49,49,49	0
57	MG	DA	3110	1/1	0.90	0.10	49,49,49,49	0
57	MG	DA	3570	1/1	0.90	0.16	43,43,43,43	0
57	MG	CA	3141	1/1	0.90	0.14	62,62,62,62	0
57	MG	CA	3089	1/1	0.90	0.23	74,74,74,74	0
57	MG	DA	3446	1/1	0.90	0.14	50,50,50,50	0
57	MG	DA	3556	1/1	0.90	0.13	55,55,55,55	0
57	MG	BA	3147	1/1	0.90	0.20	36,36,36,36	0
57	MG	CA	3126	1/1	0.90	0.09	45,45,45,45	0
57	MG	DA	3448	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3786	1/1	0.90	0.16	51,51,51,51	0
57	MG	BA	3429	1/1	0.90	0.26	50,50,50,50	0
57	MG	DA	3296	1/1	0.90	0.10	60,60,60,60	0
57	MG	BA	3410	1/1	0.90	0.16	55,55,55,55	0
57	MG	DA	3523	1/1	0.90	0.14	39,39,39,39	0
57	MG	BA	3692	1/1	0.90	0.12	58,58,58,58	0
57	MG	BA	3408	1/1	0.90	0.17	51,51,51,51	0
57	MG	DA	3243	1/1	0.90	0.12	48,48,48,48	0
57	MG	BA	3803	1/1	0.90	0.34	55,55,55,55	0
57	MG	BA	3096	1/1	0.90	0.18	60,60,60,60	0
57	MG	CA	3026	1/1	0.90	0.21	66,66,66,66	0
57	MG	DA	3388	1/1	0.90	0.14	47,47,47,47	0
57	MG	BA	3532	1/1	0.90	0.14	55,55,55,55	0
57	MG	BA	3414	1/1	0.90	0.20	54,54,54,54	0
57	MG	AA	1687	1/1	0.90	0.21	46,46,46,46	0
57	MG	AA	1756	1/1	0.90	0.33	45,45,45,45	0
57	MG	CX	3002	1/1	0.90	0.14	67,67,67,67	0
57	MG	DA	3049	1/1	0.90	0.10	47,47,47,47	0
57	MG	AA	1816	1/1	0.90	0.20	59,59,59,59	0
57	MG	CA	3121	1/1	0.90	0.13	67,67,67,67	0
57	MG	DA	3072	1/1	0.90	0.16	47,47,47,47	0
57	MG	DA	3416	1/1	0.90	0.14	52,52,52,52	0
57	MG	DA	3533	1/1	0.90	0.14	56,56,56,56	0
57	MG	BA	3769	1/1	0.90	0.20	47,47,47,47	0
57	MG	CA	3123	1/1	0.90	0.32	61,61,61,61	0
57	MG	BA	3526	1/1	0.90	0.26	41,41,41,41	0
57	MG	DA	3078	1/1	0.90	0.09	47,47,47,47	0
57	MG	DA	3482	1/1	0.90	0.15	60,60,60,60	0
57	MG	CJ	5001	1/1	0.90	0.18	77,77,77,77	0
57	MG	BA	3497	1/1	0.90	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1619	1/1	0.90	0.11	64,64,64,64	0
57	MG	CA	3027	1/1	0.90	0.19	65,65,65,65	0
57	MG	CA	3095	1/1	0.91	0.13	71,71,71,71	0
57	MG	AA	1609	1/1	0.91	0.13	63,63,63,63	0
57	MG	AT	3001	1/1	0.91	0.13	63,63,63,63	0
57	MG	DA	3554	1/1	0.91	0.09	50,50,50,50	0
57	MG	CA	3042	1/1	0.91	0.13	57,57,57,57	0
57	MG	AA	1814	1/1	0.91	0.15	57,57,57,57	0
57	MG	AA	1781	1/1	0.91	0.10	59,59,59,59	0
57	MG	BA	3645	1/1	0.91	0.18	47,47,47,47	0
57	MG	CA	3082	1/1	0.91	0.13	66,66,66,66	0
57	MG	BW	3004	1/1	0.91	0.20	45,45,45,45	0
57	MG	CA	3103	1/1	0.91	0.15	73,73,73,73	0
57	MG	DA	3154	1/1	0.91	0.08	51,51,51,51	0
57	MG	DA	3031	1/1	0.91	0.14	42,42,42,42	0
57	MG	AA	1798	1/1	0.91	0.11	62,62,62,62	0
57	MG	DO	202	1/1	0.91	0.12	60,60,60,60	0
57	MG	CA	3076	1/1	0.91	0.20	77,77,77,77	0
57	MG	DA	3260	1/1	0.91	0.17	39,39,39,39	0
57	MG	DA	3261	1/1	0.91	0.16	39,39,39,39	0
57	MG	CA	3166	1/1	0.91	0.15	55,55,55,55	0
57	MG	CA	3081	1/1	0.91	0.16	44,44,44,44	0
57	MG	BA	3126	1/1	0.91	0.23	36,36,36,36	0
57	MG	DA	3328	1/1	0.91	0.21	42,42,42,42	0
57	MG	BB	3017	1/1	0.91	0.16	81,81,81,81	0
57	MG	BA	3358	1/1	0.91	0.18	52,52,52,52	0
57	MG	BA	3446	1/1	0.91	0.09	59,59,59,59	0
57	MG	BD	3003	1/1	0.91	0.30	37,37,37,37	0
57	MG	BA	3036	1/1	0.91	0.12	56,56,56,56	0
57	MG	BA	3420	1/1	0.91	0.18	25,25,25,25	0
57	MG	CA	3152	1/1	0.91	0.10	71,71,71,71	0
57	MG	BA	3740	1/1	0.91	0.19	65,65,65,65	0
57	MG	BA	3545	1/1	0.91	0.18	28,28,28,28	0
57	MG	BA	3470	1/1	0.91	0.11	57,57,57,57	0
57	MG	AA	1753	1/1	0.91	0.20	55,55,55,55	0
57	MG	DA	3034	1/1	0.91	0.10	42,42,42,42	0
57	MG	BA	3323	1/1	0.91	0.19	57,57,57,57	0
57	MG	BA	3419	1/1	0.91	0.20	25,25,25,25	0
57	MG	CA	3100	1/1	0.91	0.15	59,59,59,59	0
57	MG	BA	3209	1/1	0.91	0.24	48,48,48,48	0
57	MG	DA	3292	1/1	0.91	0.11	29,29,29,29	0
57	MG	BA	3647	1/1	0.91	0.08	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	AX	3004	1/1	0.91	0.13	61,61,61,61	0
57	MG	BA	3435	1/1	0.91	0.22	53,53,53,53	0
57	MG	BA	3615	1/1	0.91	0.13	71,71,71,71	0
57	MG	BF	306	1/1	0.91	0.33	49,49,49,49	0
57	MG	CA	3160	1/1	0.91	0.14	73,73,73,73	0
57	MG	BA	3524	1/1	0.91	0.21	33,33,33,33	0
57	MG	AA	1705	1/1	0.91	0.23	70,70,70,70	0
57	MG	BA	3128	1/1	0.91	0.19	42,42,42,42	0
57	MG	DA	3361	1/1	0.91	0.08	33,33,33,33	0
57	MG	BB	3013	1/1	0.91	0.21	39,39,39,39	0
57	MG	BA	3388	1/1	0.91	0.20	25,25,25,25	0
57	MG	BA	3008	1/1	0.91	0.14	28,28,28,28	0
57	MG	BA	3796	1/1	0.91	0.17	47,47,47,47	0
57	MG	DA	3160	1/1	0.91	0.34	62,62,62,62	0
57	MG	DA	3197	1/1	0.91	0.20	59,59,59,59	0
57	MG	AA	1717	1/1	0.91	0.16	75,75,75,75	0
57	MG	DA	3565	1/1	0.91	0.04	52,52,52,52	0
57	MG	BA	3553	1/1	0.91	0.19	45,45,45,45	0
57	MG	DA	3308	1/1	0.91	0.21	62,62,62,62	0
57	MG	BA	3737	1/1	0.91	0.17	34,34,34,34	0
57	MG	BA	3531	1/1	0.91	0.14	60,60,60,60	0
57	MG	BA	3613	1/1	0.91	0.23	53,53,53,53	0
57	MG	DA	3479	1/1	0.91	0.10	42,42,42,42	0
57	MG	CA	3021	1/1	0.91	0.10	61,61,61,61	0
57	MG	BA	3019	1/1	0.91	0.28	54,54,54,54	0
57	MG	DA	3181	1/1	0.91	0.12	49,49,49,49	0
57	MG	BY	502	1/1	0.91	0.24	46,46,46,46	0
57	MG	BA	3378	1/1	0.91	0.24	39,39,39,39	0
57	MG	AA	1643	1/1	0.91	0.21	58,58,58,58	0
57	MG	BA	3122	1/1	0.91	0.15	35,35,35,35	0
57	MG	DA	3069	1/1	0.91	0.08	43,43,43,43	0
57	MG	AA	1729	1/1	0.91	0.15	35,35,35,35	0
57	MG	DA	3344	1/1	0.91	0.14	38,38,38,38	0
57	MG	DA	3409	1/1	0.91	0.12	54,54,54,54	0
57	MG	DA	3511	1/1	0.91	0.10	44,44,44,44	0
57	MG	DA	3593	1/1	0.91	0.08	60,60,60,60	0
59	ZN	CN	501	1/1	0.91	0.06	100,100,100,100	0
57	MG	DA	3107	1/1	0.91	0.11	61,61,61,61	0
57	MG	DA	3639	1/1	0.91	0.18	59,59,59,59	0
57	MG	BA	3517	1/1	0.91	0.23	33,33,33,33	0
57	MG	BA	3802	1/1	0.91	0.23	46,46,46,46	0
57	MG	BA	3618	1/1	0.91	0.15	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	DA	3403	1/1	0.91	0.09	49,49,49,49	0
57	MG	B7	103	1/1	0.91	0.30	40,40,40,40	0
57	MG	DA	3259	1/1	0.91	0.10	42,42,42,42	0
57	MG	BA	3507	1/1	0.91	0.26	43,43,43,43	0
57	MG	DA	3081	1/1	0.91	0.11	51,51,51,51	0
57	MG	AA	1639	1/1	0.91	0.07	54,54,54,54	0
57	MG	DA	3614	1/1	0.91	0.14	55,55,55,55	0
57	MG	DA	3030	1/1	0.91	0.17	44,44,44,44	0
57	MG	BA	3252	1/1	0.91	0.19	36,36,36,36	0
57	MG	BX	3001	1/1	0.91	0.35	44,44,44,44	0
57	MG	DA	3557	1/1	0.91	0.19	57,57,57,57	0
57	MG	AA	1721	1/1	0.91	0.16	57,57,57,57	0
57	MG	BA	3814	1/1	0.91	0.28	39,39,39,39	0
57	MG	DA	3127	1/1	0.91	0.10	52,52,52,52	0
57	MG	BA	3535	1/1	0.91	0.20	39,39,39,39	0
57	MG	CA	3055	1/1	0.91	0.18	63,63,63,63	0
57	MG	BN	3001	1/1	0.91	0.15	48,48,48,48	0
57	MG	BA	3191	1/1	0.91	0.19	40,40,40,40	0
57	MG	BA	3163	1/1	0.91	0.49	55,55,55,55	0
57	MG	DA	3524	1/1	0.91	0.17	52,52,52,52	0
57	MG	BA	3728	1/1	0.91	0.16	52,52,52,52	0
57	MG	BA	3452	1/1	0.91	0.15	56,56,56,56	0
57	MG	DA	3241	1/1	0.91	0.13	55,55,55,55	0
57	MG	AA	1801	1/1	0.91	0.09	71,71,71,71	0
57	MG	DA	3550	1/1	0.91	0.04	60,60,60,60	0
57	MG	BA	3132	1/1	0.91	0.18	50,50,50,50	0
57	MG	DA	3179	1/1	0.91	0.06	59,59,59,59	0
57	MG	DA	3159	1/1	0.91	0.11	62,62,62,62	0
57	MG	BA	3207	1/1	0.91	0.18	36,36,36,36	0
57	MG	D0	101	1/1	0.91	0.13	71,71,71,71	0
57	MG	BA	3781	1/1	0.91	0.16	56,56,56,56	0
57	MG	DA	3084	1/1	0.91	0.17	44,44,44,44	0
57	MG	AA	1714	1/1	0.91	0.20	56,56,56,56	0
57	MG	CA	3151	1/1	0.91	0.10	64,64,64,64	0
57	MG	BA	3516	1/1	0.91	0.24	46,46,46,46	0
57	MG	DA	3327	1/1	0.91	0.15	45,45,45,45	0
57	MG	BA	3685	1/1	0.91	0.20	61,61,61,61	0
57	MG	DA	3368	1/1	0.91	0.09	67,67,67,67	0
57	MG	AA	1726	1/1	0.92	0.16	58,58,58,58	0
57	MG	CT	3001	1/1	0.92	0.17	60,60,60,60	0
57	MG	BA	3156	1/1	0.92	0.23	35,35,35,35	0
57	MG	BA	3768	1/1	0.92	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3672	1/1	0.92	0.25	44,44,44,44	0
57	MG	BF	311	1/1	0.92	0.12	52,52,52,52	0
57	MG	DA	3662	1/1	0.92	0.22	50,50,50,50	0
57	MG	DA	3543	1/1	0.92	0.14	64,64,64,64	0
57	MG	BA	3314	1/1	0.92	0.18	39,39,39,39	0
57	MG	BA	3542	1/1	0.92	0.16	44,44,44,44	0
57	MG	BA	3682	1/1	0.92	0.14	60,60,60,60	0
57	MG	CA	3035	1/1	0.92	0.11	53,53,53,53	0
57	MG	DA	3405	1/1	0.92	0.07	47,47,47,47	0
57	MG	BA	3773	1/1	0.92	0.21	32,32,32,32	0
57	MG	DA	3256	1/1	0.92	0.16	51,51,51,51	0
57	MG	BA	3010	1/1	0.92	0.18	53,53,53,53	0
57	MG	BA	3500	1/1	0.92	0.20	57,57,57,57	0
57	MG	DE	3005	1/1	0.92	0.14	35,35,35,35	0
57	MG	BA	3512	1/1	0.92	0.21	23,23,23,23	0
57	MG	BZ	302	1/1	0.92	0.17	60,60,60,60	0
57	MG	DA	3022	1/1	0.92	0.45	60,60,60,60	0
57	MG	DA	3146	1/1	0.92	0.14	54,54,54,54	0
57	MG	DA	3242	1/1	0.92	0.09	52,52,52,52	0
57	MG	AA	1745	1/1	0.92	0.16	36,36,36,36	0
57	MG	DA	3362	1/1	0.92	0.24	42,42,42,42	0
57	MG	DA	3100	1/1	0.92	0.09	47,47,47,47	0
57	MG	DA	3053	1/1	0.92	0.13	47,47,47,47	0
57	MG	BA	3305	1/1	0.92	0.15	46,46,46,46	0
57	MG	DA	3470	1/1	0.92	0.08	61,61,61,61	0
57	MG	DA	3366	1/1	0.92	0.12	44,44,44,44	0
57	MG	BA	3806	1/1	0.92	0.17	43,43,43,43	0
57	MG	DF	301	1/1	0.92	0.31	48,48,48,48	0
57	MG	BA	3741	1/1	0.92	0.11	57,57,57,57	0
57	MG	BA	3729	1/1	0.92	0.14	46,46,46,46	0
57	MG	AW	3002	1/1	0.92	0.14	79,79,79,79	0
57	MG	AA	1688	1/1	0.92	0.21	66,66,66,66	0
57	MG	BA	3641	1/1	0.92	0.18	68,68,68,68	0
57	MG	DA	3094	1/1	0.92	0.06	39,39,39,39	0
57	MG	DA	3151	1/1	0.92	0.13	37,37,37,37	0
57	MG	BA	3460	1/1	0.92	0.11	52,52,52,52	0
57	MG	DA	3310	1/1	0.92	0.13	35,35,35,35	0
57	MG	AA	1692	1/1	0.92	0.15	65,65,65,65	0
57	MG	B4	502	1/1	0.92	0.09	70,70,70,70	0
57	MG	BF	307	1/1	0.92	0.13	34,34,34,34	0
57	MG	BA	3141	1/1	0.92	0.32	38,38,38,38	0
57	MG	AA	1815	1/1	0.92	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3001	1/1	0.92	0.15	43,43,43,43	0
57	MG	BA	3364	1/1	0.92	0.15	47,47,47,47	0
57	MG	DA	3425	1/1	0.92	0.16	51,51,51,51	0
57	MG	DA	3575	1/1	0.92	0.08	56,56,56,56	0
57	MG	BA	3300	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3156	1/1	0.92	0.16	52,52,52,52	0
57	MG	DA	3481	1/1	0.92	0.13	40,40,40,40	0
57	MG	DA	3431	1/1	0.92	0.23	42,42,42,42	0
57	MG	BA	3623	1/1	0.92	0.17	43,43,43,43	0
57	MG	AA	1797	1/1	0.92	0.17	59,59,59,59	0
57	MG	BA	3134	1/1	0.92	0.19	40,40,40,40	0
57	MG	BA	3124	1/1	0.92	0.28	57,57,57,57	0
57	MG	DA	3582	1/1	0.92	0.05	53,53,53,53	0
57	MG	BA	3086	1/1	0.92	0.33	42,42,42,42	0
57	MG	DA	3028	1/1	0.92	0.13	39,39,39,39	0
57	MG	CA	3113	1/1	0.92	0.16	47,47,47,47	0
57	MG	BA	3587	1/1	0.92	0.11	46,46,46,46	0
57	MG	BB	3022	1/1	0.92	0.20	60,60,60,60	0
57	MG	DA	3566	1/1	0.92	0.18	37,37,37,37	0
57	MG	DA	3189	1/1	0.92	0.23	47,47,47,47	0
57	MG	AA	1694	1/1	0.92	0.08	47,47,47,47	0
57	MG	BA	3025	1/1	0.92	0.18	43,43,43,43	0
57	MG	BA	3640	1/1	0.92	0.17	57,57,57,57	0
57	MG	DA	3561	1/1	0.92	0.16	52,52,52,52	0
57	MG	CA	3036	1/1	0.92	0.16	73,73,73,73	0
57	MG	DA	3077	1/1	0.92	0.14	38,38,38,38	0
57	MG	AL	202	1/1	0.92	0.26	56,56,56,56	0
57	MG	DA	3186	1/1	0.92	0.15	49,49,49,49	0
57	MG	BA	3431	1/1	0.92	0.28	57,57,57,57	0
57	MG	DA	3576	1/1	0.92	0.16	67,67,67,67	0
57	MG	DA	3096	1/1	0.92	0.19	68,68,68,68	0
57	MG	DA	3236	1/1	0.92	0.13	55,55,55,55	0
57	MG	DA	3478	1/1	0.92	0.17	58,58,58,58	0
57	MG	DR	3001	1/1	0.92	0.13	49,49,49,49	0
57	MG	DA	3090	1/1	0.92	0.31	50,50,50,50	0
57	MG	DA	3454	1/1	0.92	0.12	43,43,43,43	0
57	MG	BA	3348	1/1	0.92	0.18	37,37,37,37	0
57	MG	BA	3296	1/1	0.92	0.16	55,55,55,55	0
57	MG	CA	3064	1/1	0.92	0.21	55,55,55,55	0
57	MG	BA	3426	1/1	0.92	0.15	46,46,46,46	0
57	MG	BA	3137	1/1	0.92	0.25	52,52,52,52	0
57	MG	BA	3268	1/1	0.92	0.22	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	BA	3626	1/1	0.92	0.19	50,50,50,50	0
57	MG	DA	3643	1/1	0.92	0.07	54,54,54,54	0
57	MG	DA	3119	1/1	0.92	0.26	50,50,50,50	0
57	MG	DQ	3001	1/1	0.92	0.08	50,50,50,50	0
57	MG	BA	3051	1/1	0.92	0.23	37,37,37,37	0
57	MG	DA	3155	1/1	0.92	0.24	53,53,53,53	0
57	MG	BA	3483	1/1	0.92	0.17	44,44,44,44	0
57	MG	BA	3541	1/1	0.92	0.20	38,38,38,38	0
57	MG	BA	3219	1/1	0.92	0.50	58,58,58,58	0
57	MG	AA	1754	1/1	0.92	0.15	58,58,58,58	0
57	MG	DA	3553	1/1	0.92	0.07	72,72,72,72	0
57	MG	AA	1799	1/1	0.92	0.11	78,78,78,78	0
57	MG	BA	3790	1/1	0.92	0.54	66,66,66,66	0
57	MG	BA	3349	1/1	0.92	0.18	34,34,34,34	0
57	MG	BA	3528	1/1	0.92	0.20	36,36,36,36	0
57	MG	BA	3563	1/1	0.92	0.12	50,50,50,50	0
57	MG	DA	3352	1/1	0.92	0.09	34,34,34,34	0
57	MG	DA	3458	1/1	0.92	0.10	41,41,41,41	0
57	MG	BA	3170	1/1	0.92	0.17	38,38,38,38	0
57	MG	DA	3080	1/1	0.92	0.10	49,49,49,49	0
57	MG	DA	3407	1/1	0.92	0.08	58,58,58,58	0
57	MG	DA	3569	1/1	0.92	0.24	45,45,45,45	0
57	MG	DA	3506	1/1	0.92	0.08	55,55,55,55	0
57	MG	BA	3375	1/1	0.92	0.22	39,39,39,39	0
57	MG	AA	1691	1/1	0.92	0.27	62,62,62,62	0
57	MG	DA	3559	1/1	0.92	0.15	67,67,67,67	0
57	MG	DA	3001	1/1	0.92	0.14	57,57,57,57	0
57	MG	BA	3663	1/1	0.92	0.20	50,50,50,50	0
57	MG	BA	3290	1/1	0.92	0.21	57,57,57,57	0
57	MG	BA	3662	1/1	0.92	0.22	62,62,62,62	0
57	MG	BA	3436	1/1	0.92	0.15	57,57,57,57	0
57	MG	DA	3528	1/1	0.92	0.14	36,36,36,36	0
57	MG	BA	3091	1/1	0.92	0.40	42,42,42,42	0
57	MG	BA	3309	1/1	0.92	0.17	65,65,65,65	0
57	MG	DA	3357	1/1	0.92	0.13	33,33,33,33	0
57	MG	DA	3075	1/1	0.92	0.14	55,55,55,55	0
57	MG	AA	1778	1/1	0.92	0.09	51,51,51,51	0
57	MG	AA	1648	1/1	0.92	0.19	56,56,56,56	0
57	MG	DA	3339	1/1	0.92	0.20	52,52,52,52	0
57	MG	BA	3789	1/1	0.92	0.14	47,47,47,47	0
57	MG	DA	3374	1/1	0.92	0.22	62,62,62,62	0
57	MG	DA	3630	1/1	0.92	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3363	1/1	0.92	0.09	50,50,50,50	0
57	MG	CA	3062	1/1	0.92	0.11	64,64,64,64	0
57	MG	BA	3400	1/1	0.92	0.24	39,39,39,39	0
57	MG	DA	3298	1/1	0.92	0.20	55,55,55,55	0
57	MG	DA	3464	1/1	0.93	0.30	54,54,54,54	0
57	MG	BA	3101	1/1	0.93	0.24	37,37,37,37	0
57	MG	CA	3015	1/1	0.93	0.19	64,64,64,64	0
57	MG	DA	3414	1/1	0.93	0.15	42,42,42,42	0
57	MG	B6	103	1/1	0.93	0.15	52,52,52,52	0
57	MG	BA	3337	1/1	0.93	0.25	44,44,44,44	0
57	MG	DA	3622	1/1	0.93	0.10	49,49,49,49	0
57	MG	BA	3322	1/1	0.93	0.16	38,38,38,38	0
57	MG	CA	3073	1/1	0.93	0.20	55,55,55,55	0
57	MG	AA	1800	1/1	0.93	0.13	59,59,59,59	0
57	MG	BA	3624	1/1	0.93	0.13	38,38,38,38	0
57	MG	DA	3391	1/1	0.93	0.16	45,45,45,45	0
57	MG	BA	3428	1/1	0.93	0.16	51,51,51,51	0
57	MG	CA	3165	1/1	0.93	0.09	42,42,42,42	0
57	MG	DA	3499	1/1	0.93	0.14	52,52,52,52	0
57	MG	CA	3150	1/1	0.93	0.15	65,65,65,65	0
57	MG	BA	3047	1/1	0.93	0.22	43,43,43,43	0
57	MG	BA	3657	1/1	0.93	0.11	38,38,38,38	0
57	MG	BA	3282	1/1	0.93	0.24	57,57,57,57	0
57	MG	DA	3006	1/1	0.93	0.11	41,41,41,41	0
57	MG	CA	3127	1/1	0.93	0.08	59,59,59,59	0
57	MG	BA	3303	1/1	0.93	0.23	26,26,26,26	0
57	MG	BN	3003	1/1	0.93	0.21	38,38,38,38	0
57	MG	AA	1607	1/1	0.93	0.13	55,55,55,55	0
57	MG	CA	3071	1/1	0.93	0.19	56,56,56,56	0
57	MG	BA	3366	1/1	0.93	0.16	52,52,52,52	0
57	MG	BA	3247	1/1	0.93	0.17	29,29,29,29	0
57	MG	CA	3124	1/1	0.93	0.22	69,69,69,69	0
57	MG	DA	3207	1/1	0.93	0.14	48,48,48,48	0
57	MG	DA	3335	1/1	0.93	0.25	49,49,49,49	0
57	MG	BA	3321	1/1	0.93	0.13	53,53,53,53	0
57	MG	BA	3754	1/1	0.93	0.14	42,42,42,42	0
57	MG	CA	3120	1/1	0.93	0.12	68,68,68,68	0
57	MG	BA	3599	1/1	0.93	0.16	60,60,60,60	0
57	MG	BA	3543	1/1	0.93	0.23	52,52,52,52	0
57	MG	BA	3150	1/1	0.93	0.17	39,39,39,39	0
57	MG	DA	3342	1/1	0.93	0.10	53,53,53,53	0
57	MG	BE	304	1/1	0.93	0.23	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3054	1/1	0.93	0.33	69,69,69,69	0
57	MG	DA	3222	1/1	0.93	0.23	58,58,58,58	0
57	MG	DA	3504	1/1	0.93	0.09	52,52,52,52	0
57	MG	BA	3161	1/1	0.93	0.29	44,44,44,44	0
57	MG	AA	1690	1/1	0.93	0.42	52,52,52,52	0
57	MG	BA	3330	1/1	0.93	0.15	27,27,27,27	0
57	MG	BA	3301	1/1	0.93	0.18	62,62,62,62	0
57	MG	AA	1654	1/1	0.93	0.23	65,65,65,65	0
57	MG	BA	3649	1/1	0.93	0.14	55,55,55,55	0
57	MG	AA	1791	1/1	0.93	0.08	54,54,54,54	0
57	MG	DA	3083	1/1	0.93	0.26	41,41,41,41	0
57	MG	DA	3210	1/1	0.93	0.08	52,52,52,52	0
57	MG	DA	3449	1/1	0.93	0.13	34,34,34,34	0
57	MG	BA	3195	1/1	0.93	0.18	36,36,36,36	0
57	MG	BA	3179	1/1	0.93	0.23	43,43,43,43	0
57	MG	DA	3371	1/1	0.93	0.17	34,34,34,34	0
57	MG	AA	1641	1/1	0.93	0.17	65,65,65,65	0
57	MG	DA	3466	1/1	0.93	0.11	48,48,48,48	0
57	MG	BA	3302	1/1	0.93	0.15	49,49,49,49	0
57	MG	DA	3305	1/1	0.93	0.12	53,53,53,53	0
57	MG	AA	1751	1/1	0.93	0.23	53,53,53,53	0
57	MG	DA	3249	1/1	0.93	0.08	65,65,65,65	0
57	MG	CA	3078	1/1	0.93	0.16	65,65,65,65	0
57	MG	BA	3785	1/1	0.93	0.14	56,56,56,56	0
57	MG	BA	3659	1/1	0.93	0.11	47,47,47,47	0
57	MG	BA	3651	1/1	0.93	0.14	66,66,66,66	0
57	MG	DA	3644	1/1	0.93	0.24	58,58,58,58	0
57	MG	AK	3101	1/1	0.93	0.17	69,69,69,69	0
57	MG	BA	3403	1/1	0.93	0.29	33,33,33,33	0
57	MG	DA	3579	1/1	0.93	0.16	62,62,62,62	0
57	MG	DA	3048	1/1	0.93	0.12	59,59,59,59	0
57	MG	DY	502	1/1	0.93	0.17	55,55,55,55	0
57	MG	AA	1657	1/1	0.93	0.12	64,64,64,64	0
57	MG	BA	3177	1/1	0.93	0.23	46,46,46,46	0
57	MG	BA	3775	1/1	0.93	0.33	39,39,39,39	0
57	MG	DA	3595	1/1	0.93	0.13	57,57,57,57	0
57	MG	BA	3055	1/1	0.93	0.23	37,37,37,37	0
57	MG	BR	5001	1/1	0.93	0.20	50,50,50,50	0
57	MG	BA	3462	1/1	0.93	0.11	53,53,53,53	0
57	MG	AA	1782	1/1	0.93	0.14	54,54,54,54	0
57	MG	BA	3746	1/1	0.93	0.14	78,78,78,78	0
57	MG	B0	3001	1/1	0.93	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3315	1/1	0.93	0.13	44,44,44,44	0
57	MG	BA	3686	1/1	0.93	0.19	27,27,27,27	0
57	MG	BA	3757	1/1	0.93	0.18	43,43,43,43	0
57	MG	BA	3066	1/1	0.93	0.24	58,58,58,58	0
57	MG	DA	3104	1/1	0.93	0.11	57,57,57,57	0
57	MG	DA	3396	1/1	0.93	0.17	46,46,46,46	0
57	MG	AA	1752	1/1	0.93	0.14	48,48,48,48	0
57	MG	BA	3269	1/1	0.93	0.25	45,45,45,45	0
57	MG	BA	3540	1/1	0.93	0.16	31,31,31,31	0
57	MG	BA	3552	1/1	0.93	0.15	55,55,55,55	0
57	MG	BA	3798	1/1	0.93	0.24	22,22,22,22	0
57	MG	DA	3433	1/1	0.93	0.17	59,59,59,59	0
57	MG	BA	3661	1/1	0.93	0.24	25,25,25,25	0
57	MG	BA	3092	1/1	0.93	0.29	40,40,40,40	0
57	MG	CA	3025	1/1	0.93	0.24	53,53,53,53	0
57	MG	B5	102	1/1	0.93	0.19	43,43,43,43	0
57	MG	AY	3002	1/1	0.93	0.31	52,52,52,52	0
57	MG	DF	305	1/1	0.93	0.59	45,45,45,45	0
57	MG	BA	3220	1/1	0.93	0.16	35,35,35,35	0
57	MG	DA	3421	1/1	0.93	0.12	56,56,56,56	0
57	MG	DA	3105	1/1	0.93	0.22	45,45,45,45	0
57	MG	BA	3697	1/1	0.93	0.18	41,41,41,41	0
57	MG	BA	3123	1/1	0.93	0.09	43,43,43,43	0
57	MG	CA	3159	1/1	0.93	0.13	62,62,62,62	0
57	MG	DA	3536	1/1	0.93	0.08	52,52,52,52	0
57	MG	AA	1737	1/1	0.93	0.09	60,60,60,60	0
57	MG	BA	3684	1/1	0.93	0.22	51,51,51,51	0
57	MG	BA	3699	1/1	0.93	0.20	67,67,67,67	0
57	MG	DA	3177	1/1	0.93	0.13	58,58,58,58	0
57	MG	DA	3539	1/1	0.93	0.08	55,55,55,55	0
57	MG	CA	3117	1/1	0.93	0.09	63,63,63,63	0
57	MG	AA	1656	1/1	0.93	0.16	63,63,63,63	0
57	MG	BA	3081	1/1	0.93	0.30	48,48,48,48	0
57	MG	BA	3289	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3449	1/1	0.93	0.23	62,62,62,62	0
57	MG	BA	3218	1/1	0.93	0.15	45,45,45,45	0
57	MG	BA	3432	1/1	0.93	0.22	32,32,32,32	0
57	MG	DA	3571	1/1	0.93	0.28	45,45,45,45	0
57	MG	AA	1638	1/1	0.93	0.23	60,60,60,60	0
57	MG	AA	1802	1/1	0.93	0.10	54,54,54,54	0
57	MG	BA	3181	1/1	0.93	0.10	40,40,40,40	0
57	MG	DA	3282	1/1	0.93	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3304	1/1	0.93	0.18	39,39,39,39	0
57	MG	AX	3011	1/1	0.93	0.13	60,60,60,60	0
57	MG	BA	3237	1/1	0.93	0.17	44,44,44,44	0
57	MG	DA	3563	1/1	0.93	0.10	70,70,70,70	0
57	MG	AA	1790	1/1	0.93	0.08	81,81,81,81	0
57	MG	DA	3133	1/1	0.93	0.18	60,60,60,60	0
57	MG	DA	3026	1/1	0.93	0.72	50,50,50,50	0
57	MG	BB	3005	1/1	0.93	0.28	51,51,51,51	0
57	MG	DA	3441	1/1	0.93	0.20	58,58,58,58	0
57	MG	DA	3461	1/1	0.93	0.13	51,51,51,51	0
57	MG	DA	3131	1/1	0.93	0.25	49,49,49,49	0
57	MG	DD	303	1/1	0.93	0.34	51,51,51,51	0
57	MG	DA	3587	1/1	0.93	0.12	51,51,51,51	0
57	MG	B6	101	1/1	0.93	0.32	60,60,60,60	0
57	MG	CA	3101	1/1	0.93	0.11	65,65,65,65	0
57	MG	DA	3646	1/1	0.93	0.15	56,56,56,56	0
57	MG	BA	3148	1/1	0.93	0.28	38,38,38,38	0
57	MG	AA	1675	1/1	0.93	0.24	61,61,61,61	0
57	MG	BA	3415	1/1	0.93	0.23	35,35,35,35	0
57	MG	BA	3673	1/1	0.93	0.28	61,61,61,61	0
57	MG	DA	3613	1/1	0.93	0.11	56,56,56,56	0
57	MG	BA	3690	1/1	0.93	0.13	39,39,39,39	0
57	MG	BA	3279	1/1	0.93	0.32	52,52,52,52	0
57	MG	CA	3098	1/1	0.93	0.11	54,54,54,54	0
57	MG	AA	1645	1/1	0.93	0.15	61,61,61,61	0
57	MG	AA	1765	1/1	0.93	0.13	65,65,65,65	0
57	MG	AX	3014	1/1	0.93	0.24	61,61,61,61	0
57	MG	BA	3527	1/1	0.93	0.19	24,24,24,24	0
57	MG	DA	3273	1/1	0.93	0.12	62,62,62,62	0
57	MG	DA	3367	1/1	0.93	0.17	49,49,49,49	0
57	MG	DA	3139	1/1	0.94	0.11	44,44,44,44	0
57	MG	BA	3294	1/1	0.94	0.16	43,43,43,43	0
57	MG	AA	1728	1/1	0.94	0.25	49,49,49,49	0
57	MG	DA	3526	1/1	0.94	0.12	52,52,52,52	0
57	MG	BA	3804	1/1	0.94	0.16	36,36,36,36	0
57	MG	BB	3012	1/1	0.94	0.19	56,56,56,56	0
57	MG	DA	3475	1/1	0.94	0.18	56,56,56,56	0
57	MG	DA	3012	1/1	0.94	0.11	43,43,43,43	0
57	MG	BA	3012	1/1	0.94	0.17	25,25,25,25	0
57	MG	AA	1806	1/1	0.94	0.18	74,74,74,74	0
57	MG	BA	3620	1/1	0.94	0.14	29,29,29,29	0
57	MG	BF	302	1/1	0.94	0.31	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3126	1/1	0.94	0.15	59,59,59,59	0
57	MG	BF	301	1/1	0.94	0.25	40,40,40,40	0
57	MG	AA	1659	1/1	0.94	0.19	65,65,65,65	0
57	MG	AA	1733	1/1	0.94	0.12	50,50,50,50	0
57	MG	DA	3018	1/1	0.94	0.10	31,31,31,31	0
57	MG	DA	3551	1/1	0.94	0.17	49,49,49,49	0
57	MG	BA	3242	1/1	0.94	0.69	55,55,55,55	0
57	MG	BA	3703	1/1	0.94	0.33	28,28,28,28	0
57	MG	DA	3564	1/1	0.94	0.17	53,53,53,53	0
57	MG	DA	3176	1/1	0.94	0.24	38,38,38,38	0
57	MG	BW	3002	1/1	0.94	0.27	58,58,58,58	0
57	MG	BA	3187	1/1	0.94	0.22	38,38,38,38	0
57	MG	DA	3220	1/1	0.94	0.32	50,50,50,50	0
57	MG	CA	3144	1/1	0.94	0.13	82,82,82,82	0
57	MG	BA	3165	1/1	0.94	0.31	52,52,52,52	0
57	MG	DA	3138	1/1	0.94	0.14	54,54,54,54	0
57	MG	AA	1649	1/1	0.94	0.18	28,28,28,28	0
57	MG	DA	3142	1/1	0.94	0.13	51,51,51,51	0
57	MG	DA	3419	1/1	0.94	0.14	50,50,50,50	0
57	MG	AM	3001	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3285	1/1	0.94	0.12	50,50,50,50	0
57	MG	BA	3334	1/1	0.94	0.21	56,56,56,56	0
57	MG	BB	3003	1/1	0.94	0.18	30,30,30,30	0
57	MG	AA	1805	1/1	0.94	0.07	48,48,48,48	0
57	MG	BA	3298	1/1	0.94	0.15	27,27,27,27	0
57	MG	CA	3072	1/1	0.94	0.14	62,62,62,62	0
57	MG	BA	3244	1/1	0.94	0.26	31,31,31,31	0
57	MG	BA	3241	1/1	0.94	0.16	56,56,56,56	0
57	MG	DA	3226	1/1	0.94	0.18	57,57,57,57	0
57	MG	BA	3236	1/1	0.94	0.13	52,52,52,52	0
57	MG	BA	3048	1/1	0.94	0.22	29,29,29,29	0
57	MG	BA	3437	1/1	0.94	0.23	62,62,62,62	0
57	MG	BA	3084	1/1	0.94	0.18	42,42,42,42	0
57	MG	D3	3001	1/1	0.94	0.27	63,63,63,63	0
57	MG	DA	3540	1/1	0.94	0.06	50,50,50,50	0
57	MG	DA	3074	1/1	0.94	0.08	59,59,59,59	0
57	MG	BA	3373	1/1	0.94	0.22	34,34,34,34	0
57	MG	DA	3223	1/1	0.94	0.19	39,39,39,39	0
57	MG	BU	201	1/1	0.94	0.36	43,43,43,43	0
57	MG	BA	3722	1/1	0.94	0.19	64,64,64,64	0
57	MG	AA	1808	1/1	0.94	0.14	49,49,49,49	0
57	MG	DB	3004	1/1	0.94	0.21	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	BA	3193	1/1	0.94	0.13	37,37,37,37	0
57	MG	DA	3548	1/1	0.94	0.10	66,66,66,66	0
57	MG	AA	1646	1/1	0.94	0.23	58,58,58,58	0
57	MG	BE	303	1/1	0.94	0.15	43,43,43,43	0
57	MG	DA	3585	1/1	0.94	0.25	55,55,55,55	0
57	MG	DA	3288	1/1	0.94	0.16	39,39,39,39	0
57	MG	BA	3292	1/1	0.94	0.24	26,26,26,26	0
57	MG	DA	3517	1/1	0.94	0.12	48,48,48,48	0
57	MG	DA	3240	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3105	1/1	0.94	0.12	46,46,46,46	0
57	MG	CA	3106	1/1	0.94	0.13	58,58,58,58	0
57	MG	BA	3771	1/1	0.94	0.11	41,41,41,41	0
57	MG	BA	3097	1/1	0.94	0.12	41,41,41,41	0
57	MG	DA	3004	1/1	0.94	0.20	53,53,53,53	0
57	MG	BA	3206	1/1	0.94	0.16	34,34,34,34	0
57	MG	DA	3534	1/1	0.94	0.10	46,46,46,46	0
57	MG	DA	3268	1/1	0.94	0.12	41,41,41,41	0
57	MG	BA	3100	1/1	0.94	0.25	61,61,61,61	0
57	MG	DA	3635	1/1	0.94	0.11	43,43,43,43	0
57	MG	BA	3210	1/1	0.94	0.25	41,41,41,41	0
57	MG	AX	3002	1/1	0.94	0.30	71,71,71,71	0
57	MG	DA	3283	1/1	0.94	0.07	27,27,27,27	0
57	MG	BA	3332	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3474	1/1	0.94	0.27	33,33,33,33	0
57	MG	AB	3001	1/1	0.94	0.13	77,77,77,77	0
57	MG	CA	3046	1/1	0.94	0.18	61,61,61,61	0
57	MG	DA	3609	1/1	0.94	0.10	61,61,61,61	0
57	MG	BA	3733	1/1	0.94	0.15	42,42,42,42	0
57	MG	DA	3567	1/1	0.94	0.26	44,44,44,44	0
57	MG	DA	3164	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3134	1/1	0.94	0.21	52,52,52,52	0
57	MG	BA	3399	1/1	0.94	0.20	41,41,41,41	0
57	MG	BA	3098	1/1	0.94	0.22	23,23,23,23	0
57	MG	BA	3192	1/1	0.94	0.20	19,19,19,19	0
57	MG	DA	3401	1/1	0.94	0.06	69,69,69,69	0
57	MG	BA	3038	1/1	0.94	0.23	20,20,20,20	0
57	MG	BA	3009	1/1	0.94	0.17	31,31,31,31	0
57	MG	BA	3384	1/1	0.94	0.11	45,45,45,45	0
57	MG	BA	3706	1/1	0.94	0.16	47,47,47,47	0
57	MG	DA	3631	1/1	0.94	0.12	49,49,49,49	0
57	MG	BA	3799	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3743	1/1	0.94	0.59	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3040	1/1	0.94	0.27	33,33,33,33	0
57	MG	BA	3758	1/1	0.94	0.12	41,41,41,41	0
57	MG	DA	3148	1/1	0.94	0.21	49,49,49,49	0
57	MG	BA	3069	1/1	0.94	0.34	48,48,48,48	0
57	MG	BA	3095	1/1	0.94	0.23	53,53,53,53	0
57	MG	BA	3113	1/1	0.94	0.14	50,50,50,50	0
57	MG	DA	3047	1/1	0.94	0.16	45,45,45,45	0
57	MG	BA	3679	1/1	0.94	0.22	52,52,52,52	0
57	MG	DA	3602	1/1	0.94	0.26	62,62,62,62	0
57	MG	DA	3202	1/1	0.94	0.20	62,62,62,62	0
57	MG	DA	3483	1/1	0.94	0.09	53,53,53,53	0
57	MG	BA	3714	1/1	0.94	0.12	46,46,46,46	0
57	MG	BA	3211	1/1	0.94	0.18	43,43,43,43	0
57	MG	DA	3605	1/1	0.94	0.12	45,45,45,45	0
57	MG	CA	3114	1/1	0.94	0.14	71,71,71,71	0
57	MG	DA	3659	1/1	0.94	0.14	41,41,41,41	0
57	MG	BA	3450	1/1	0.94	0.25	54,54,54,54	0
57	MG	BA	3616	1/1	0.94	0.20	59,59,59,59	0
57	MG	BA	3596	1/1	0.94	0.17	59,59,59,59	0
57	MG	BA	3784	1/1	0.94	0.18	52,52,52,52	0
57	MG	DB	3006	1/1	0.94	0.14	55,55,55,55	0
57	MG	DA	3660	1/1	0.94	0.52	46,46,46,46	0
57	MG	DA	3372	1/1	0.94	0.13	53,53,53,53	0
59	ZN	B4	501	1/1	0.94	0.10	118,118,118,118	0
57	MG	DA	3206	1/1	0.94	0.08	50,50,50,50	0
57	MG	BA	3584	1/1	0.94	0.12	55,55,55,55	0
57	MG	BA	3280	1/1	0.94	0.21	25,25,25,25	0
57	MG	BA	3317	1/1	0.94	0.21	43,43,43,43	0
57	MG	DA	3535	1/1	0.94	0.19	44,44,44,44	0
57	MG	CA	3169	1/1	0.94	0.18	62,62,62,62	0
57	MG	BA	3489	1/1	0.94	0.25	50,50,50,50	0
57	MG	DA	3608	1/1	0.94	0.09	57,57,57,57	0
57	MG	BA	3198	1/1	0.94	0.16	44,44,44,44	0
57	MG	BA	3695	1/1	0.94	0.15	40,40,40,40	0
57	MG	AA	1731	1/1	0.94	0.18	56,56,56,56	0
57	MG	DA	3255	1/1	0.94	0.24	47,47,47,47	0
57	MG	DA	3251	1/1	0.94	0.15	40,40,40,40	0
57	MG	CA	3069	1/1	0.94	0.22	58,58,58,58	0
57	MG	DA	3467	1/1	0.94	0.24	52,52,52,52	0
57	MG	DE	3003	1/1	0.94	0.12	43,43,43,43	0
57	MG	DA	3185	1/1	0.94	0.15	51,51,51,51	0
57	MG	BA	3394	1/1	0.94	0.28	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	3064	1/1	0.94	0.23	45,45,45,45	0
57	MG	BA	3112	1/1	0.94	0.26	41,41,41,41	0
57	MG	BA	3059	1/1	0.94	0.14	36,36,36,36	0
57	MG	BA	3246	1/1	0.94	0.31	55,55,55,55	0
57	MG	BA	3027	1/1	0.94	0.41	64,64,64,64	0
57	MG	DA	3128	1/1	0.94	0.28	56,56,56,56	0
57	MG	BA	3744	1/1	0.94	0.18	55,55,55,55	0
57	MG	BO	5001	1/1	0.94	0.13	61,61,61,61	0
57	MG	BA	3601	1/1	0.94	0.32	40,40,40,40	0
57	MG	BA	3044	1/1	0.94	0.35	43,43,43,43	0
57	MG	DB	3002	1/1	0.94	0.26	63,63,63,63	0
57	MG	DA	3438	1/1	0.94	0.08	42,42,42,42	0
57	MG	DA	3247	1/1	0.94	0.16	49,49,49,49	0
57	MG	BA	3788	1/1	0.94	0.24	44,44,44,44	0
57	MG	BE	306	1/1	0.94	0.10	38,38,38,38	0
57	MG	DA	3113	1/1	0.94	0.13	35,35,35,35	0
57	MG	AA	1673	1/1	0.94	0.13	48,48,48,48	0
57	MG	BA	3555	1/1	0.94	0.19	50,50,50,50	0
57	MG	BV	201	1/1	0.94	0.36	31,31,31,31	0
57	MG	AA	1683	1/1	0.94	0.13	62,62,62,62	0
57	MG	CA	3037	1/1	0.94	0.21	53,53,53,53	0
57	MG	BA	3519	1/1	0.94	0.19	45,45,45,45	0
57	MG	CA	3056	1/1	0.94	0.10	64,64,64,64	0
57	MG	AA	1715	1/1	0.94	0.23	45,45,45,45	0
57	MG	DA	3009	1/1	0.94	0.17	61,61,61,61	0
57	MG	DA	3060	1/1	0.94	0.28	60,60,60,60	0
57	MG	BA	3070	1/1	0.94	0.24	41,41,41,41	0
57	MG	BA	3030	1/1	0.94	0.24	39,39,39,39	0
57	MG	BA	3135	1/1	0.94	0.45	56,56,56,56	0
57	MG	BB	3010	1/1	0.94	0.18	53,53,53,53	0
57	MG	BA	3445	1/1	0.94	0.23	54,54,54,54	0
57	MG	BA	3320	1/1	0.94	0.16	55,55,55,55	0
57	MG	DA	3621	1/1	0.94	0.49	52,52,52,52	0
57	MG	CA	3147	1/1	0.94	0.10	70,70,70,70	0
57	MG	BA	3422	1/1	0.94	0.16	36,36,36,36	0
57	MG	DA	3230	1/1	0.94	0.14	46,46,46,46	0
57	MG	DA	3402	1/1	0.94	0.09	48,48,48,48	0
57	MG	BA	3028	1/1	0.94	0.20	37,37,37,37	0
57	MG	DB	3009	1/1	0.94	0.14	58,58,58,58	0
57	MG	DA	3277	1/1	0.94	0.13	50,50,50,50	0
57	MG	BA	3581	1/1	0.94	0.12	59,59,59,59	0
57	MG	BA	3675	1/1	0.94	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	AA	1676	1/1	0.94	0.16	58,58,58,58	0
57	MG	BA	3480	1/1	0.94	0.18	47,47,47,47	0
57	MG	B8	5001	1/1	0.94	0.20	42,42,42,42	0
57	MG	BA	3509	1/1	0.94	0.18	50,50,50,50	0
57	MG	AA	1749	1/1	0.94	0.19	50,50,50,50	0
57	MG	AA	1698	1/1	0.94	0.23	58,58,58,58	0
57	MG	DA	3529	1/1	0.94	0.07	76,76,76,76	0
57	MG	BA	3351	1/1	0.94	0.19	45,45,45,45	0
57	MG	AA	1785	1/1	0.94	0.11	72,72,72,72	0
57	MG	CA	3060	1/1	0.94	0.08	71,71,71,71	0
57	MG	BA	3202	1/1	0.94	0.15	62,62,62,62	0
57	MG	CA	3075	1/1	0.94	0.24	65,65,65,65	0
57	MG	BA	3386	1/1	0.94	0.14	28,28,28,28	0
57	MG	CA	3136	1/1	0.94	0.14	48,48,48,48	0
57	MG	AA	1617	1/1	0.94	0.10	58,58,58,58	0
57	MG	BA	3427	1/1	0.94	0.17	33,33,33,33	0
57	MG	DA	3616	1/1	0.94	0.20	63,63,63,63	0
57	MG	CA	3018	1/1	0.94	0.13	63,63,63,63	0
57	MG	DA	3531	1/1	0.94	0.07	48,48,48,48	0
57	MG	BA	3395	1/1	0.94	0.20	30,30,30,30	0
57	MG	BA	3589	1/1	0.94	0.23	59,59,59,59	0
57	MG	AA	1780	1/1	0.94	0.11	69,69,69,69	0
57	MG	DA	3460	1/1	0.94	0.18	37,37,37,37	0
57	MG	BA	3677	1/1	0.94	0.10	44,44,44,44	0
57	MG	DA	3642	1/1	0.94	0.21	62,62,62,62	0
57	MG	DA	3019	1/1	0.94	0.08	42,42,42,42	0
57	MG	DA	3465	1/1	0.94	0.17	42,42,42,42	0
57	MG	DA	3166	1/1	0.94	0.16	55,55,55,55	0
57	MG	AA	1636	1/1	0.94	0.31	52,52,52,52	0
57	MG	BA	3556	1/1	0.94	0.07	46,46,46,46	0
57	MG	BA	3562	1/1	0.94	0.16	55,55,55,55	0
57	MG	DA	3272	1/1	0.94	0.19	49,49,49,49	0
57	MG	CA	3024	1/1	0.94	0.16	67,67,67,67	0
57	MG	BR	5002	1/1	0.94	0.14	50,50,50,50	0
57	MG	DA	3167	1/1	0.94	0.21	40,40,40,40	0
57	MG	BA	3353	1/1	0.94	0.12	55,55,55,55	0
57	MG	DA	3496	1/1	0.95	0.17	56,56,56,56	0
57	MG	DA	3269	1/1	0.95	0.11	50,50,50,50	0
57	MG	AA	1786	1/1	0.95	0.14	69,69,69,69	0
57	MG	DE	3002	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3716	1/1	0.95	0.25	45,45,45,45	0
57	MG	DA	3610	1/1	0.95	0.09	47,47,47,47	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	0.95	0.12	47,47,47,47	0
57	MG	BW	3003	1/1	0.95	0.15	35,35,35,35	0
57	MG	BA	3118	1/1	0.95	0.21	35,35,35,35	0
57	MG	DA	3385	1/1	0.95	0.07	60,60,60,60	0
57	MG	BA	3421	1/1	0.95	0.26	62,62,62,62	0
59	ZN	BY	501	1/1	0.95	0.18	68,68,68,68	0
57	MG	BA	3228	1/1	0.95	0.10	65,65,65,65	0
57	MG	DB	3008	1/1	0.95	0.17	56,56,56,56	0
57	MG	BA	3208	1/1	0.95	0.11	43,43,43,43	0
57	MG	CA	3057	1/1	0.95	0.14	84,84,84,84	0
57	MG	BA	3708	1/1	0.95	0.21	33,33,33,33	0
57	MG	DA	3003	1/1	0.95	0.23	36,36,36,36	0
57	MG	BA	3752	1/1	0.95	0.12	34,34,34,34	0
57	MG	BA	3277	1/1	0.95	0.43	52,52,52,52	0
57	MG	BA	3607	1/1	0.95	0.17	36,36,36,36	0
57	MG	BA	3801	1/1	0.95	0.16	71,71,71,71	0
57	MG	BA	3061	1/1	0.95	0.30	25,25,25,25	0
57	MG	BA	3199	1/1	0.95	0.30	64,64,64,64	0
57	MG	BA	3284	1/1	0.95	0.10	57,57,57,57	0
57	MG	AA	1709	1/1	0.95	0.26	55,55,55,55	0
57	MG	BA	3037	1/1	0.95	0.28	42,42,42,42	0
57	MG	AA	1769	1/1	0.95	0.19	50,50,50,50	0
57	MG	AX	3006	1/1	0.95	0.15	68,68,68,68	0
57	MG	BA	3116	1/1	0.95	0.35	46,46,46,46	0
57	MG	DA	3102	1/1	0.95	0.32	40,40,40,40	0
57	MG	DA	3583	1/1	0.95	0.12	52,52,52,52	0
57	MG	BA	3238	1/1	0.95	0.48	44,44,44,44	0
57	MG	BA	3617	1/1	0.95	0.10	42,42,42,42	0
57	MG	DA	3043	1/1	0.95	0.19	53,53,53,53	0
57	MG	DA	3252	1/1	0.95	0.07	50,50,50,50	0
57	MG	AA	1807	1/1	0.95	0.07	68,68,68,68	0
57	MG	BA	3153	1/1	0.95	0.15	45,45,45,45	0
57	MG	DA	3145	1/1	0.95	0.32	48,48,48,48	0
57	MG	BA	3401	1/1	0.95	0.25	26,26,26,26	0
57	MG	BA	3478	1/1	0.95	0.15	54,54,54,54	0
57	MG	DA	3184	1/1	0.95	0.12	52,52,52,52	0
57	MG	BA	3363	1/1	0.95	0.17	52,52,52,52	0
57	MG	BA	3580	1/1	0.95	0.15	48,48,48,48	0
57	MG	DA	3287	1/1	0.95	0.21	52,52,52,52	0
57	MG	DA	3076	1/1	0.95	0.18	52,52,52,52	0
57	MG	BA	3511	1/1	0.95	0.18	50,50,50,50	0
57	MG	CA	3093	1/1	0.95	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1757	1/1	0.95	0.25	68,68,68,68	0
57	MG	BA	3178	1/1	0.95	0.17	32,32,32,32	0
57	MG	AA	1700	1/1	0.95	0.08	71,71,71,71	0
57	MG	DA	3641	1/1	0.95	0.07	46,46,46,46	0
57	MG	BA	3017	1/1	0.95	0.28	65,65,65,65	0
57	MG	DA	3346	1/1	0.95	0.14	49,49,49,49	0
57	MG	BA	3158	1/1	0.95	0.17	41,41,41,41	0
57	MG	DA	3278	1/1	0.95	0.10	39,39,39,39	0
57	MG	DA	3389	1/1	0.95	0.19	59,59,59,59	0
57	MG	DA	3404	1/1	0.95	0.08	43,43,43,43	0
57	MG	BA	3459	1/1	0.95	0.15	31,31,31,31	0
57	MG	DA	3193	1/1	0.95	0.15	47,47,47,47	0
57	MG	BA	3093	1/1	0.95	0.24	41,41,41,41	0
57	MG	BB	3018	1/1	0.95	0.06	54,54,54,54	0
57	MG	DA	3656	1/1	0.95	0.25	41,41,41,41	0
57	MG	CA	3033	1/1	0.95	0.10	54,54,54,54	0
57	MG	BB	3014	1/1	0.95	0.12	67,67,67,67	0
57	MG	BA	3169	1/1	0.95	0.24	50,50,50,50	0
57	MG	AA	1750	1/1	0.95	0.14	49,49,49,49	0
57	MG	BA	3709	1/1	0.95	0.34	48,48,48,48	0
57	MG	BA	3812	1/1	0.95	0.12	42,42,42,42	0
57	MG	BA	3753	1/1	0.95	0.19	68,68,68,68	0
57	MG	BA	3251	1/1	0.95	0.25	43,43,43,43	0
57	MG	DA	3423	1/1	0.95	0.20	37,37,37,37	0
57	MG	AA	1804	1/1	0.95	0.12	70,70,70,70	0
57	MG	DA	3149	1/1	0.95	0.08	46,46,46,46	0
57	MG	CA	3097	1/1	0.95	0.27	60,60,60,60	0
57	MG	BA	3664	1/1	0.95	0.21	69,69,69,69	0
57	MG	BA	3575	1/1	0.95	0.12	50,50,50,50	0
57	MG	DA	3038	1/1	0.95	0.14	56,56,56,56	0
57	MG	DA	3115	1/1	0.95	0.29	55,55,55,55	0
57	MG	CA	3142	1/1	0.95	0.18	50,50,50,50	0
57	MG	BA	3071	1/1	0.95	0.31	59,59,59,59	0
57	MG	BA	3537	1/1	0.95	0.08	43,43,43,43	0
57	MG	CX	3001	1/1	0.95	0.18	57,57,57,57	0
57	MG	DA	3322	1/1	0.95	0.16	42,42,42,42	0
57	MG	B7	101	1/1	0.95	0.12	41,41,41,41	0
57	MG	BA	3774	1/1	0.95	0.32	27,27,27,27	0
57	MG	BA	3042	1/1	0.95	0.13	37,37,37,37	0
57	MG	DA	3359	1/1	0.95	0.16	40,40,40,40	0
57	MG	BA	3328	1/1	0.95	0.19	27,27,27,27	0
57	MG	AA	1794	1/1	0.95	0.16	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	3080	1/1	0.95	0.14	31,31,31,31	0
57	MG	BA	3444	1/1	0.95	0.15	48,48,48,48	0
57	MG	DA	3337	1/1	0.95	0.06	48,48,48,48	0
57	MG	BA	3261	1/1	0.95	0.21	18,18,18,18	0
57	MG	DA	3225	1/1	0.95	0.10	55,55,55,55	0
57	MG	BA	3335	1/1	0.95	0.15	40,40,40,40	0
57	MG	BA	3578	1/1	0.95	0.35	39,39,39,39	0
57	MG	BA	3188	1/1	0.95	0.19	32,32,32,32	0
57	MG	BA	3152	1/1	0.95	0.26	23,23,23,23	0
57	MG	BA	3629	1/1	0.95	0.25	58,58,58,58	0
57	MG	BA	3481	1/1	0.95	0.12	54,54,54,54	0
57	MG	BU	202	1/1	0.95	0.15	40,40,40,40	0
57	MG	BA	3032	1/1	0.95	0.21	33,33,33,33	0
57	MG	BA	3465	1/1	0.95	0.09	48,48,48,48	0
57	MG	BB	3008	1/1	0.95	0.36	59,59,59,59	0
57	MG	DA	3295	1/1	0.95	0.19	67,67,67,67	0
57	MG	DA	3378	1/1	0.95	0.14	52,52,52,52	0
57	MG	DA	3509	1/1	0.95	0.06	49,49,49,49	0
57	MG	BA	3213	1/1	0.95	0.15	43,43,43,43	0
57	MG	DA	3224	1/1	0.95	0.08	39,39,39,39	0
57	MG	DA	3589	1/1	0.95	0.08	29,29,29,29	0
57	MG	BA	3567	1/1	0.95	0.25	32,32,32,32	0
57	MG	BA	3293	1/1	0.95	0.11	58,58,58,58	0
57	MG	BA	3324	1/1	0.95	0.15	60,60,60,60	0
57	MG	DA	3165	1/1	0.95	0.21	55,55,55,55	0
57	MG	BV	202	1/1	0.95	0.26	32,32,32,32	0
57	MG	DA	3410	1/1	0.95	0.22	40,40,40,40	0
57	MG	BA	3691	1/1	0.95	0.11	43,43,43,43	0
57	MG	CA	3074	1/1	0.95	0.14	60,60,60,60	0
57	MG	DN	5001	1/1	0.95	0.11	63,63,63,63	0
57	MG	BA	3748	1/1	0.95	0.17	61,61,61,61	0
57	MG	CA	3040	1/1	0.95	0.12	56,56,56,56	0
57	MG	BA	3223	1/1	0.95	0.18	41,41,41,41	0
57	MG	CA	3168	1/1	0.95	0.20	41,41,41,41	0
57	MG	DA	3171	1/1	0.95	0.17	40,40,40,40	0
57	MG	AA	1742	1/1	0.95	0.14	52,52,52,52	0
57	MG	DA	3474	1/1	0.95	0.09	53,53,53,53	0
57	MG	AA	1746	1/1	0.95	0.10	56,56,56,56	0
57	MG	CD	502	1/1	0.95	0.27	53,53,53,53	0
57	MG	BA	3433	1/1	0.95	0.20	27,27,27,27	0
57	MG	BA	3350	1/1	0.95	0.12	34,34,34,34	0
57	MG	DA	3325	1/1	0.95	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3175	1/1	0.95	0.14	41,41,41,41	0
57	MG	DA	3586	1/1	0.95	0.08	50,50,50,50	0
57	MG	BA	3469	1/1	0.95	0.16	61,61,61,61	0
57	MG	DA	3594	1/1	0.95	0.09	58,58,58,58	0
57	MG	DD	301	1/1	0.95	0.22	44,44,44,44	0
57	MG	BA	3451	1/1	0.95	0.25	44,44,44,44	0
57	MG	AA	1774	1/1	0.95	0.17	51,51,51,51	0
57	MG	CA	3134	1/1	0.95	0.12	64,64,64,64	0
57	MG	BA	3495	1/1	0.95	0.16	43,43,43,43	0
57	MG	DA	3429	1/1	0.95	0.15	36,36,36,36	0
57	MG	DA	3527	1/1	0.95	0.13	52,52,52,52	0
57	MG	DA	3082	1/1	0.95	0.22	47,47,47,47	0
57	MG	DA	3510	1/1	0.95	0.26	64,64,64,64	0
57	MG	AA	1776	1/1	0.95	0.16	73,73,73,73	0
57	MG	AA	1783	1/1	0.95	0.17	35,35,35,35	0
57	MG	BA	3520	1/1	0.95	0.25	29,29,29,29	0
57	MG	BA	3043	1/1	0.95	0.17	31,31,31,31	0
57	MG	BA	3471	1/1	0.95	0.19	27,27,27,27	0
57	MG	BA	3572	1/1	0.95	0.26	39,39,39,39	0
57	MG	DA	3266	1/1	0.95	0.12	37,37,37,37	0
57	MG	DA	3124	1/1	0.95	0.17	43,43,43,43	0
57	MG	BE	305	1/1	0.95	0.07	48,48,48,48	0
57	MG	DA	3299	1/1	0.95	0.09	46,46,46,46	0
57	MG	DA	3364	1/1	0.95	0.10	45,45,45,45	0
57	MG	DA	3331	1/1	0.95	0.15	47,47,47,47	0
57	MG	BA	3780	1/1	0.95	0.13	42,42,42,42	0
57	MG	CA	3088	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3355	1/1	0.95	0.15	35,35,35,35	0
57	MG	BD	3007	1/1	0.95	0.30	46,46,46,46	0
57	MG	BA	3297	1/1	0.95	0.22	42,42,42,42	0
57	MG	BA	3276	1/1	0.95	0.40	44,44,44,44	0
57	MG	AA	1615	1/1	0.95	0.21	51,51,51,51	0
57	MG	BA	3258	1/1	0.95	0.35	44,44,44,44	0
57	MG	BA	3550	1/1	0.95	0.16	50,50,50,50	0
57	MG	DA	3490	1/1	0.95	0.13	33,33,33,33	0
57	MG	CA	3053	1/1	0.95	0.12	41,41,41,41	0
57	MG	DA	3329	1/1	0.95	0.10	47,47,47,47	0
57	MG	BA	3455	1/1	0.95	0.14	52,52,52,52	0
57	MG	CA	3116	1/1	0.95	0.20	57,57,57,57	0
57	MG	BA	3023	1/1	0.95	0.17	41,41,41,41	0
57	MG	DA	3555	1/1	0.95	0.21	46,46,46,46	0
57	MG	BA	3479	1/1	0.95	0.06	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	3498	1/1	0.95	0.17	35,35,35,35	0
57	MG	AX	3009	1/1	0.95	0.37	65,65,65,65	0
57	MG	BA	3671	1/1	0.95	0.19	24,24,24,24	0
57	MG	BQ	3002	1/1	0.95	0.28	46,46,46,46	0
57	MG	BA	3143	1/1	0.95	0.10	41,41,41,41	0
57	MG	BA	3168	1/1	0.95	0.24	45,45,45,45	0
57	MG	DA	3434	1/1	0.95	0.07	60,60,60,60	0
57	MG	DA	3147	1/1	0.95	0.14	44,44,44,44	0
57	MG	AA	1670	1/1	0.95	0.17	67,67,67,67	0
57	MG	BA	3120	1/1	0.95	0.18	45,45,45,45	0
57	MG	DA	3443	1/1	0.95	0.19	51,51,51,51	0
57	MG	DA	3588	1/1	0.95	0.15	59,59,59,59	0
57	MG	AA	1775	1/1	0.95	0.11	73,73,73,73	0
57	MG	DA	3382	1/1	0.95	0.12	41,41,41,41	0
57	MG	DA	3312	1/1	0.95	0.12	42,42,42,42	0
57	MG	BA	3262	1/1	0.96	0.27	31,31,31,31	0
57	MG	BA	3724	1/1	0.96	0.18	20,20,20,20	0
57	MG	DA	3573	1/1	0.96	0.05	61,61,61,61	0
57	MG	BA	3590	1/1	0.96	0.15	33,33,33,33	0
57	MG	BA	3031	1/1	0.96	0.27	36,36,36,36	0
57	MG	BA	3502	1/1	0.96	0.19	30,30,30,30	0
57	MG	BA	3602	1/1	0.96	0.11	47,47,47,47	0
57	MG	BA	3082	1/1	0.96	0.18	28,28,28,28	0
57	MG	DW	3001	1/1	0.96	0.21	41,41,41,41	0
57	MG	BA	3648	1/1	0.96	0.22	58,58,58,58	0
57	MG	BA	3464	1/1	0.96	0.13	44,44,44,44	0
57	MG	DA	3215	1/1	0.96	0.18	40,40,40,40	0
57	MG	AA	1647	1/1	0.96	0.22	44,44,44,44	0
57	MG	DA	3293	1/1	0.96	0.15	61,61,61,61	0
57	MG	BA	3787	1/1	0.96	0.14	45,45,45,45	0
57	MG	BB	3015	1/1	0.96	0.26	45,45,45,45	0
57	MG	DA	3011	1/1	0.96	0.07	35,35,35,35	0
57	MG	BA	3336	1/1	0.96	0.17	20,20,20,20	0
57	MG	AA	1725	1/1	0.96	0.22	51,51,51,51	0
57	MG	BG	201	1/1	0.96	0.14	39,39,39,39	0
57	MG	B7	105	1/1	0.96	0.20	28,28,28,28	0
57	MG	BA	3307	1/1	0.96	0.19	28,28,28,28	0
57	MG	BA	3119	1/1	0.96	0.15	46,46,46,46	0
57	MG	BF	303	1/1	0.96	0.26	33,33,33,33	0
57	MG	AA	1767	1/1	0.96	0.11	67,67,67,67	0
57	MG	DA	3638	1/1	0.96	0.09	47,47,47,47	0
57	MG	BA	3201	1/1	0.96	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3432	1/1	0.96	0.17	52,52,52,52	0
57	MG	BA	3397	1/1	0.96	0.15	28,28,28,28	0
57	MG	CA	3066	1/1	0.96	0.14	48,48,48,48	0
57	MG	BA	3151	1/1	0.96	0.17	36,36,36,36	0
57	MG	DA	3157	1/1	0.96	0.13	34,34,34,34	0
57	MG	DA	3044	1/1	0.96	0.19	53,53,53,53	0
57	MG	DA	3263	1/1	0.96	0.13	65,65,65,65	0
57	MG	BA	3308	1/1	0.96	0.23	39,39,39,39	0
57	MG	DA	3117	1/1	0.96	0.09	56,56,56,56	0
57	MG	BF	304	1/1	0.96	0.39	41,41,41,41	0
57	MG	BA	3791	1/1	0.96	0.38	49,49,49,49	0
57	MG	BA	3396	1/1	0.96	0.23	25,25,25,25	0
57	MG	BA	3172	1/1	0.96	0.26	40,40,40,40	0
57	MG	BA	3402	1/1	0.96	0.18	27,27,27,27	0
57	MG	BA	3144	1/1	0.96	0.18	41,41,41,41	0
57	MG	AA	1706	1/1	0.96	0.22	60,60,60,60	0
57	MG	DA	3430	1/1	0.96	0.13	47,47,47,47	0
57	MG	DA	3380	1/1	0.96	0.04	66,66,66,66	0
57	MG	CF	3001	1/1	0.96	0.12	51,51,51,51	0
57	MG	DA	3457	1/1	0.96	0.18	44,44,44,44	0
57	MG	DA	3503	1/1	0.96	0.22	38,38,38,38	0
57	MG	BA	3409	1/1	0.96	0.23	22,22,22,22	0
57	MG	BA	3392	1/1	0.96	0.18	26,26,26,26	0
57	MG	BA	3046	1/1	0.96	0.15	43,43,43,43	0
57	MG	BA	3482	1/1	0.96	0.16	51,51,51,51	0
57	MG	BA	3610	1/1	0.96	0.09	61,61,61,61	0
57	MG	AA	1773	1/1	0.96	0.10	61,61,61,61	0
57	MG	DA	3059	1/1	0.96	0.10	50,50,50,50	0
57	MG	DA	3473	1/1	0.96	0.22	50,50,50,50	0
57	MG	BA	3643	1/1	0.96	0.12	52,52,52,52	0
57	MG	CA	3155	1/1	0.96	0.15	57,57,57,57	0
57	MG	DA	3258	1/1	0.96	0.16	45,45,45,45	0
57	MG	DA	3137	1/1	0.96	0.17	52,52,52,52	0
57	MG	DA	3450	1/1	0.96	0.06	50,50,50,50	0
57	MG	BA	3196	1/1	0.96	0.23	56,56,56,56	0
57	MG	BA	3034	1/1	0.96	0.23	35,35,35,35	0
57	MG	DA	3525	1/1	0.96	0.15	28,28,28,28	0
57	MG	AA	1716	1/1	0.96	0.17	50,50,50,50	0
57	MG	DA	3098	1/1	0.96	0.10	66,66,66,66	0
57	MG	BA	3215	1/1	0.96	0.42	37,37,37,37	0
57	MG	BA	3050	1/1	0.96	0.15	32,32,32,32	0
57	MG	BF	308	1/1	0.96	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	DA	3265	1/1	0.96	0.16	57,57,57,57	0
57	MG	BP	3001	1/1	0.96	0.14	34,34,34,34	0
57	MG	BA	3090	1/1	0.96	0.26	38,38,38,38	0
57	MG	DA	3360	1/1	0.96	0.09	31,31,31,31	0
57	MG	CA	3138	1/1	0.96	0.10	65,65,65,65	0
57	MG	BA	3762	1/1	0.96	0.18	20,20,20,20	0
57	MG	BA	3521	1/1	0.96	0.22	40,40,40,40	0
57	MG	DA	3152	1/1	0.96	0.17	45,45,45,45	0
57	MG	BA	3405	1/1	0.96	0.16	52,52,52,52	0
57	MG	AA	1779	1/1	0.96	0.14	59,59,59,59	0
57	MG	AA	1685	1/1	0.96	0.21	62,62,62,62	0
57	MG	BA	3568	1/1	0.96	0.23	24,24,24,24	0
57	MG	BA	3249	1/1	0.96	0.23	53,53,53,53	0
57	MG	BA	3438	1/1	0.96	0.20	35,35,35,35	0
57	MG	BA	3398	1/1	0.96	0.22	32,32,32,32	0
57	MG	BA	3503	1/1	0.96	0.10	51,51,51,51	0
57	MG	DA	3276	1/1	0.96	0.16	28,28,28,28	0
57	MG	DA	3162	1/1	0.96	0.14	57,57,57,57	0
57	MG	DA	3228	1/1	0.96	0.16	44,44,44,44	0
57	MG	BA	3130	1/1	0.96	0.46	48,48,48,48	0
57	MG	BA	3454	1/1	0.96	0.17	46,46,46,46	0
57	MG	AA	1608	1/1	0.96	0.22	43,43,43,43	0
57	MG	DE	3004	1/1	0.96	0.17	31,31,31,31	0
57	MG	DA	3246	1/1	0.96	0.06	46,46,46,46	0
57	MG	BA	3795	1/1	0.96	0.25	19,19,19,19	0
57	MG	B9	502	1/1	0.96	0.34	46,46,46,46	0
57	MG	BA	3035	1/1	0.96	0.27	49,49,49,49	0
57	MG	BA	3808	1/1	0.96	0.15	38,38,38,38	0
57	MG	AA	1736	1/1	0.96	0.10	49,49,49,49	0
57	MG	BA	3565	1/1	0.96	0.14	61,61,61,61	0
57	MG	BA	3013	1/1	0.96	0.20	28,28,28,28	0
57	MG	AA	1813	1/1	0.96	0.21	38,38,38,38	0
57	MG	DA	3270	1/1	0.96	0.09	42,42,42,42	0
57	MG	CA	3028	1/1	0.96	0.27	48,48,48,48	0
57	MG	BA	3493	1/1	0.96	0.21	38,38,38,38	0
57	MG	BA	3167	1/1	0.96	0.18	45,45,45,45	0
57	MG	DA	3183	1/1	0.96	0.17	41,41,41,41	0
57	MG	AA	1793	1/1	0.96	0.17	63,63,63,63	0
57	MG	CA	3149	1/1	0.96	0.12	54,54,54,54	0
57	MG	DA	3664	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3595	1/1	0.96	0.09	61,61,61,61	0
57	MG	BA	3797	1/1	0.96	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1811	1/1	0.96	0.21	49,49,49,49	0
57	MG	BA	3468	1/1	0.96	0.19	45,45,45,45	0
57	MG	BA	3756	1/1	0.96	0.19	18,18,18,18	0
57	MG	BA	3142	1/1	0.96	0.31	46,46,46,46	0
57	MG	BA	3440	1/1	0.96	0.20	35,35,35,35	0
57	MG	DA	3343	1/1	0.96	0.15	34,34,34,34	0
57	MG	BA	3783	1/1	0.96	0.15	37,37,37,37	0
57	MG	AA	1744	1/1	0.96	0.17	44,44,44,44	0
57	MG	CA	3038	1/1	0.96	0.09	57,57,57,57	0
57	MG	BA	3430	1/1	0.96	0.24	34,34,34,34	0
57	MG	BA	3720	1/1	0.96	0.12	38,38,38,38	0
57	MG	AA	1748	1/1	0.96	0.16	64,64,64,64	0
57	MG	DA	3121	1/1	0.96	0.10	40,40,40,40	0
57	MG	DA	3507	1/1	0.96	0.07	59,59,59,59	0
57	MG	BA	3319	1/1	0.96	0.22	23,23,23,23	0
57	MG	BA	3514	1/1	0.96	0.19	43,43,43,43	0
57	MG	BA	3306	1/1	0.96	0.17	15,15,15,15	0
57	MG	BA	3204	1/1	0.96	0.27	67,67,67,67	0
57	MG	BE	302	1/1	0.96	0.16	35,35,35,35	0
57	MG	BA	3291	1/1	0.96	0.26	53,53,53,53	0
57	MG	DA	3350	1/1	0.96	0.18	31,31,31,31	0
57	MG	BA	3447	1/1	0.96	0.32	52,52,52,52	0
57	MG	AA	1760	1/1	0.96	0.15	65,65,65,65	0
57	MG	CA	3156	1/1	0.96	0.08	59,59,59,59	0
57	MG	DA	3029	1/1	0.96	0.57	45,45,45,45	0
57	MG	CK	5001	1/1	0.96	0.05	61,61,61,61	0
57	MG	BA	3214	1/1	0.96	0.50	43,43,43,43	0
57	MG	DA	3349	1/1	0.96	0.16	34,34,34,34	0
57	MG	BF	309	1/1	0.96	0.18	31,31,31,31	0
57	MG	DA	3058	1/1	0.96	0.08	61,61,61,61	0
57	MG	BA	3216	1/1	0.96	0.28	39,39,39,39	0
57	MG	DA	3652	1/1	0.96	0.16	31,31,31,31	0
57	MG	BA	3374	1/1	0.96	0.19	50,50,50,50	0
57	MG	DA	3214	1/1	0.96	0.08	51,51,51,51	0
57	MG	DE	3007	1/1	0.96	0.11	58,58,58,58	0
57	MG	AA	1637	1/1	0.96	0.10	61,61,61,61	0
57	MG	BA	3205	1/1	0.96	0.43	57,57,57,57	0
57	MG	AA	1719	1/1	0.96	0.16	63,63,63,63	0
57	MG	BA	3159	1/1	0.96	0.18	27,27,27,27	0
57	MG	DA	3109	1/1	0.96	0.13	49,49,49,49	0
57	MG	BA	3352	1/1	0.96	0.16	68,68,68,68	0
57	MG	DA	3221	1/1	0.96	0.10	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	3076	1/1	0.96	0.38	42,42,42,42	0
57	MG	BA	3226	1/1	0.96	0.22	25,25,25,25	0
57	MG	BA	3361	1/1	0.96	0.08	56,56,56,56	0
57	MG	BA	3585	1/1	0.96	0.16	29,29,29,29	0
57	MG	BA	3486	1/1	0.96	0.13	41,41,41,41	0
57	MG	AE	3001	1/1	0.96	0.07	63,63,63,63	0
57	MG	BA	3654	1/1	0.96	0.11	59,59,59,59	0
57	MG	BA	3022	1/1	0.96	0.11	25,25,25,25	0
57	MG	DA	3598	1/1	0.96	0.10	55,55,55,55	0
57	MG	BA	3285	1/1	0.96	0.15	58,58,58,58	0
57	MG	BA	3764	1/1	0.96	0.20	66,66,66,66	0
57	MG	DA	3231	1/1	0.96	0.18	61,61,61,61	0
57	MG	AA	1734	1/1	0.96	0.12	43,43,43,43	0
57	MG	BA	3278	1/1	0.96	0.78	54,54,54,54	0
57	MG	BA	3380	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3108	1/1	0.96	0.21	42,42,42,42	0
57	MG	BA	3711	1/1	0.96	0.25	44,44,44,44	0
57	MG	BA	3376	1/1	0.96	0.19	29,29,29,29	0
57	MG	DA	3437	1/1	0.96	0.18	48,48,48,48	0
57	MG	DA	3484	1/1	0.96	0.07	46,46,46,46	0
57	MG	DA	3365	1/1	0.96	0.14	19,19,19,19	0
57	MG	CA	3083	1/1	0.96	0.16	50,50,50,50	0
57	MG	BA	3466	1/1	0.96	0.17	51,51,51,51	0
57	MG	BA	3234	1/1	0.96	0.12	52,52,52,52	0
57	MG	DA	3387	1/1	0.96	0.10	59,59,59,59	0
57	MG	DA	3354	1/1	0.96	0.11	41,41,41,41	0
57	MG	DA	3216	1/1	0.96	0.15	35,35,35,35	0
57	MG	BA	3492	1/1	0.96	0.12	38,38,38,38	0
57	MG	DA	3309	1/1	0.96	0.12	48,48,48,48	0
57	MG	DA	3647	1/1	0.96	0.11	52,52,52,52	0
57	MG	CA	3140	1/1	0.96	0.16	57,57,57,57	0
57	MG	DA	3213	1/1	0.97	0.18	37,37,37,37	0
57	MG	BA	3341	1/1	0.97	0.20	18,18,18,18	0
57	MG	BQ	3001	1/1	0.97	0.26	37,37,37,37	0
57	MG	DF	304	1/1	0.97	0.07	51,51,51,51	0
57	MG	DA	3120	1/1	0.97	0.33	56,56,56,56	0
57	MG	CA	3105	1/1	0.97	0.11	75,75,75,75	0
57	MG	CA	3048	1/1	0.97	0.12	58,58,58,58	0
57	MG	BD	3005	1/1	0.97	0.24	44,44,44,44	0
57	MG	BA	3190	1/1	0.97	0.28	54,54,54,54	0
57	MG	DA	3180	1/1	0.97	0.21	48,48,48,48	0
57	MG	BA	3331	1/1	0.97	0.20	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	CA	3128	1/1	0.97	0.13	52,52,52,52	0
57	MG	BA	3448	1/1	0.97	0.18	17,17,17,17	0
57	MG	BA	3136	1/1	0.97	0.36	49,49,49,49	0
57	MG	BA	3548	1/1	0.97	0.13	35,35,35,35	0
57	MG	DA	3492	1/1	0.97	0.07	48,48,48,48	0
57	MG	BA	3669	1/1	0.97	0.20	28,28,28,28	0
57	MG	DA	3039	1/1	0.97	0.16	38,38,38,38	0
57	MG	BA	3077	1/1	0.97	0.20	15,15,15,15	0
57	MG	AA	1653	1/1	0.97	0.23	54,54,54,54	0
57	MG	BA	3004	1/1	0.97	0.22	36,36,36,36	0
57	MG	BA	3810	1/1	0.97	0.21	35,35,35,35	0
57	MG	DA	3040	1/1	0.97	0.14	28,28,28,28	0
57	MG	BB	3021	1/1	0.97	0.18	41,41,41,41	0
57	MG	AA	1661	1/1	0.97	0.37	54,54,54,54	0
57	MG	AN	502	1/1	0.97	0.29	62,62,62,62	0
57	MG	DD	304	1/1	0.97	0.09	36,36,36,36	0
57	MG	DA	3302	1/1	0.97	0.23	53,53,53,53	0
57	MG	BA	3634	1/1	0.97	0.14	55,55,55,55	0
57	MG	CA	3043	1/1	0.97	0.18	44,44,44,44	0
57	MG	AA	1727	1/1	0.97	0.14	50,50,50,50	0
57	MG	BA	3736	1/1	0.97	0.16	22,22,22,22	0
57	MG	DA	3386	1/1	0.97	0.10	44,44,44,44	0
57	MG	BA	3053	1/1	0.97	0.27	23,23,23,23	0
57	MG	BB	3007	1/1	0.97	0.17	41,41,41,41	0
57	MG	B7	102	1/1	0.97	0.17	41,41,41,41	0
57	MG	DA	3036	1/1	0.97	0.17	35,35,35,35	0
57	MG	DA	3303	1/1	0.97	0.12	43,43,43,43	0
57	MG	BA	3083	1/1	0.97	0.34	60,60,60,60	0
57	MG	BA	3157	1/1	0.97	0.20	46,46,46,46	0
57	MG	DA	3144	1/1	0.97	0.23	41,41,41,41	0
57	MG	BA	3011	1/1	0.97	0.15	30,30,30,30	0
57	MG	BA	3725	1/1	0.97	0.18	31,31,31,31	0
57	MG	AA	1703	1/1	0.97	0.29	43,43,43,43	0
57	MG	BA	3621	1/1	0.97	0.19	43,43,43,43	0
57	MG	DA	3045	1/1	0.97	0.22	51,51,51,51	0
57	MG	DA	3501	1/1	0.97	0.10	49,49,49,49	0
57	MG	CA	3084	1/1	0.97	0.14	56,56,56,56	0
57	MG	DA	3629	1/1	0.97	0.12	57,57,57,57	0
57	MG	BA	3385	1/1	0.97	0.23	30,30,30,30	0
57	MG	BA	3256	1/1	0.97	0.34	34,34,34,34	0
57	MG	DA	3290	1/1	0.97	0.14	33,33,33,33	0
57	MG	BA	3628	1/1	0.97	0.28	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	BA	3473	1/1	0.97	0.19	28,28,28,28	0
57	MG	DA	3203	1/1	0.97	0.18	53,53,53,53	0
57	MG	DA	3661	1/1	0.97	0.10	62,62,62,62	0
57	MG	BB	3011	1/1	0.97	0.20	47,47,47,47	0
57	MG	DA	3062	1/1	0.97	0.11	53,53,53,53	0
57	MG	BA	3760	1/1	0.97	0.17	50,50,50,50	0
57	MG	BA	3174	1/1	0.97	0.53	38,38,38,38	0
57	MG	BA	3496	1/1	0.97	0.12	51,51,51,51	0
57	MG	AA	1611	1/1	0.97	0.19	20,20,20,20	0
57	MG	DA	3307	1/1	0.97	0.12	51,51,51,51	0
57	MG	BA	3287	1/1	0.97	0.17	27,27,27,27	0
57	MG	BA	3315	1/1	0.97	0.18	40,40,40,40	0
57	MG	DA	3304	1/1	0.97	0.14	42,42,42,42	0
57	MG	BA	3490	1/1	0.97	0.17	43,43,43,43	0
57	MG	DA	3348	1/1	0.97	0.21	53,53,53,53	0
57	MG	BA	3606	1/1	0.97	0.16	36,36,36,36	0
57	MG	DA	3495	1/1	0.97	0.05	50,50,50,50	0
57	MG	BA	3045	1/1	0.97	0.17	39,39,39,39	0
57	MG	CA	3047	1/1	0.97	0.16	50,50,50,50	0
57	MG	DE	3006	1/1	0.97	0.21	38,38,38,38	0
57	MG	CA	3096	1/1	0.97	0.18	43,43,43,43	0
57	MG	DA	3264	1/1	0.97	0.18	51,51,51,51	0
57	MG	DA	3370	1/1	0.97	0.13	59,59,59,59	0
57	MG	BA	3362	1/1	0.97	0.22	47,47,47,47	0
57	MG	BA	3356	1/1	0.97	0.24	31,31,31,31	0
57	MG	BH	201	1/1	0.97	0.19	56,56,56,56	0
57	MG	BA	3461	1/1	0.97	0.11	45,45,45,45	0
57	MG	BA	3387	1/1	0.97	0.20	29,29,29,29	0
57	MG	BA	3749	1/1	0.97	0.16	52,52,52,52	0
57	MG	BA	3612	1/1	0.97	0.10	60,60,60,60	0
57	MG	BA	3260	1/1	0.97	0.20	19,19,19,19	0
57	MG	BA	3544	1/1	0.97	0.18	52,52,52,52	0
57	MG	DA	3267	1/1	0.97	0.12	44,44,44,44	0
57	MG	DA	3323	1/1	0.97	0.21	49,49,49,49	0
57	MG	BA	3560	1/1	0.97	0.14	63,63,63,63	0
57	MG	BA	3776	1/1	0.97	0.22	60,60,60,60	0
57	MG	BA	3180	1/1	0.97	0.27	46,46,46,46	0
57	MG	DA	3316	1/1	0.97	0.20	57,57,57,57	0
57	MG	DA	3248	1/1	0.97	0.11	58,58,58,58	0
57	MG	BA	3566	1/1	0.97	0.21	31,31,31,31	0
57	MG	BA	3186	1/1	0.97	0.27	41,41,41,41	0
57	MG	BA	3770	1/1	0.97	0.44	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	AA	1624	1/1	0.97	0.25	66,66,66,66	0
57	MG	BB	3023	1/1	0.97	0.16	47,47,47,47	0
57	MG	B5	104	1/1	0.97	0.09	58,58,58,58	0
57	MG	DA	3037	1/1	0.97	0.12	26,26,26,26	0
57	MG	CA	3158	1/1	0.97	0.20	55,55,55,55	0
57	MG	BA	3221	1/1	0.97	0.21	29,29,29,29	0
57	MG	AA	1627	1/1	0.97	0.14	54,54,54,54	0
57	MG	BA	3357	1/1	0.97	0.07	34,34,34,34	0
57	MG	DA	3073	1/1	0.97	0.08	33,33,33,33	0
57	MG	BA	3683	1/1	0.97	0.21	62,62,62,62	0
57	MG	BA	3412	1/1	0.97	0.17	30,30,30,30	0
57	MG	BA	3434	1/1	0.97	0.12	19,19,19,19	0
57	MG	BA	3185	1/1	0.97	0.15	33,33,33,33	0
57	MG	AA	1803	1/1	0.97	0.12	46,46,46,46	0
57	MG	BD	3001	1/1	0.97	0.14	34,34,34,34	0
57	MG	DA	3294	1/1	0.97	0.12	40,40,40,40	0
57	MG	BA	3316	1/1	0.97	0.20	54,54,54,54	0
57	MG	DA	3326	1/1	0.97	0.10	46,46,46,46	0
57	MG	DA	3640	1/1	0.97	0.10	62,62,62,62	0
57	MG	CA	3132	1/1	0.97	0.14	64,64,64,64	0
57	MG	AA	1642	1/1	0.97	0.23	59,59,59,59	0
57	MG	BA	3184	1/1	0.97	0.21	42,42,42,42	0
57	MG	DA	3544	1/1	0.97	0.12	53,53,53,53	0
57	MG	DA	3198	1/1	0.97	0.16	52,52,52,52	0
59	ZN	DY	501	1/1	0.97	0.11	90,90,90,90	0
57	MG	BA	3627	1/1	0.97	0.21	56,56,56,56	0
57	MG	AA	1668	1/1	0.97	0.10	63,63,63,63	0
57	MG	CA	3133	1/1	0.97	0.17	82,82,82,82	0
57	MG	BA	3635	1/1	0.97	0.12	42,42,42,42	0
57	MG	BV	203	1/1	0.97	0.21	23,23,23,23	0
57	MG	BU	203	1/1	0.97	0.31	34,34,34,34	0
57	MG	CA	3118	1/1	0.97	0.18	60,60,60,60	0
57	MG	DA	3334	1/1	0.97	0.22	57,57,57,57	0
57	MG	BA	3311	1/1	0.97	0.19	56,56,56,56	0
57	MG	DA	3436	1/1	0.97	0.11	35,35,35,35	0
57	MG	DA	3229	1/1	0.97	0.12	38,38,38,38	0
57	MG	AA	1809	1/1	0.97	0.17	42,42,42,42	0
57	MG	DA	3654	1/1	0.97	0.19	35,35,35,35	0
57	MG	BA	3413	1/1	0.97	0.17	37,37,37,37	0
57	MG	BA	3072	1/1	0.97	0.24	49,49,49,49	0
57	MG	AA	1665	1/1	0.97	0.16	55,55,55,55	0
57	MG	BA	3494	1/1	0.97	0.11	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	3424	1/1	0.97	0.29	31,31,31,31	0
57	MG	BA	3777	1/1	0.97	0.10	41,41,41,41	0
57	MG	DA	3007	1/1	0.97	0.13	30,30,30,30	0
57	MG	DA	3005	1/1	0.97	0.16	54,54,54,54	0
57	MG	DA	3537	1/1	0.97	0.16	45,45,45,45	0
57	MG	BA	3586	1/1	0.97	0.11	55,55,55,55	0
57	MG	BA	3391	1/1	0.97	0.15	41,41,41,41	0
59	ZN	D9	501	1/1	0.97	0.12	64,64,64,64	0
57	MG	BA	3370	1/1	0.97	0.24	50,50,50,50	0
57	MG	DA	3169	1/1	0.97	0.28	41,41,41,41	0
57	MG	BA	3603	1/1	0.97	0.28	42,42,42,42	0
57	MG	BA	3393	1/1	0.97	0.20	23,23,23,23	0
57	MG	BA	3227	1/1	0.97	0.17	33,33,33,33	0
57	MG	DA	3321	1/1	0.97	0.15	29,29,29,29	0
57	MG	BA	3547	1/1	0.97	0.16	45,45,45,45	0
57	MG	BA	3639	1/1	0.97	0.18	49,49,49,49	0
57	MG	BA	3162	1/1	0.97	0.29	41,41,41,41	0
57	MG	DA	3655	1/1	0.97	0.08	38,38,38,38	0
57	MG	BA	3089	1/1	0.97	0.19	36,36,36,36	0
57	MG	BD	3004	1/1	0.97	0.20	28,28,28,28	0
57	MG	AA	1735	1/1	0.97	0.12	45,45,45,45	0
57	MG	DA	3518	1/1	0.97	0.10	56,56,56,56	0
57	MG	BA	3576	1/1	0.97	0.24	30,30,30,30	0
57	MG	AU	101	1/1	0.97	0.12	56,56,56,56	0
57	MG	BA	3630	1/1	0.97	0.25	39,39,39,39	0
57	MG	DA	3319	1/1	0.97	0.14	33,33,33,33	0
57	MG	BA	3463	1/1	0.97	0.21	56,56,56,56	0
57	MG	DA	3182	1/1	0.97	0.21	52,52,52,52	0
57	MG	BA	3133	1/1	0.97	0.27	37,37,37,37	0
59	ZN	D6	501	1/1	0.97	0.18	65,65,65,65	0
57	MG	BA	3007	1/1	0.97	0.23	21,21,21,21	0
57	MG	BA	3054	1/1	0.97	0.22	30,30,30,30	0
57	MG	DA	3440	1/1	0.97	0.13	36,36,36,36	0
57	MG	BA	3698	1/1	0.97	0.11	47,47,47,47	0
57	MG	DA	3353	1/1	0.97	0.13	47,47,47,47	0
57	MG	BA	3342	1/1	0.97	0.29	67,67,67,67	0
57	MG	CA	3167	1/1	0.97	0.30	57,57,57,57	0
57	MG	DA	3027	1/1	0.97	0.53	43,43,43,43	0
57	MG	BA	3674	1/1	0.97	0.34	48,48,48,48	0
57	MG	BA	3033	1/1	0.97	0.40	31,31,31,31	0
57	MG	DA	3340	1/1	0.97	0.14	27,27,27,27	0
57	MG	BA	3559	1/1	0.97	0.22	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	3489	1/1	0.97	0.09	48,48,48,48	0
59	ZN	AN	501	1/1	0.97	0.16	77,77,77,77	0
57	MG	DA	3428	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3605	1/1	0.97	0.18	47,47,47,47	0
57	MG	BD	3010	1/1	0.97	0.20	46,46,46,46	0
57	MG	BA	3344	1/1	0.97	0.10	71,71,71,71	0
57	MG	DA	3262	1/1	0.97	0.13	20,20,20,20	0
57	MG	DA	3014	1/1	0.97	0.22	44,44,44,44	0
57	MG	DA	3297	1/1	0.98	0.18	51,51,51,51	0
57	MG	BA	3368	1/1	0.98	0.24	32,32,32,32	0
57	MG	DA	3521	1/1	0.98	0.09	57,57,57,57	0
57	MG	BA	3533	1/1	0.98	0.18	23,23,23,23	0
57	MG	BA	3772	1/1	0.98	0.15	36,36,36,36	0
58	SF4	AD	501	8/8	0.98	0.15	59,68,73,79	0
57	MG	BA	3813	1/1	0.98	0.13	29,29,29,29	0
57	MG	DA	3178	1/1	0.98	0.17	40,40,40,40	0
57	MG	BA	3146	1/1	0.98	0.17	41,41,41,41	0
57	MG	DA	3584	1/1	0.98	0.09	31,31,31,31	0
57	MG	DA	3547	1/1	0.98	0.08	48,48,48,48	0
57	MG	DE	3001	1/1	0.98	0.44	31,31,31,31	0
57	MG	DA	3300	1/1	0.98	0.10	38,38,38,38	0
57	MG	BA	3182	1/1	0.98	0.67	52,52,52,52	0
57	MG	BA	3425	1/1	0.98	0.25	48,48,48,48	0
57	MG	DA	3013	1/1	0.98	0.13	39,39,39,39	0
57	MG	BB	3002	1/1	0.98	0.28	55,55,55,55	0
57	MG	BA	3467	1/1	0.98	0.13	46,46,46,46	0
57	MG	BA	3779	1/1	0.98	0.19	17,17,17,17	0
57	MG	DA	3581	1/1	0.98	0.07	44,44,44,44	0
57	MG	AA	1732	1/1	0.98	0.20	63,63,63,63	0
57	MG	AA	1792	1/1	0.98	0.12	47,47,47,47	0
57	MG	BA	3312	1/1	0.98	0.19	31,31,31,31	0
57	MG	BA	3382	1/1	0.98	0.12	55,55,55,55	0
57	MG	DA	3477	1/1	0.98	0.11	53,53,53,53	0
57	MG	AA	1730	1/1	0.98	0.25	27,27,27,27	0
57	MG	DA	3093	1/1	0.98	0.13	47,47,47,47	0
57	MG	DA	3453	1/1	0.98	0.17	54,54,54,54	0
57	MG	DA	3615	1/1	0.98	0.09	62,62,62,62	0
57	MG	BA	3701	1/1	0.98	0.23	39,39,39,39	0
58	SF4	CD	501	8/8	0.98	0.14	64,67,74,91	0
57	MG	DA	3085	1/1	0.98	0.18	28,28,28,28	0
57	MG	BD	3002	1/1	0.98	0.21	28,28,28,28	0
57	MG	CA	3163	1/1	0.98	0.19	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	3054	1/1	0.98	0.10	27,27,27,27	0
57	MG	AA	1702	1/1	0.98	0.27	47,47,47,47	0
57	MG	DA	3163	1/1	0.98	0.21	34,34,34,34	0
57	MG	BA	3472	1/1	0.98	0.20	24,24,24,24	0
57	MG	DA	3217	1/1	0.98	0.24	57,57,57,57	0
57	MG	DA	3050	1/1	0.98	0.25	44,44,44,44	0
57	MG	AA	1677	1/1	0.98	0.21	43,43,43,43	0
57	MG	DA	3408	1/1	0.98	0.23	55,55,55,55	0
57	MG	DA	3168	1/1	0.98	0.12	44,44,44,44	0
57	MG	AA	1796	1/1	0.98	0.07	64,64,64,64	0
57	MG	DA	3025	1/1	0.98	0.45	47,47,47,47	0
57	MG	AA	1795	1/1	0.98	0.12	55,55,55,55	0
57	MG	BA	3326	1/1	0.98	0.15	24,24,24,24	0
57	MG	BA	3750	1/1	0.98	0.22	46,46,46,46	0
57	MG	DA	3195	1/1	0.98	0.13	42,42,42,42	0
57	MG	DA	3447	1/1	0.98	0.16	59,59,59,59	0
57	MG	DA	3597	1/1	0.98	0.15	48,48,48,48	0
57	MG	DA	3188	1/1	0.98	0.24	35,35,35,35	0
57	MG	AA	1740	1/1	0.98	0.17	41,41,41,41	0
57	MG	BA	3782	1/1	0.98	0.16	38,38,38,38	0
57	MG	BA	3075	1/1	0.98	0.20	24,24,24,24	0
57	MG	AA	1722	1/1	0.98	0.18	57,57,57,57	0
57	MG	BA	3371	1/1	0.98	0.10	49,49,49,49	0
57	MG	DA	3373	1/1	0.98	0.09	31,31,31,31	0
57	MG	BA	3751	1/1	0.98	0.23	37,37,37,37	0
57	MG	BA	3020	1/1	0.98	0.21	25,25,25,25	0
57	MG	BA	3259	1/1	0.98	0.18	25,25,25,25	0
57	MG	BA	3267	1/1	0.98	0.30	61,61,61,61	0
57	MG	BA	3173	1/1	0.98	0.28	32,32,32,32	0
57	MG	BD	3009	1/1	0.98	0.16	37,37,37,37	0
57	MG	DO	201	1/1	0.98	0.12	49,49,49,49	0
57	MG	DA	3381	1/1	0.98	0.15	40,40,40,40	0
57	MG	BA	3534	1/1	0.98	0.23	26,26,26,26	0
57	MG	BA	3742	1/1	0.98	0.21	48,48,48,48	0
57	MG	BA	3539	1/1	0.98	0.14	42,42,42,42	0
57	MG	DA	3245	1/1	0.98	0.08	58,58,58,58	0
57	MG	BD	3008	1/1	0.98	0.30	45,45,45,45	0
57	MG	DA	3546	1/1	0.98	0.04	47,47,47,47	0
57	MG	DA	3599	1/1	0.98	0.09	48,48,48,48	0
57	MG	BA	3793	1/1	0.98	0.22	11,11,11,11	0
57	MG	CA	3104	1/1	0.98	0.23	37,37,37,37	0
57	MG	BA	3719	1/1	0.98	0.20	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	BU	204	1/1	0.98	0.31	47,47,47,47	0
57	MG	AA	1720	1/1	0.98	0.19	55,55,55,55	0
57	MG	AA	1718	1/1	0.98	0.11	66,66,66,66	0
57	MG	BA	3039	1/1	0.98	0.19	36,36,36,36	0
57	MG	CA	3145	1/1	0.98	0.12	65,65,65,65	0
57	MG	BA	3457	1/1	0.98	0.19	48,48,48,48	0
57	MG	DA	3562	1/1	0.98	0.12	31,31,31,31	0
57	MG	DA	3103	1/1	0.98	0.22	56,56,56,56	0
57	MG	BA	3591	1/1	0.98	0.39	41,41,41,41	0
57	MG	CA	3067	1/1	0.98	0.24	46,46,46,46	0
57	MG	DA	3274	1/1	0.98	0.22	40,40,40,40	0
57	MG	BA	3189	1/1	0.98	0.22	39,39,39,39	0
57	MG	DA	3632	1/1	0.98	0.17	52,52,52,52	0
57	MG	AA	1724	1/1	0.98	0.17	39,39,39,39	0
57	MG	BA	3739	1/1	0.98	0.11	21,21,21,21	0
57	MG	BA	3650	1/1	0.98	0.17	45,45,45,45	0
57	MG	BA	3488	1/1	0.98	0.13	20,20,20,20	0
57	MG	DA	3345	1/1	0.98	0.15	58,58,58,58	0
57	MG	AA	1762	1/1	0.98	0.21	66,66,66,66	0
57	MG	DA	3020	1/1	0.98	0.12	26,26,26,26	0
57	MG	DA	3469	1/1	0.98	0.07	50,50,50,50	0
57	MG	BA	3339	1/1	0.98	0.21	43,43,43,43	0
57	MG	BA	3114	1/1	0.98	0.20	39,39,39,39	0
57	MG	AA	1761	1/1	0.98	0.20	70,70,70,70	0
57	MG	BA	3345	1/1	0.98	0.19	51,51,51,51	0
57	MG	BA	3665	1/1	0.98	0.17	42,42,42,42	0
57	MG	BF	305	1/1	0.98	0.14	36,36,36,36	0
57	MG	BA	3067	1/1	0.98	0.21	43,43,43,43	0
57	MG	BA	3021	1/1	0.98	0.12	43,43,43,43	0
57	MG	CA	3079	1/1	0.98	0.12	49,49,49,49	0
57	MG	BA	3811	1/1	0.98	0.21	48,48,48,48	0
57	MG	CA	3080	1/1	0.98	0.10	49,49,49,49	0
57	MG	DB	3013	1/1	0.99	0.12	66,66,66,66	0
57	MG	CA	3092	1/1	0.99	0.24	51,51,51,51	0
57	MG	BA	3104	1/1	0.99	0.19	24,24,24,24	0
59	ZN	D5	501	1/1	0.99	0.19	57,57,57,57	0
57	MG	DA	3355	1/1	0.99	0.11	43,43,43,43	0
57	MG	BA	3551	1/1	0.99	0.15	44,44,44,44	0
57	MG	BA	3718	1/1	0.99	0.17	47,47,47,47	0
57	MG	BA	3085	1/1	0.99	0.29	31,31,31,31	0
57	MG	BA	3583	1/1	0.99	0.15	33,33,33,33	0
57	MG	DA	3398	1/1	0.99	0.08	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	CA	3085	1/1	0.99	0.15	41,41,41,41	0
57	MG	AA	1772	1/1	0.99	0.20	47,47,47,47	0
57	MG	BA	3476	1/1	0.99	0.16	48,48,48,48	0
57	MG	BV	205	1/1	0.99	0.12	34,34,34,34	0
57	MG	AA	1770	1/1	0.99	0.13	51,51,51,51	0
57	MG	DA	3392	1/1	0.99	0.19	53,53,53,53	0
57	MG	BA	3731	1/1	0.99	0.14	32,32,32,32	0
59	ZN	B6	102	1/1	0.99	0.26	50,50,50,50	0
57	MG	AA	1758	1/1	0.99	0.09	37,37,37,37	0
57	MG	BA	3800	1/1	0.99	0.19	29,29,29,29	0
57	MG	DA	3472	1/1	0.99	0.14	25,25,25,25	0
57	MG	AA	1678	1/1	0.99	0.25	47,47,47,47	0
57	MG	CA	3010	1/1	0.99	0.10	49,49,49,49	0
57	MG	CA	3044	1/1	0.99	0.16	47,47,47,47	0
57	MG	BA	3310	1/1	0.99	0.23	26,26,26,26	0
57	MG	B5	101	1/1	0.99	0.27	30,30,30,30	0
57	MG	DA	3209	1/1	0.99	0.09	49,49,49,49	0
59	ZN	B5	103	1/1	0.99	0.21	40,40,40,40	0
57	MG	DA	3383	1/1	0.99	0.13	28,28,28,28	0
57	MG	AA	1681	1/1	0.99	0.12	38,38,38,38	0
57	MG	BD	3006	1/1	0.99	0.09	34,34,34,34	0
57	MG	BA	3417	1/1	0.99	0.21	24,24,24,24	0
57	MG	BA	3707	1/1	0.99	0.19	39,39,39,39	0
57	MG	BA	3499	1/1	0.99	0.13	39,39,39,39	0
57	MG	AA	1672	1/1	0.99	0.17	45,45,45,45	0
57	MG	BA	3582	1/1	0.99	0.12	31,31,31,31	0
57	MG	DA	3412	1/1	0.99	0.14	41,41,41,41	0
57	MG	BA	3003	1/1	0.99	0.17	33,33,33,33	0
59	ZN	B9	501	1/1	1.00	0.23	49,49,49,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.