



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 12:34 am BST

PDB ID : 1VY5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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

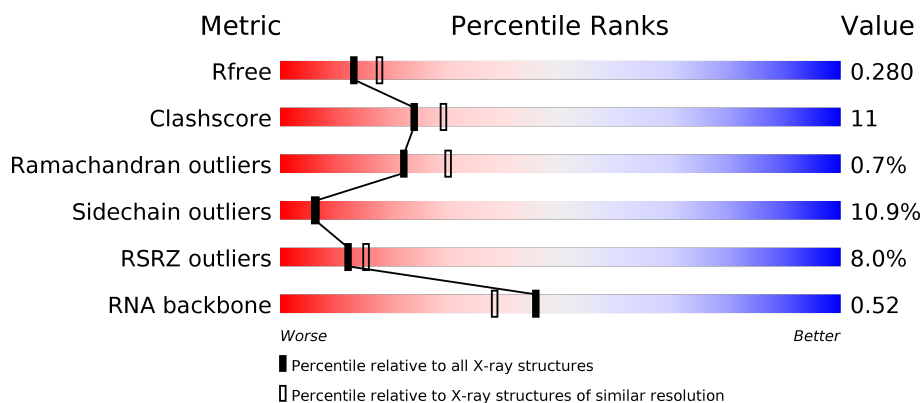
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>2%</div> <div>52% 37% 9%</div> </div>
1	CA	1521	<div> <div>4%</div> <div>45% 42% 10%</div> </div>
2	AB	256	<div> <div>12%</div> <div>42% 41% 6% 10%</div> </div>
2	CB	256	<div> <div>20%</div> <div>36% 43% 11% 10%</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	5MU	CY	54	-	-	-	X
25	PSU	CY	55	-	-	-	X
57	MG	DA	3651	-	-	-	X
57	MG	DD	303	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	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
			1607	727	288	516	73	3			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1560	702	281	503	72	2			

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

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

- Molecule 25 is a RNA chain called 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
			2136	1349	423	361	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			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
			511	328	99	82	2			
55	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	812	Total	Mg	0	0
			812	812		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	4	Total	Mg	0	0
			4	4		
57	D3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DF	4	Total 4	Mg 4	0	0
57	CV	1	Total 1	Mg 1	0	0
57	B8	1	Total 1	Mg 1	0	0
57	BE	8	Total 8	Mg 8	0	0
57	AW	4	Total 4	Mg 4	0	0
57	DU	2	Total 2	Mg 2	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	5	Total 5	Mg 5	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	170	Total 170	Mg 170	0	0
57	B5	1	Total 1	Mg 1	0	0
57	BB	20	Total 20	Mg 20	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	3	Total 3	Mg 3	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	9	Total 9	Mg 9	0	0
57	BX	3	Total 3	Mg 3	0	0
57	B2	1	Total 1	Mg 1	0	0

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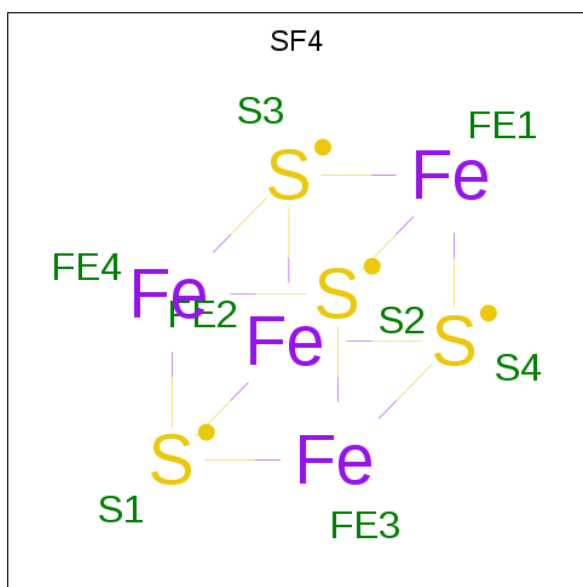
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	214	Total 214	Mg 214	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	3	Total 3	Mg 3	0	0
57	DV	3	Total 3	Mg 3	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	3	Total 3	Mg 3	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	677	Total 677	Mg 677	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	4	Total 4	Mg 4	0	0
57	B7	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	5	Total 5	Mg 5	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	9	Total 9	Mg 9	0	0
57	B0	3	Total 3	Mg 3	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	9	Total 9	Mg 9	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0

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



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	227	Total 227	O 227	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	3	Total 3	O 3	0	0
61	AX	6	Total 6	O 6	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1383	Total 1383	O 1383	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BE	14	Total 14	O 14	0	0
61	BF	8	Total 8	O 8	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	16	Total 16	O 16	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	4	Total 4	O 4	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	3	Total 3	O 3	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CA	185	Total 185	O 185	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	DA	1025	Total 1025	O 1025	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	19	Total 19	O 19	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	3	Total 3	O 3	0	0
61	DN	2	Total 2	O 2	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	16	Total 16	O 16	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	3	Total 3	O 3	0	0
61	DU	2	Total 2	O 2	0	0
61	DX	3	Total 3	O 3	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0

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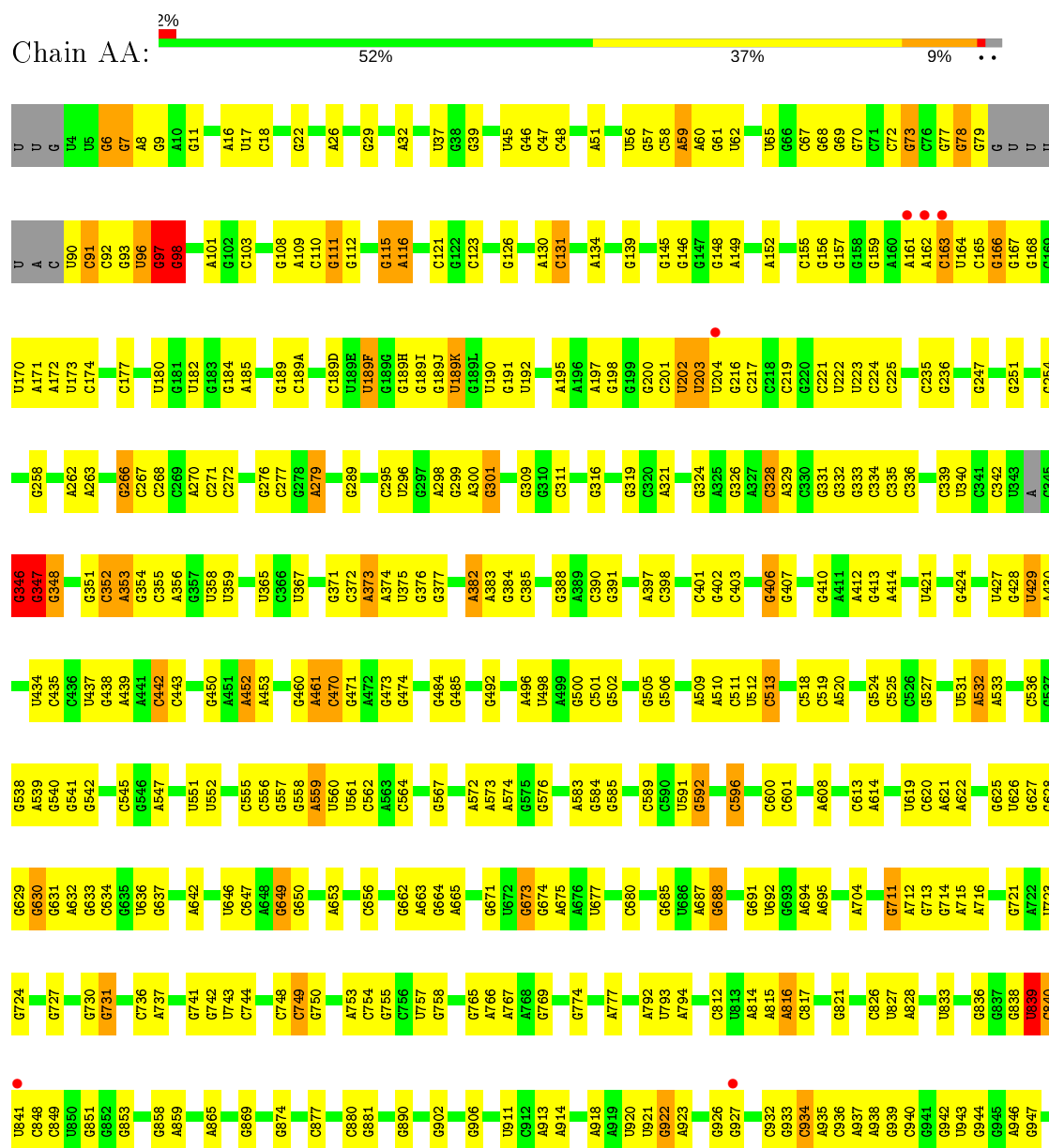
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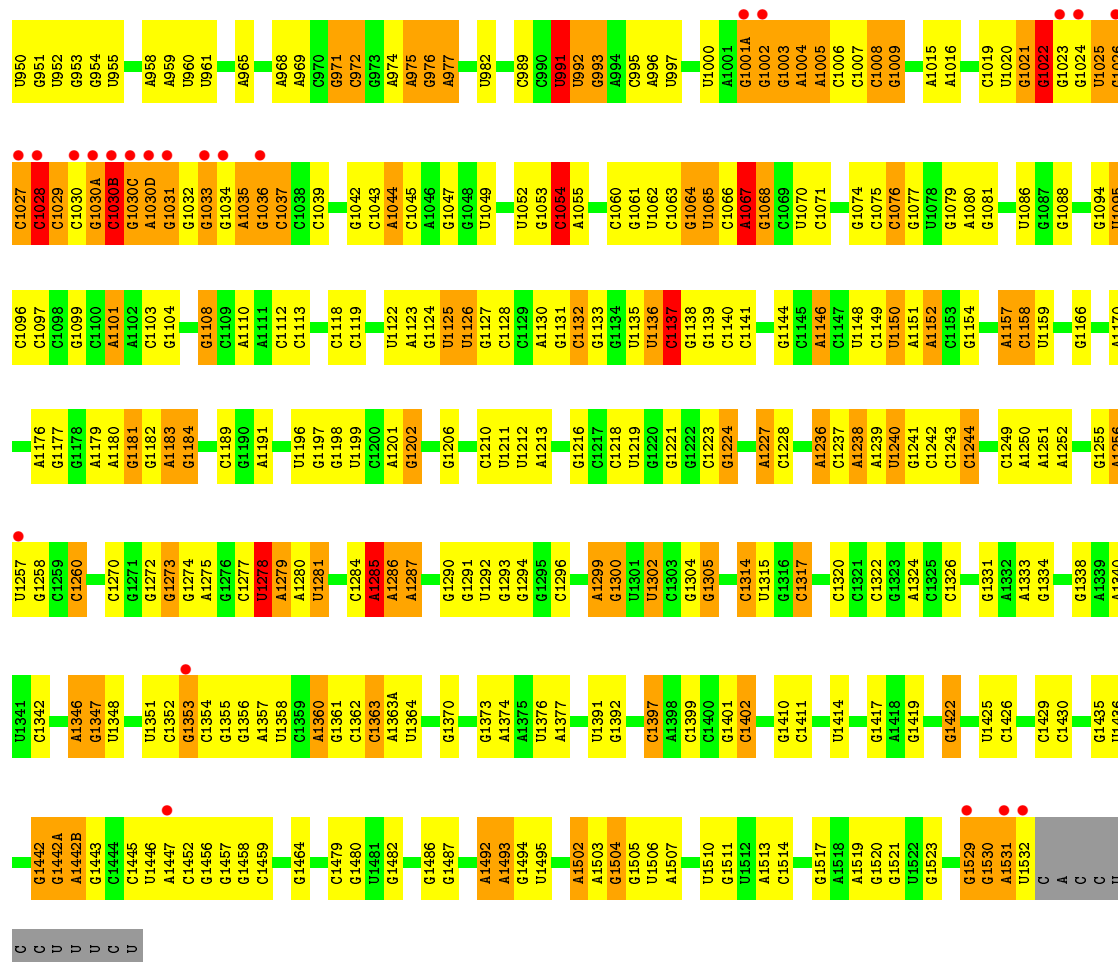
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

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.

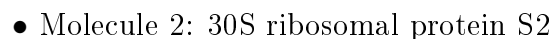
• Molecule 1: 16S Ribosomal RNA



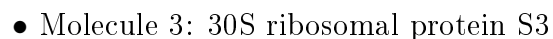


C1514	G1410	G1384	C1262	U1186	G1128	U1062	A1005	A946	U841	A737	C543	A448
G1515	C1411	G1338	C1263	G1197	C1129	C1063	C1006	G947	C848	G741	G544	C449
G1516	C1412	A1339	A1269	G1198	A1130	G1064	C1008	G948	G851	G742	G545	G450
G1517	C1413	A1340	C1270	G1199	G1131	U1065	G1008	A949	G852	G743	G546	A451
A1518	U1414	U1341	G1271	C1200	G1132	C1066	G1010	U950	G853	G744	A547	A452
A1519	G1419	C1342	G1272	A1201	G1134	G1068	G1011	G951	G854	G745	U551	G460
G1520	G1422	G1343	G1273	G1202	U1135	C1203	U1012	U952	C857	G746	U552	A461
G1529	C1423	U1345	A1204	C1203	U1136	U1070	G1013	G953	G858	G747	C556	C470
G1530	C1424	U1346	U1205	A1205	G1137	C1071	A1014	U954	A859	G748	C556	G471
A1531	U1532	G1347	C1277	G1206	G1139	U1073	A1016	U955	A860	G749	U551	G472
C	C	U1348	U1278	U1206	G1140	G1074	G1017	U956	G861	G750	U552	G473
A	C	A1279	U1279	U1206	C1141	C1075	C1018	U957	C866	G751	U560	G474
C	C	A1280	U1280	U1211	G1142	G1076	C1019	A958	C867	G752	U561	G475
C	C	U1281	U1281	U1212	G1143	C1076	U1020	A959	C868	G753	C562	G485
C	C	G1282	G1283	A1213	G1144	U1079	G1021	U960	G869	G754	A572	G485
U	U	C1284	C1284	C1214	C1145	A1080	G1022	U961	G870	G755	A573	C488
C	C	G1285	A1285	G1215	G1146	G1081	G1023	G962	G871	G756	G576	C488
U	U	A1286	A1286	G1216	C1147	U1082	G1024	G963	C874	G757	C576	G492
U	U	A1287	C1217	C1217	U1148	U1083	U1025	A964	C875	G758	U580	A496
U	U	A1288	U1219	C1218	C1149	G1084	G1026	A965	C876	G759	U581	U498
U	U	A1289	U1220	U1219	U1150	U1085	C1027	A966	C879	G760	U582	U499
U	U	A1290	G1221	G1221	A1151	U1086	C1028	A967	C880	G761	A583	G500
U	U	U1291	G1222	G1222	A1152	U1087	C1029	G970	C885	G762	U584	G501
U	U	U1292	C1223	C1223	C1153	G1088	G1030	G971	C886	G763	G587	G502
U	U	G1293	G1224	A1225	G1154	A1092	G1030A	G972	C887	G764	G588	C503
U	U	G1294	A1225	A1225	G1155	A1093	G1030B	G973	C888	G765	G589	C504
U	U	C1297	A1226	C1226	G1156	U1094	A1030C	A974	C889	G766	G592	G505
U	U	C1298	A1227	C1227	A1157	U1095	A1030D	A975	C890	G767	C596	A509
U	U	A1299	C1228	C1228	G1158	U1096	G1031	G976	C891	G768	A607	A510
U	U	G1300	G1231	G1231	U1159	C1097	G1032	A977	C892	G769	A608	C511
U	U	U1301	U1232	U1232	C1162	U1098	G1033	C978	C893	G770	A609	U512
U	U	G1303	G1233	G1233	G1163	C1099	G1034	C979	C894	G771	G610	C513
U	U	G1304	C1234	C1234	G1164	G1101	A1030E	C980	C895	G772	G610	C514
U	U	G1305	U1235	U1235	C1165	A1101	G1037	U981	C896	G773	C620	C518
U	U	G1305	A1236	A1236	G1165	A1102	C1038	U982	C897	G774	G625	G521
U	U	G1312	C1237	C1237	A1169	C1103	C1039	U983	C898	G775	G626	C522
U	U	U1313	A1238	A1238	A1170	G1104	U1040	C984	C899	G776	G627	A523
U	U	C1314	U1239	U1239	G1171	C1104	A1041	A986	C900	G777	G628	C528
U	U	U1315	U1240	U1240	G1172	G1108	G1042	C987	C901	G778	G629	G529
U	U	G1316	G1243	G1243	G1173	C1109	C1043	G988	C902	G779	G630	G530
U	U	C1317	C1244	C1244	G1174	A1110	A1044	C989	C903	G780	G631	U531
U	U	A1318	A1245	A1245	G1175	C1113	G1047	U991	C904	G781	G632	A532
U	U	A1319	C1246	C1246	G1176	C1114	U1048	U992	C905	G782	G633	A533
U	U	C1320	C1247	C1247	G1177	C1115	U1049	G993	C906	G783	G641	U534
U	U	C1321	G1249	G1249	G1178	C1116	G1050	G994	C907	G784	G642	A535
U	U	C1322	A1250	A1250	A1179	C1117	C1051	C995	C908	G785	G643	C536
U	U	G1323	A1251	A1251	A1180	G1118	U1052	C996	C909	G786	G644	C537
U	U	A1324	A1252	A1252	G1181	C1119	G1053	U997	C910	G787	G645	G538
U	U	C1325	G1255	G1255	A1182	G1120	C1054	U998	C911	G788	G646	A539
U	U	C1326	G1256	G1256	A1183	U1121	A1055	C999	C912	G789	G647	G540
U	U	C1327	A1256	A1256	G1184	U1122	U1056	C999	C913	G790	A648	G541
U	U	C1328	U1257	U1257	G1185	A1123	G1057	U1000	C914	G791	G650	G542
U	U	C1331	G1258	G1258	G1186	G1124	G1058	A1001	C915	G792	G651	G543
U	U	A1332	C1259	C1259	G1190	U1125	C1059	G1002	C916	G793	G652	G544
U	U	A1333	U1260	U1260	A1191	U1126	C1060	G1003	C917	G794	G653	G545
U	U		A1261	A1261	C1192	G1127	G1061	A1004	C918	G795	G654	G546

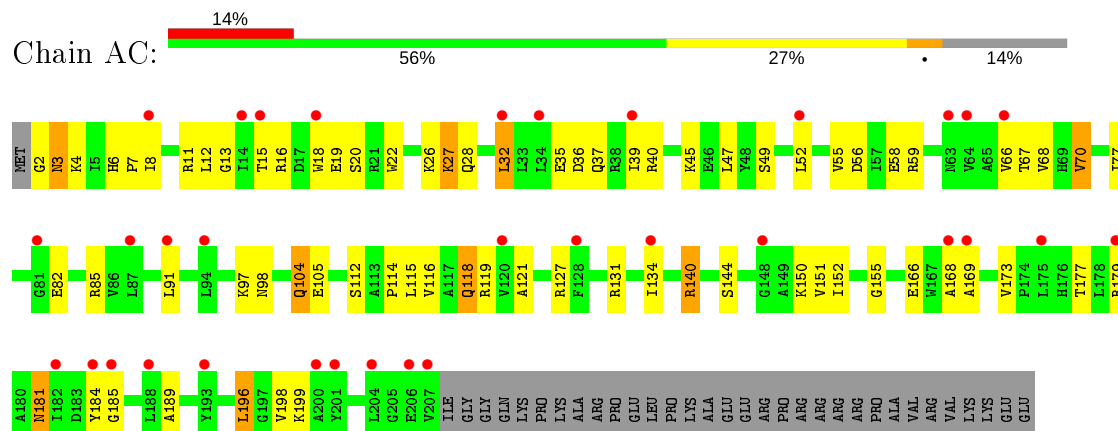
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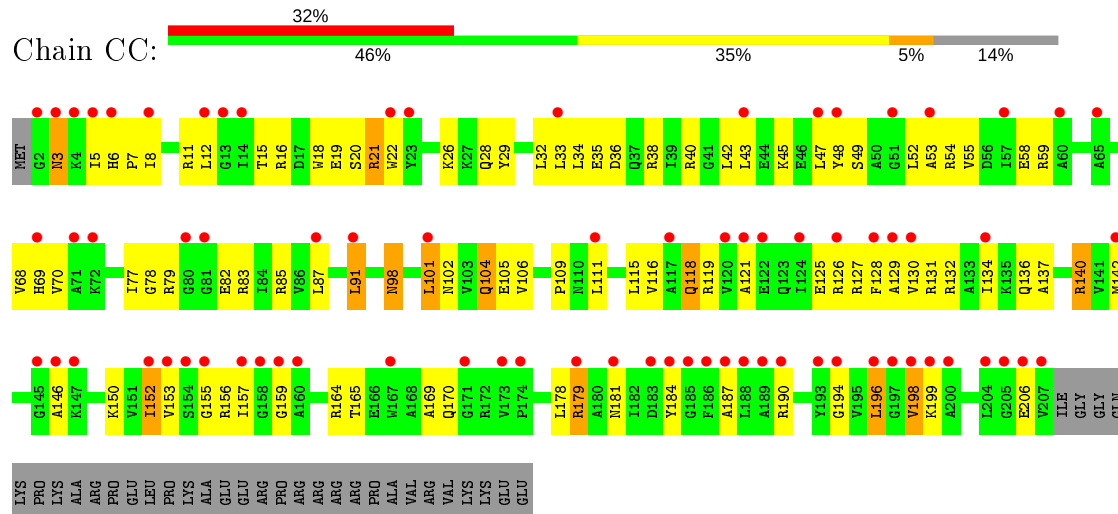
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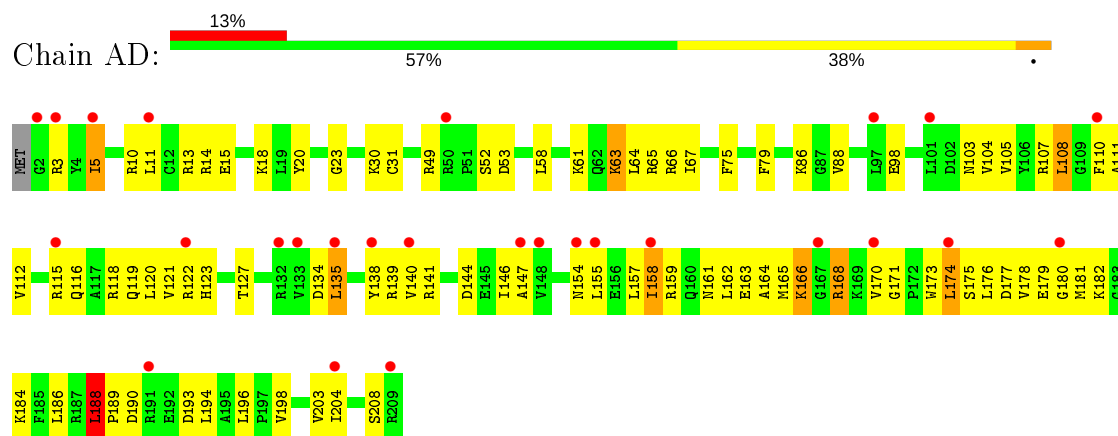
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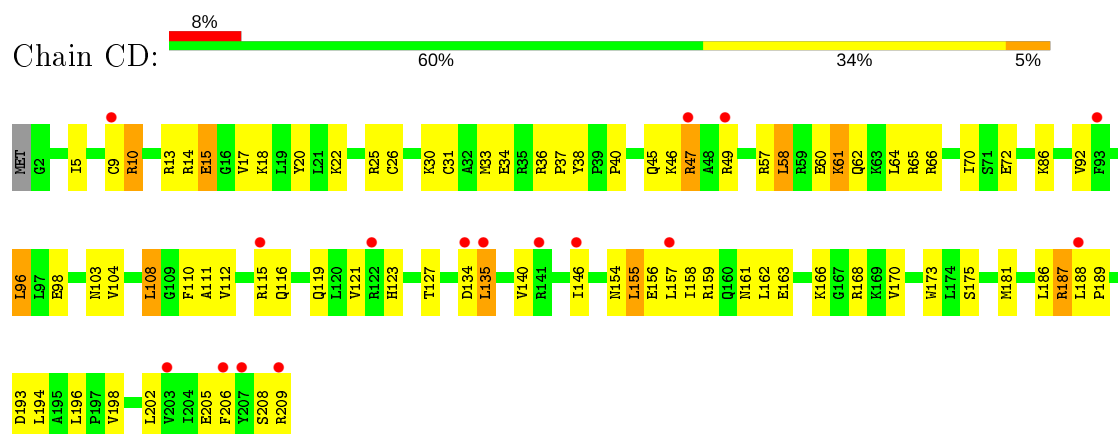
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

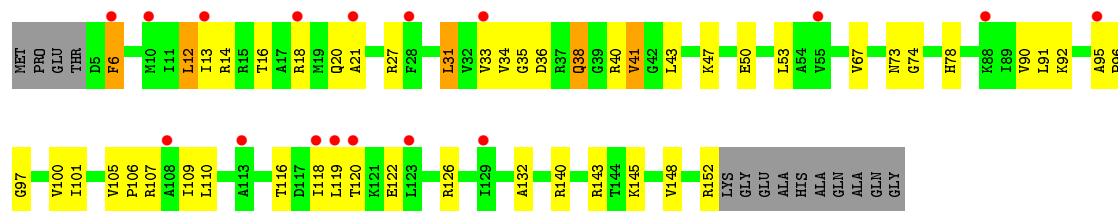


- Molecule 4: 30S ribosomal protein S4

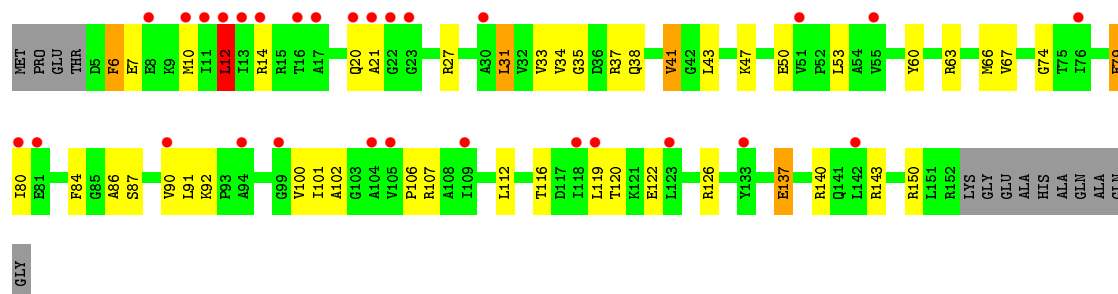


- Molecule 5: 30S ribosomal protein S5

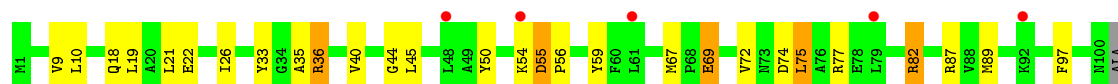
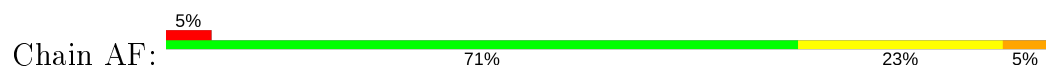




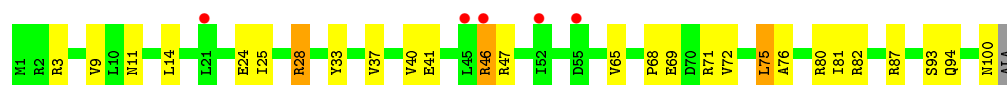
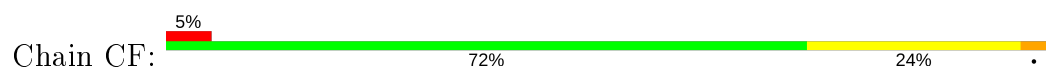
• Molecule 5: 30S ribosomal protein S5



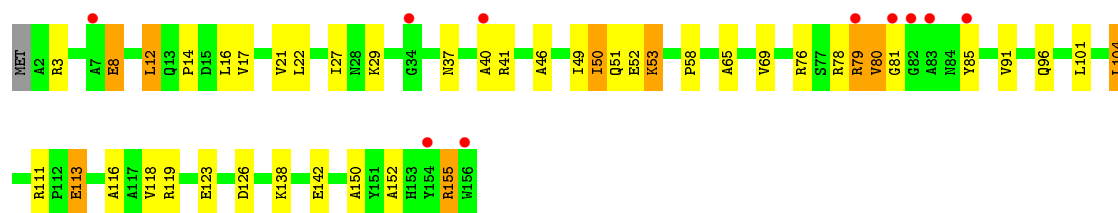
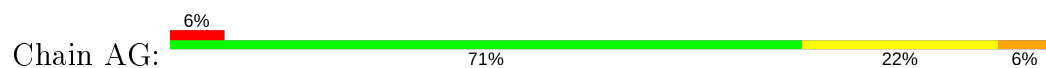
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

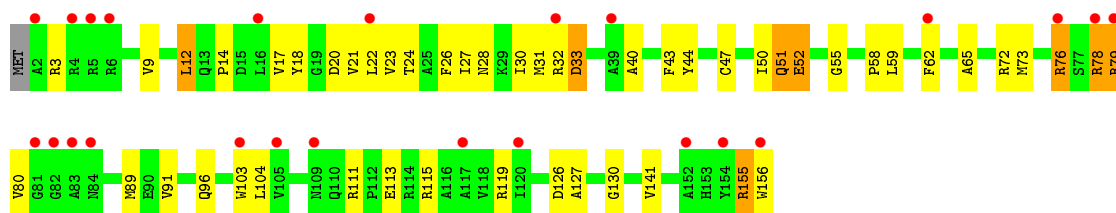


• Molecule 7: 30S ribosomal protein S7

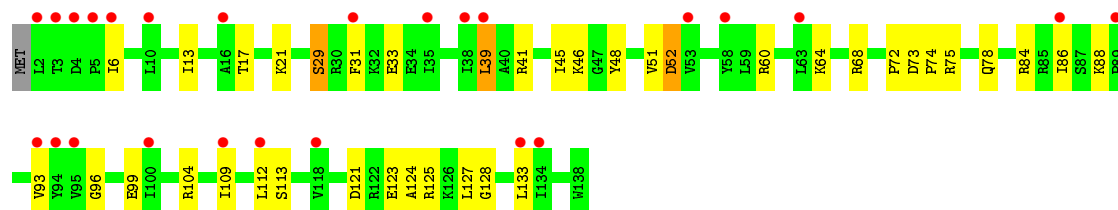
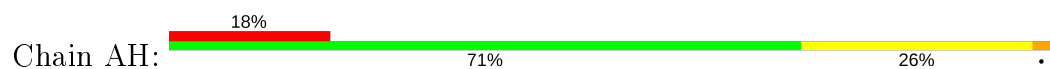


• Molecule 7: 30S ribosomal protein S7

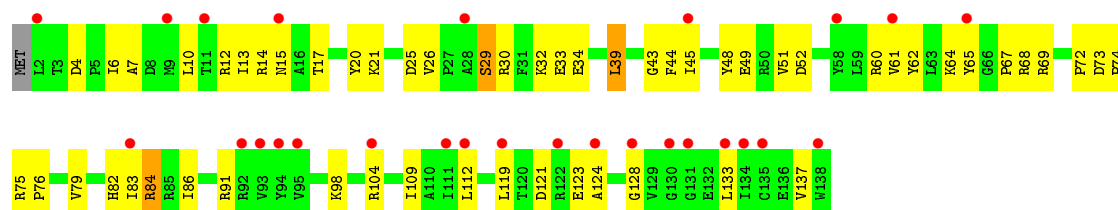




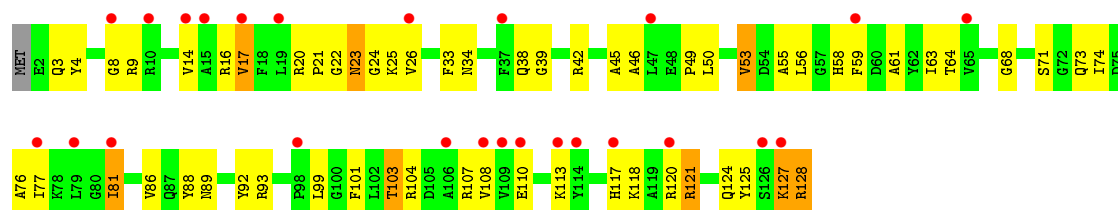
• Molecule 8: 30S ribosomal protein S8



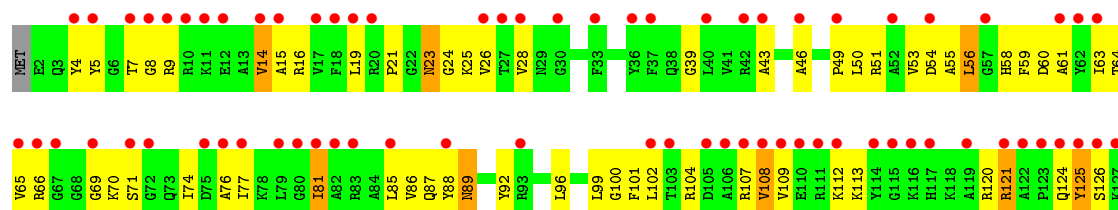
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

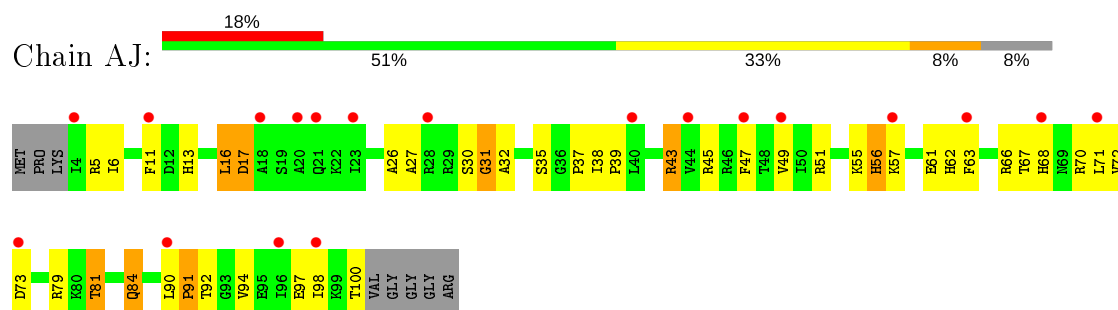


• Molecule 9: 30S ribosomal protein S9

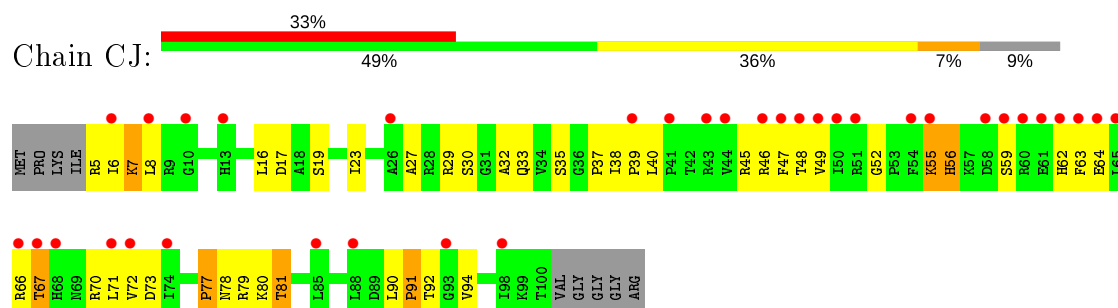




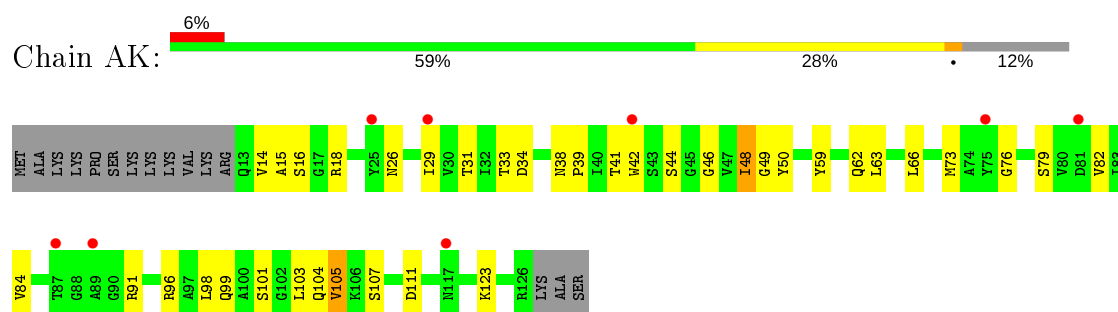
- Molecule 10: 30S ribosomal protein S10



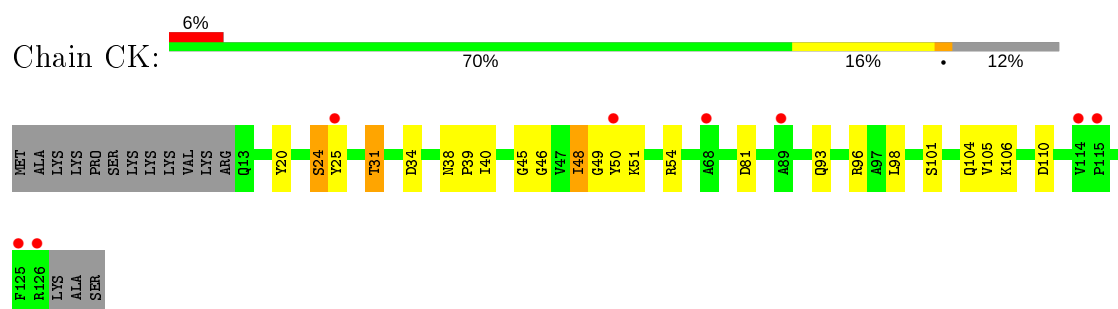
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

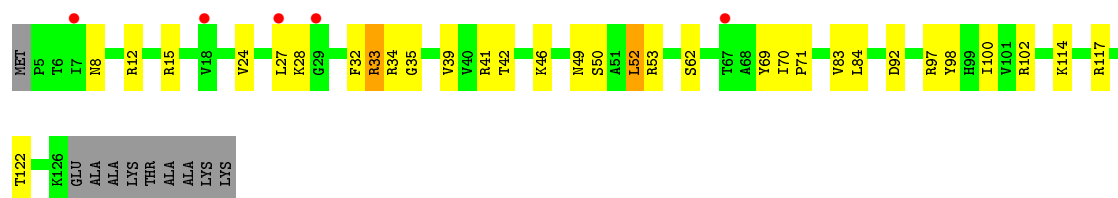


- Molecule 11: 30S ribosomal protein S11

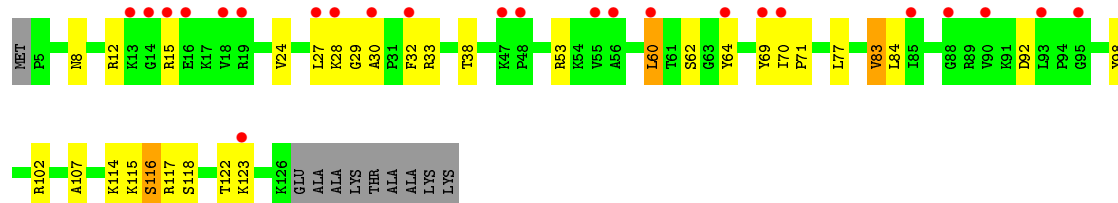


- Molecule 12: 30S ribosomal protein S12

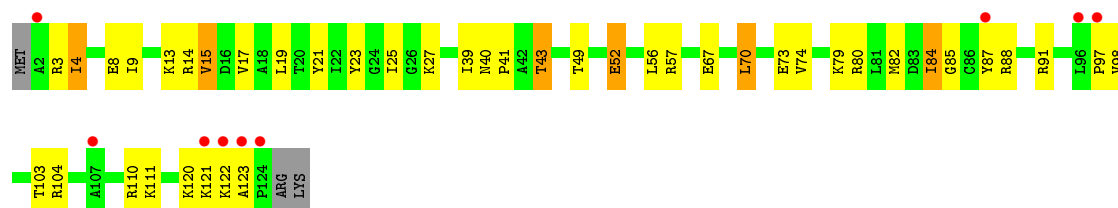




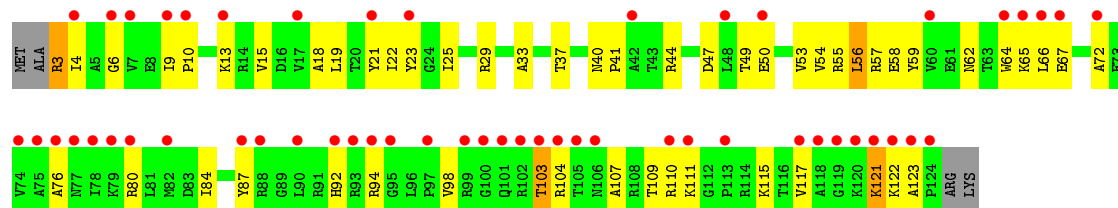
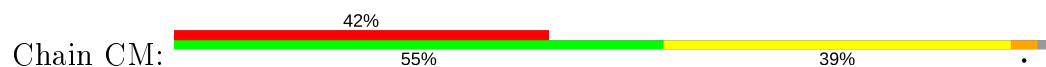
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

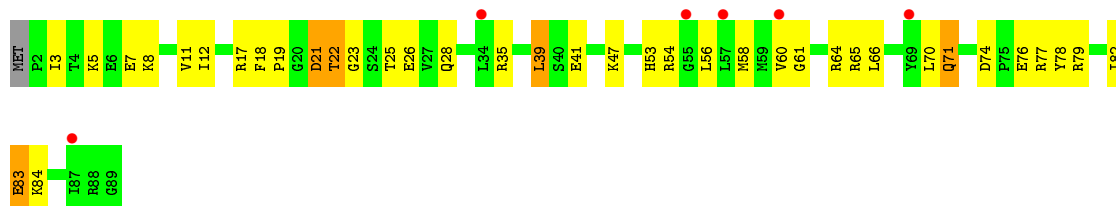


- Molecule 14: 30S ribosomal protein S14 type Z

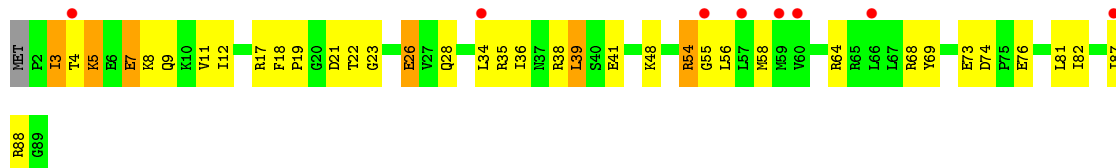




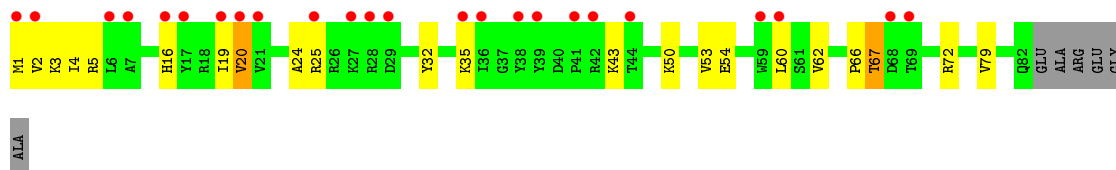
- Molecule 15: 30S ribosomal protein S15



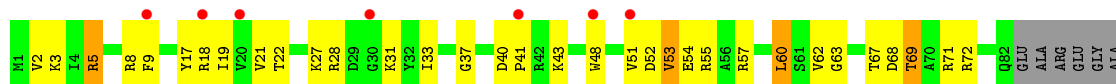
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

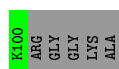


- Molecule 16: 30S ribosomal protein S16

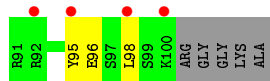
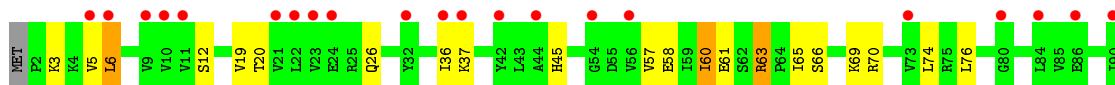
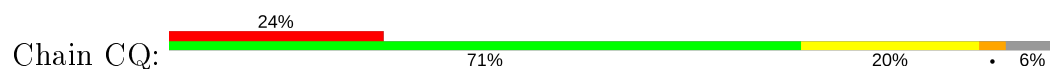


- Molecule 17: 30S ribosomal protein S17

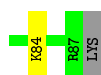
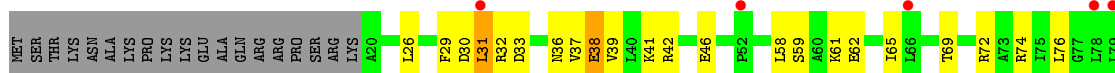




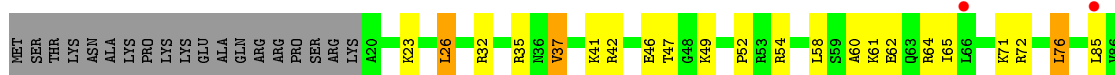
- Molecule 17: 30S ribosomal protein S17



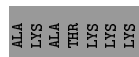
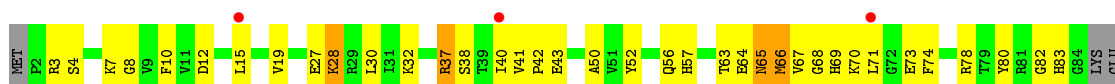
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

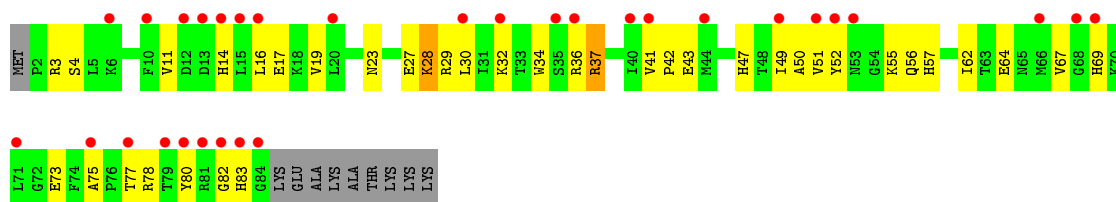


- Molecule 19: 30S ribosomal protein S19

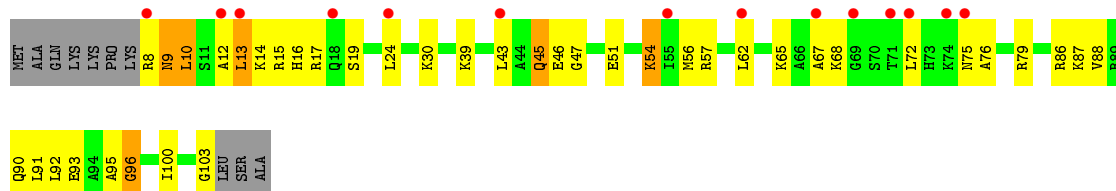


- Molecule 19: 30S ribosomal protein S19

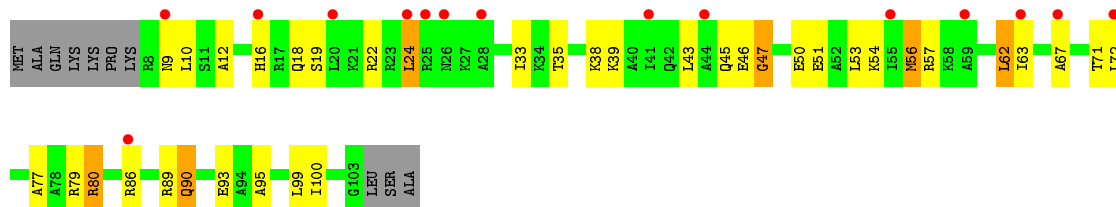




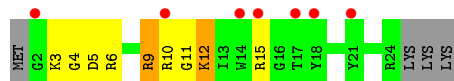
- Molecule 20: 30S ribosomal protein S20



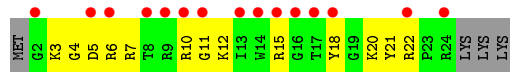
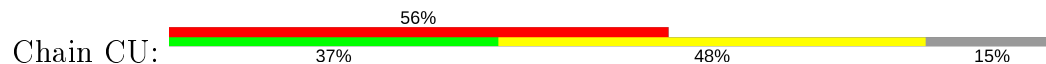
- Molecule 20: 30S ribosomal protein S20



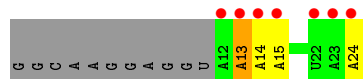
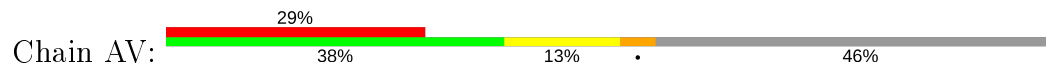
- Molecule 21: 30S ribosomal protein Thx



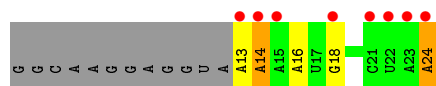
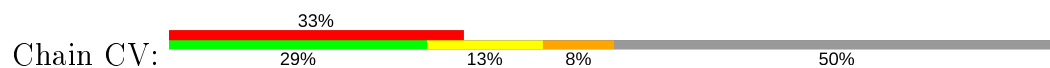
- Molecule 21: 30S ribosomal protein Thx



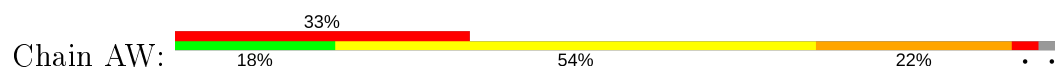
- Molecule 22: mRNA



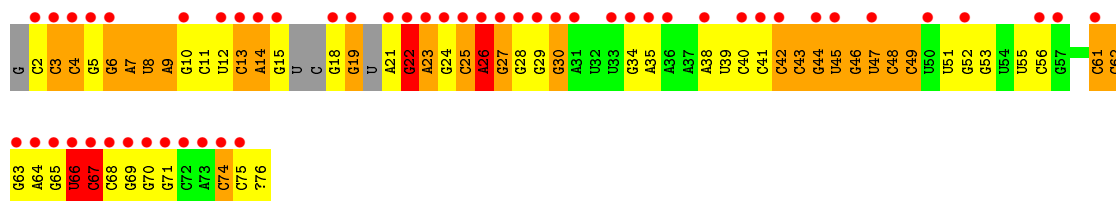
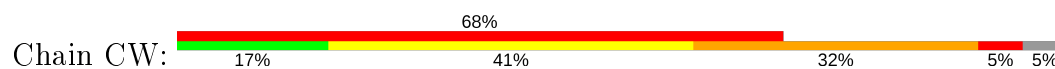
- Molecule 22: mRNA



- Molecule 23: A-site tRNA



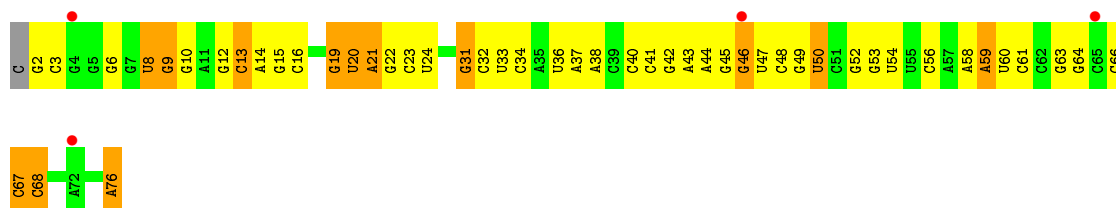
- Molecule 23: A-site tRNA



- Molecule 24: P-site tRNA



- Molecule 24: P-site tRNA

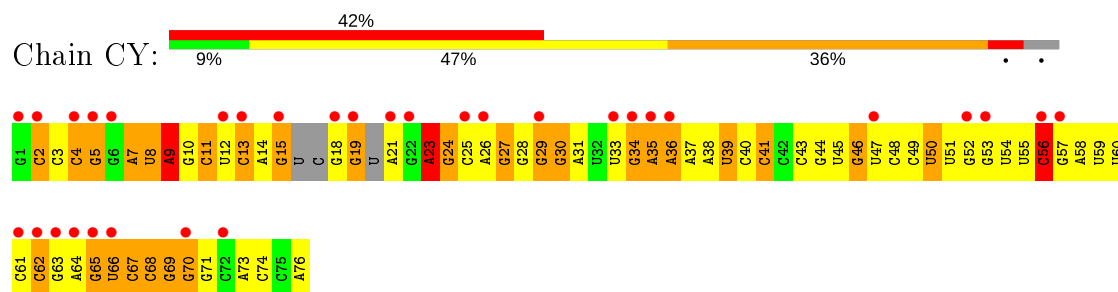


- Molecule 25: E-site tRNA

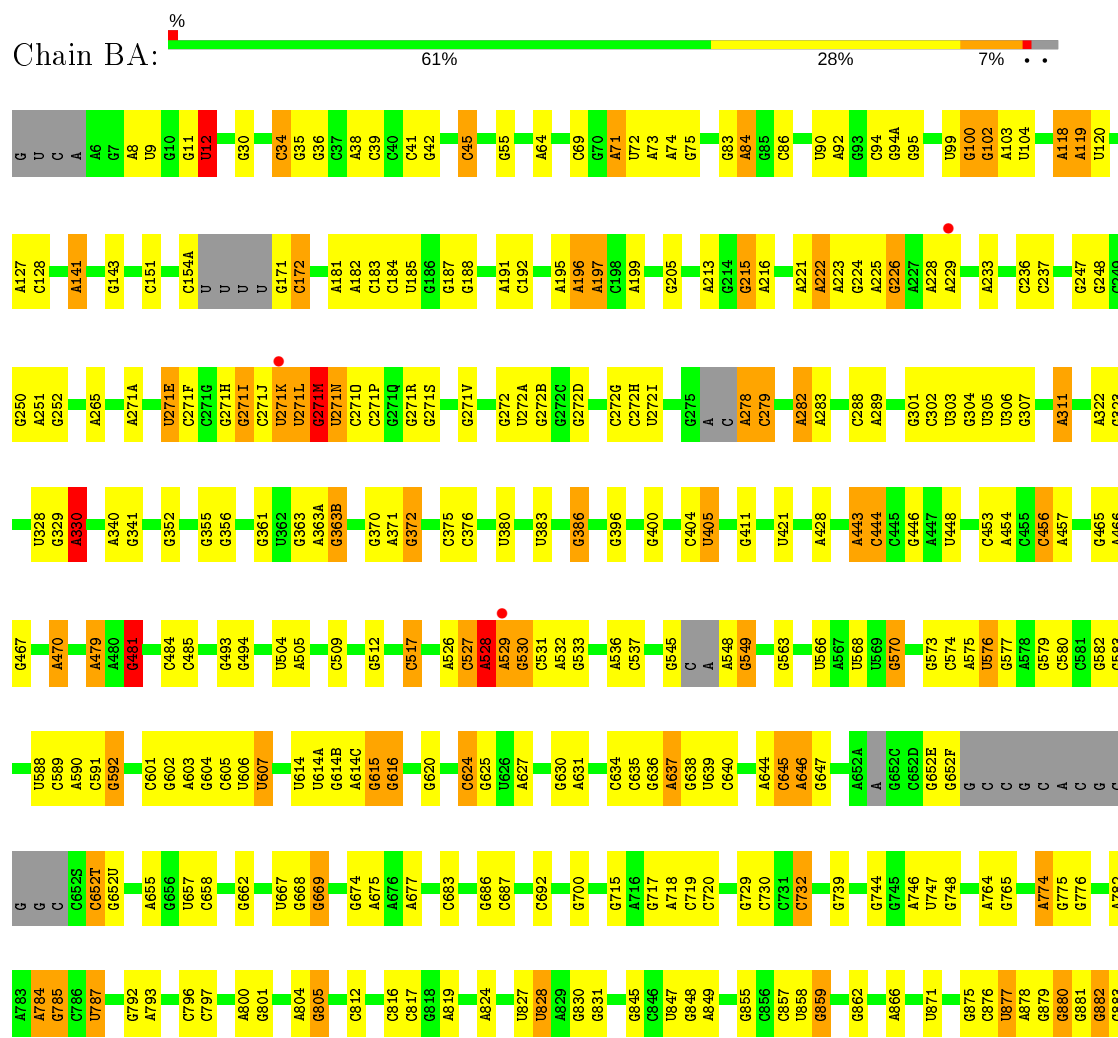




• Molecule 25: E-site tRNA



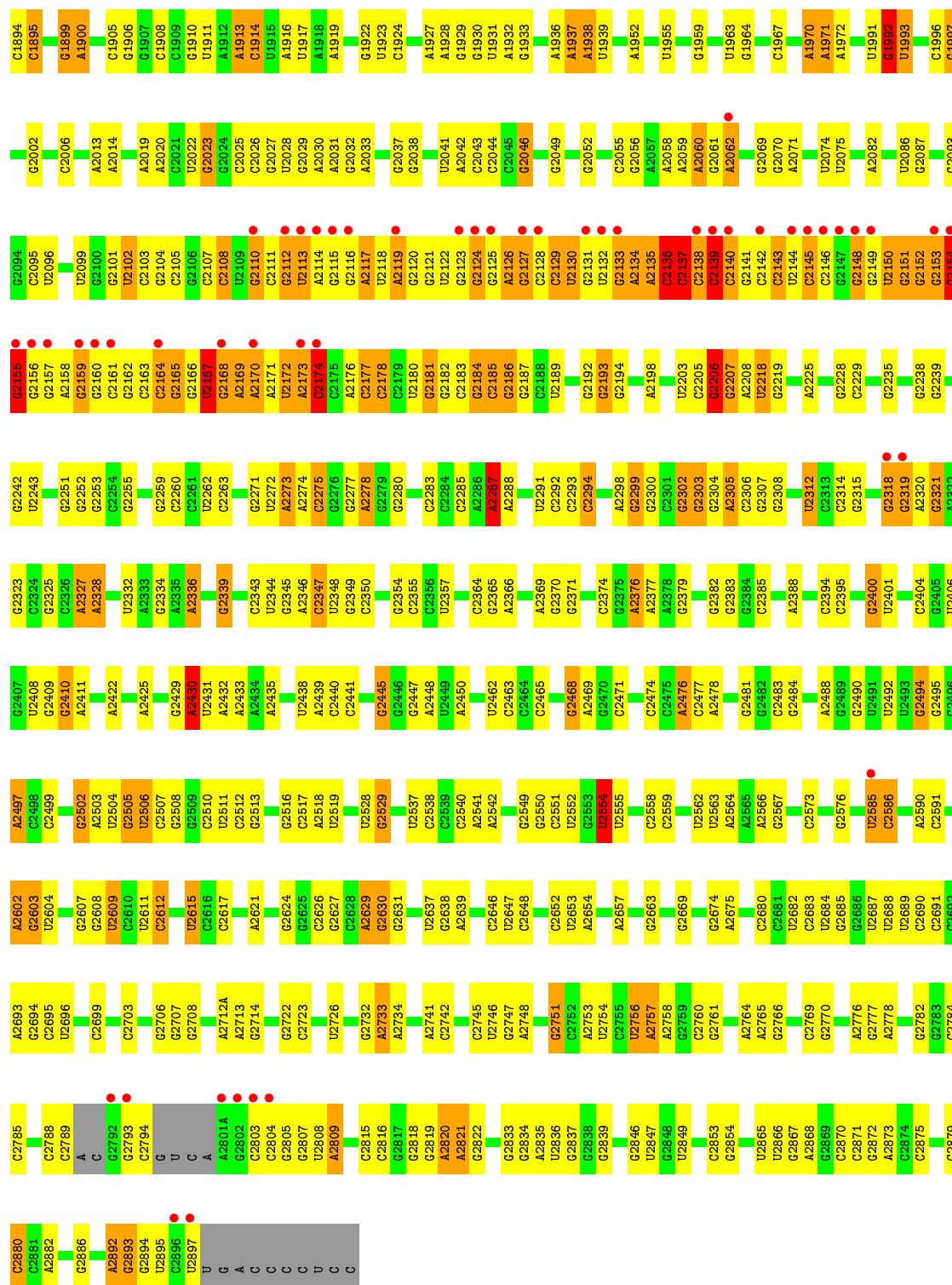
• Molecule 26: 23S Ribosomal RNA



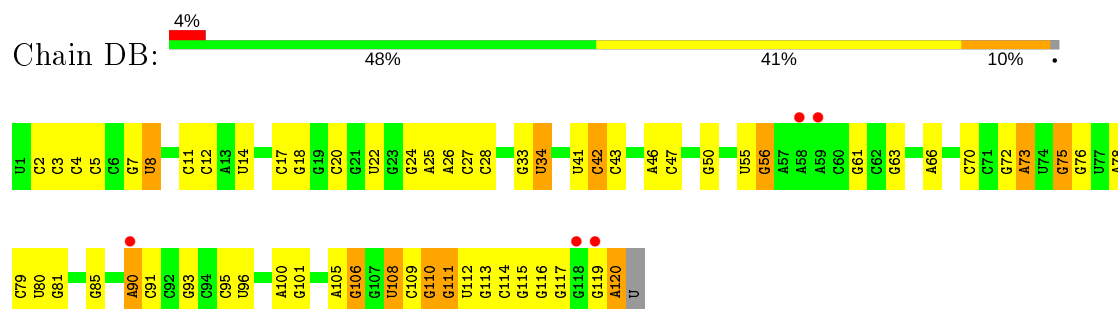
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C2275	C2160	A1848	G1746	A1610	A1494	A1379	A1253	G993	C886
G2276	G2161	A1849	G1747	A1611	A1495	G1380	G1254	C994	A887
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C2283	G2010	G1860	G1751	A1631A	A1508	U1396	G1258	C998	C892
G2284	U2011	G1861	U1752	A1632	C1509	A1403	G1259	A1001	C893
C2285	G2012	G1862	A1753	G1633	A1509A	U1404	U1267	A1002	C894
A2286	A2013	A1876	A1754	A1634	U1512	U1405	A1268	A1009	A896
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G2289	A2114	A1883	G1764	A1641	G1520	C1408	G1271	A1013	A899
G2290	C2020	G1886	A1773	G1642	C1530	G1416	A1272	A1014	A900
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C2292	G2022	A1899	U1775	G1649	C1532	G1418	A1274	A1020	U907
C2293	G2023	G1899	U1776	A1654	U	A1419	U1289	A1021	A910
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G2304	A2032	G1906	A1780	A1665	G1538	G1422	C1293	U1026	U1027
A2305	C2036	A1913	C1781	G1666	G1539	G1423	U1297	A1028	C923
G2308	U2041	A1914	A1782	G1667	U1540	C1428	C1297	A1029	C924
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G2345	U2144	U1938	U1805	G1702	A1577	G1456	G1338	C1052	A953
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A2247	G2151	G1965	G1828	U1714	A1584	A1471	G1135	C	A959
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G2259	G2153	A1970	U1840	G1721	A1586	G1482	G1140	G	C970
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	G2157				A1590				C975



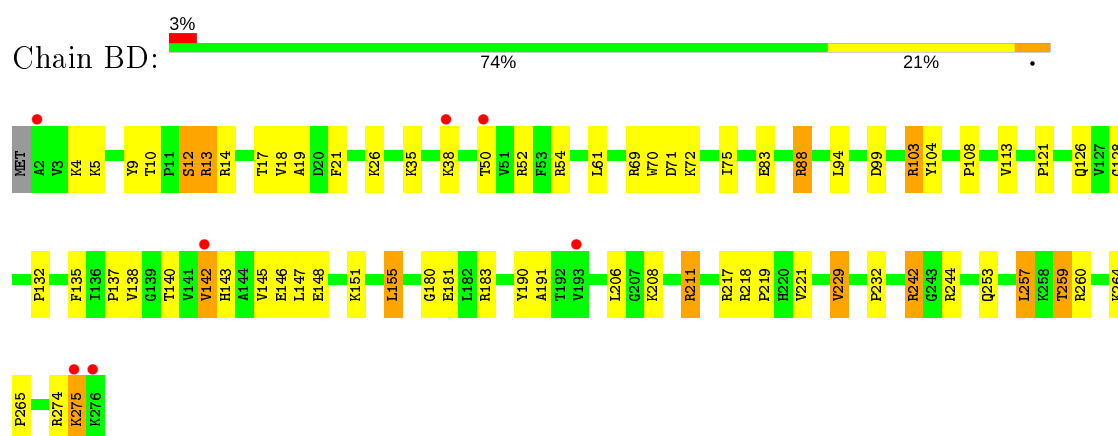
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U1798	C1657	C1547	A1477	U1287	C1288	G1185	G	G974	C883	U813	G726	G641
G1799	C1658	A1547	G1477	A1378	A1289	C1186	A	C975	C894	U814	G727	G642
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A1801	A1669	A1549	G1479	A1380	A1291	U1188	C	A984	C896	C817	C730	C644
A1802	C1670	A1550	A1480	G1381	G1292	A1189	A	A985	C897	C818	C731	C645
A1803	A1671	A1551	A1481	A1382	U1293	A1190	C	G987	C898	A819	G647	A646
C1804	C1672	A1552	G1482	U1383	A1294	G1191	C	A988	A899	A820	A734	G648
U1805	G1673	A1553	A1483	A1384	U1295	G1192	C	G989	A900	A821	G649	A647
G1806	G1674	A1554	A1484	A1385	U1296	U1193	C	A990	A901	U740	U740	G650
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A1836	C1722	A1602	A1514	U1415	U1326	U1223	C	C1019	U855	U773	G773	C
A1837	U1723	A1603	A1515	U1416	U1327	U1224	A	C1020	U856	U774	G774	C
A1838	A1724	A1604	A1516	U1417	U1328	U1225	C	C1021	U857	U775	G775	C
A1839	C1725	A1605	A1517	U1418	U1329	U1226	C	C1022	U858	U776	G776	C
A1840	U1726	A1606	A1518	U1419	U1330	U1227	A	C1023	U859	U777	G777	C
A1841	C1727	A1607	A1519	U1420	U1331	U1228	C	C1024	U860	U778	G778	C
A1842	A1728	A1608	A1520	U1421	U1332	U1229	C	C1025	U861	U779	G779	C
A1843	U1729	A1609	A1521	U1422	U1333	U1230	A	C1026	U862	U780	G780	C
A1844	C1729	A1610	A1522	U1423	U1334	U1231	C	C1027	U863	U781	G781	C
A1845	A1730	A1611	A1523	U1424	U1335	U1232	A	C1028	U864	U782	G782	C
A1846	U1731	A1612	A1524	U1425	U1336	U1233	C	C1029	U865	U783	G783	C
A1847	C1732	A1613	A1525	U1426	U1337	U1234	A	C1030	U866	U784	G784	C
A1848	A1733	A1614	A1526	U1427	U1338	U1235	C	C1031	U867	U785	G785	C
A1849	U1734	A1615	A1527	U1428	U1339	U1236	A	C1032	U868	U786	G786	C
A1850	C1735	A1616	A1528	U1429	U1340	U1237	C	C1033	U869	U787	G787	C
A1851	A1736	A1617	A1529	U1430	U1341	U1238	A	C1034	U870	U788	G788	C
A1852	U1737	A1618	A1530	U1431	U1342	U1239	C	C1035	U871	U789	G789	C
A1853	C1736	A1619	A1531	U1432	U1343	U1240	A	C1036	U872	U790	G790	C
A1854	A1737	A1620	A1532	U1433	U1344	U1241	C	C1037	U873	U791	G791	C
A1855	U1738	A1621	A1533	U1434	U1345	U1242	A	C1038	U874	U792	G792	C
A1856	C1739	A1622	A1534	U1435	U1346	U1243	C	C1039	U875	U793	G793	C
A1857	A1739	A1623	A1535	U1436	U1347	U1244	A	C1040	U876	U794	G794	C
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A1898	C1776	A1664	A1576	U1477	U1388	U1285	C	C1081	U917	U835	G835	C
A1899	A1778	A1665	A1577	U1478	U1389	U1286	A	C1082	U918	U836	G836	C
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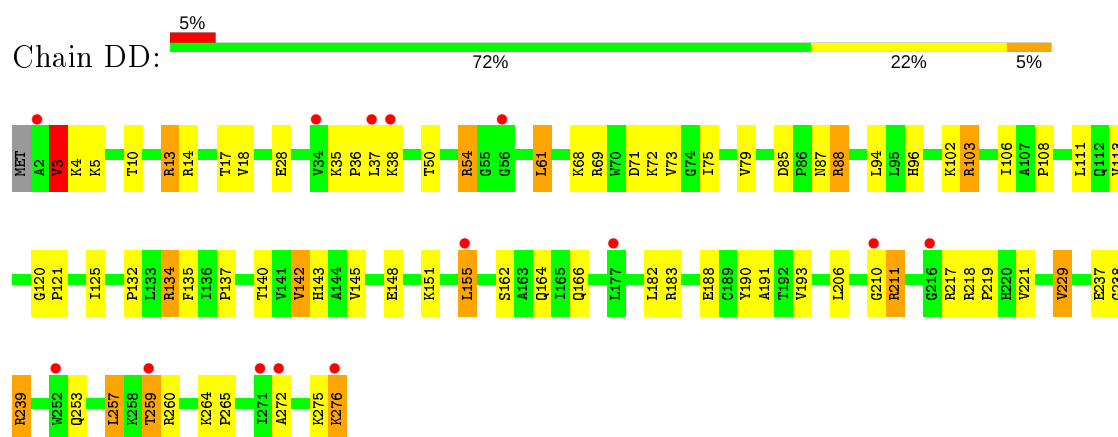
- Molecule 27: 5S Ribosomal RNA



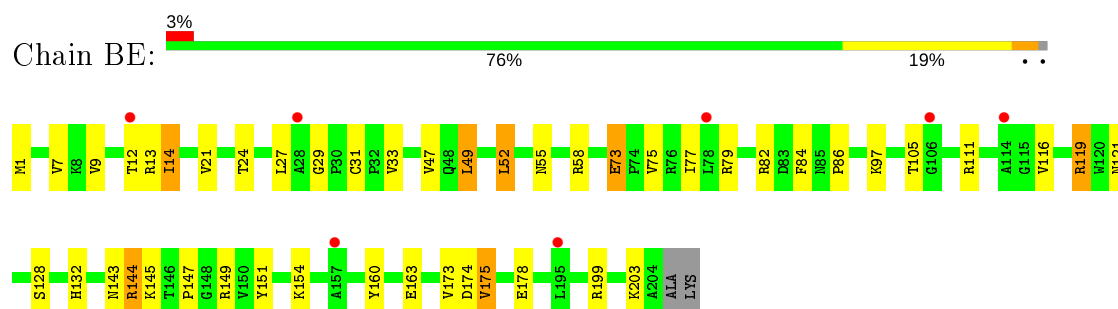
- Molecule 28: 50S ribosomal protein L2



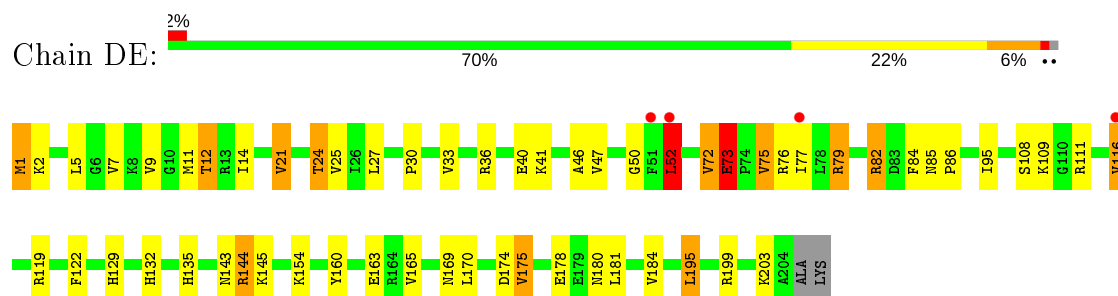
- Molecule 28: 50S ribosomal protein L2



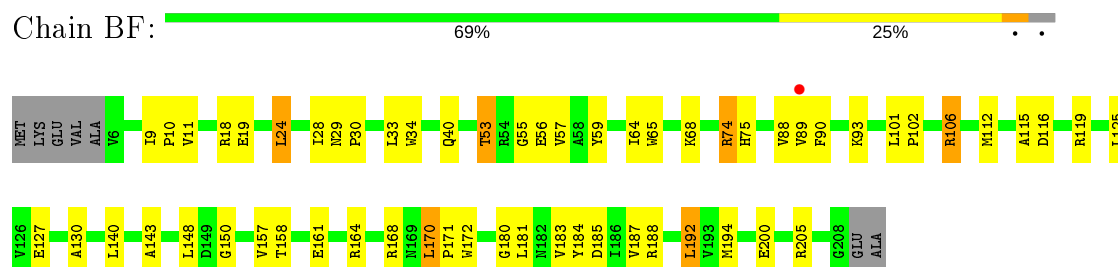
- Molecule 29: 50S ribosomal protein L3



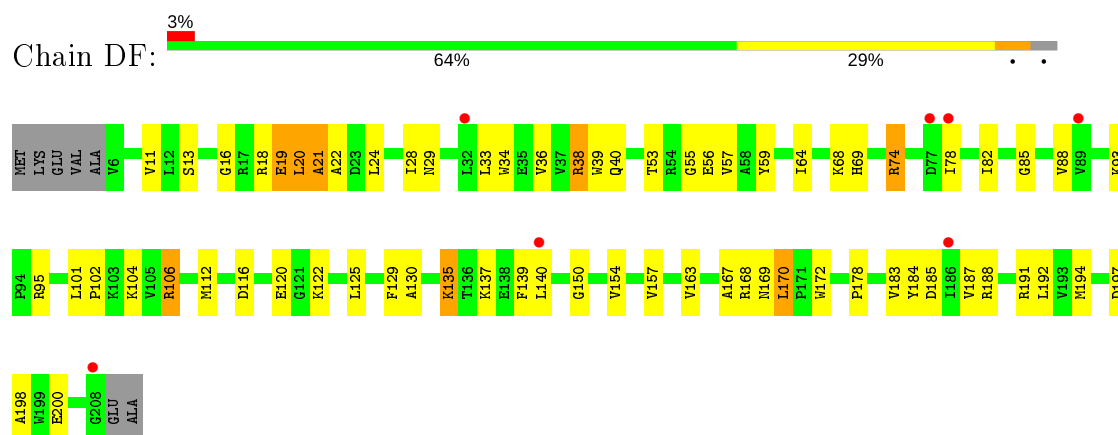
- Molecule 29: 50S ribosomal protein L3



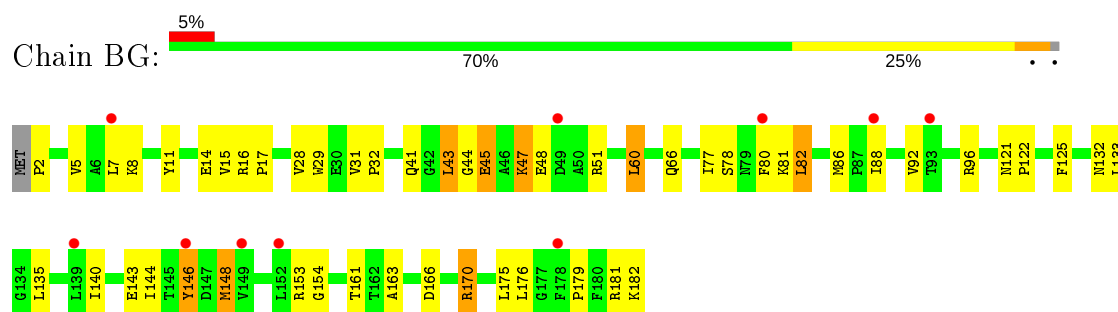
- Molecule 30: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L4

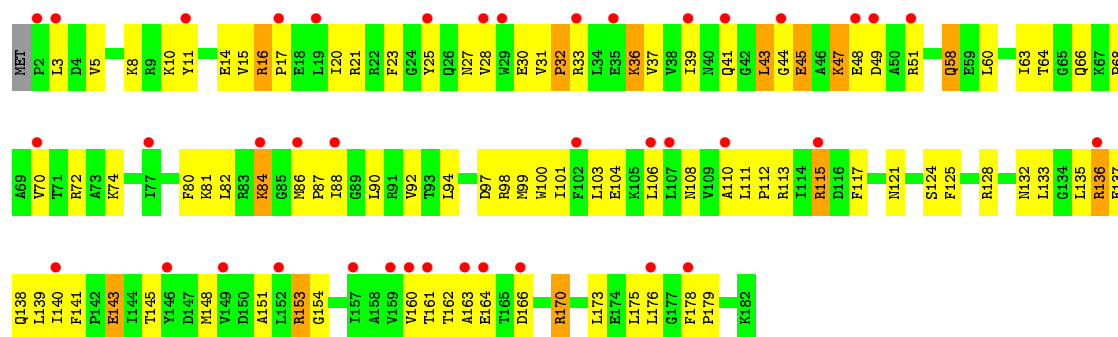


- Molecule 31: 50S ribosomal protein L5

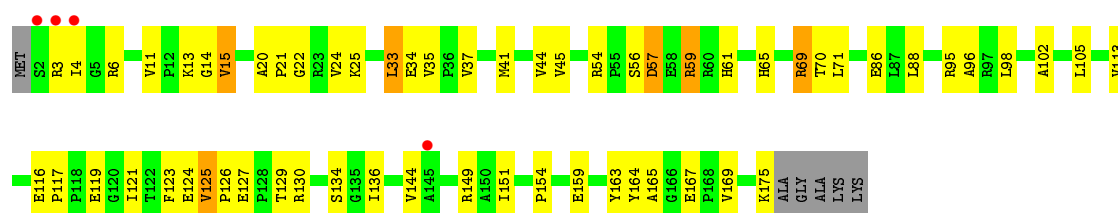


- Molecule 31: 50S ribosomal protein L5

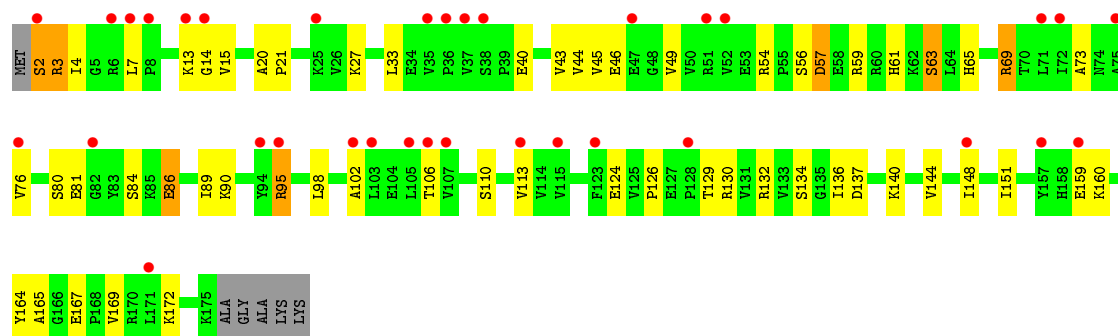




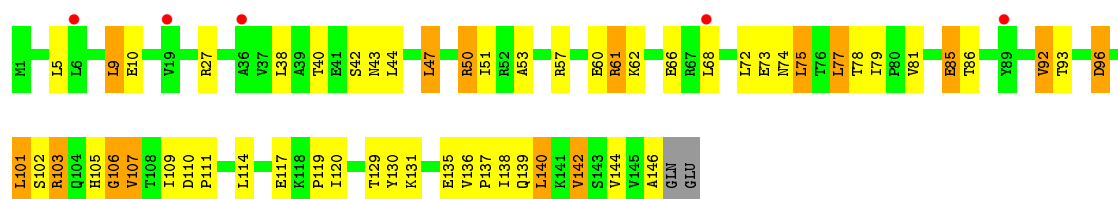
• Molecule 32: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L6

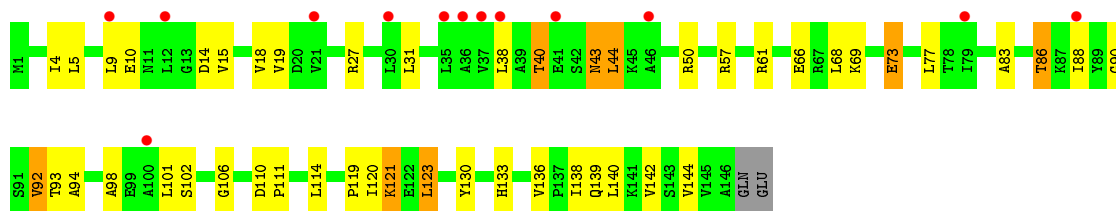


• Molecule 33: 50S ribosomal protein L9

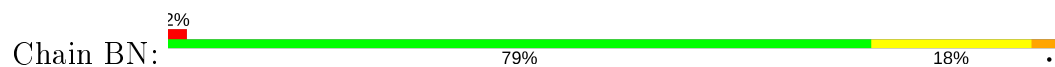


• Molecule 33: 50S ribosomal protein L9

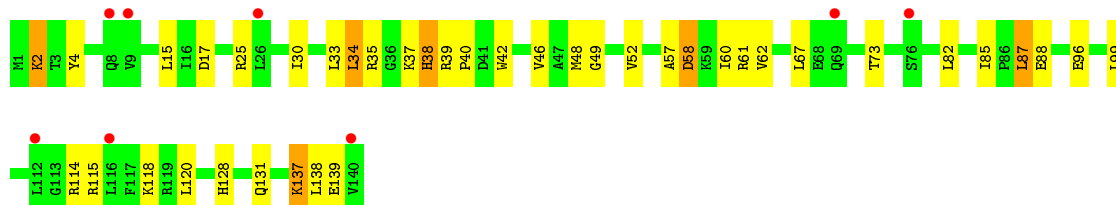
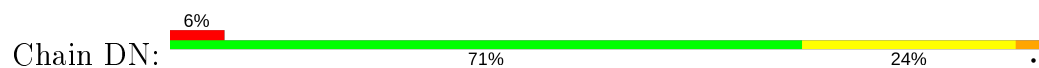




- Molecule 34: 50S ribosomal protein L13



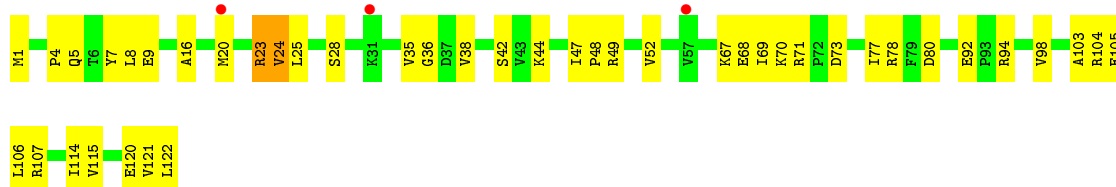
- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L14

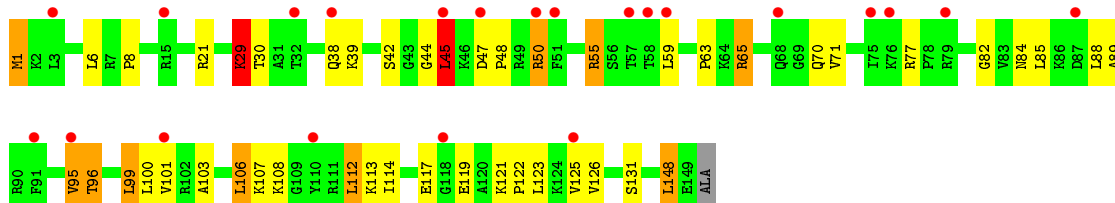


- Molecule 36: 50S ribosomal protein L15

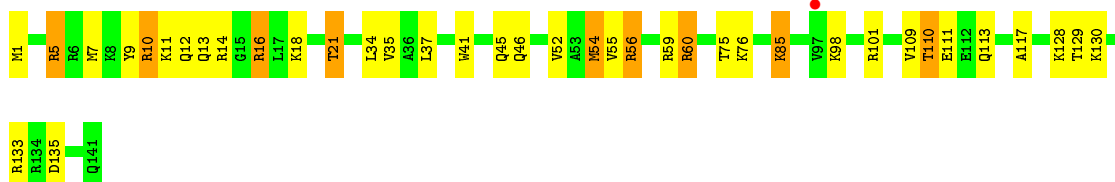
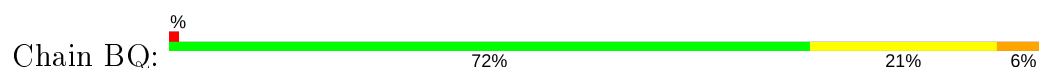




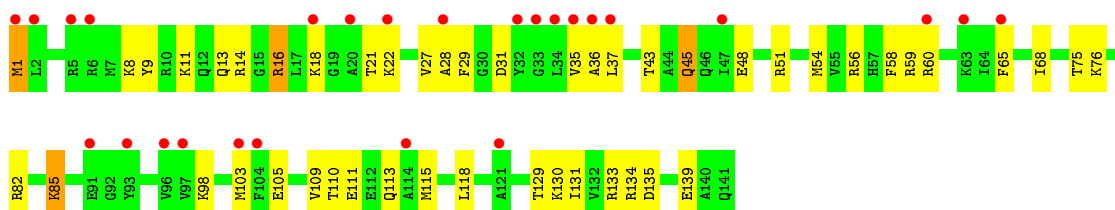
- Molecule 36: 50S ribosomal protein L15



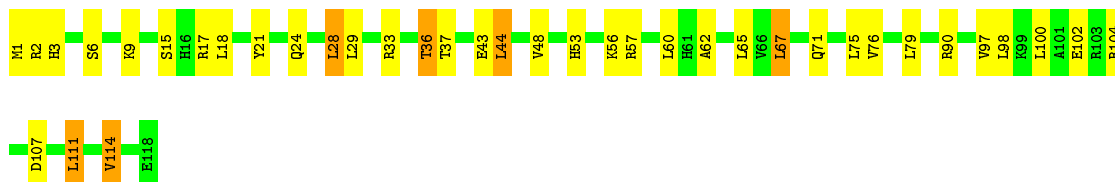
- Molecule 37: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L16

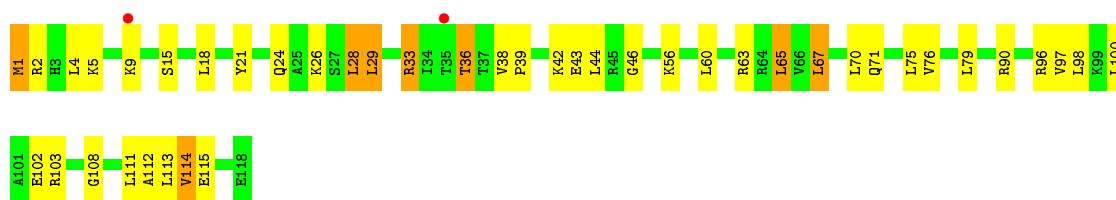


- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

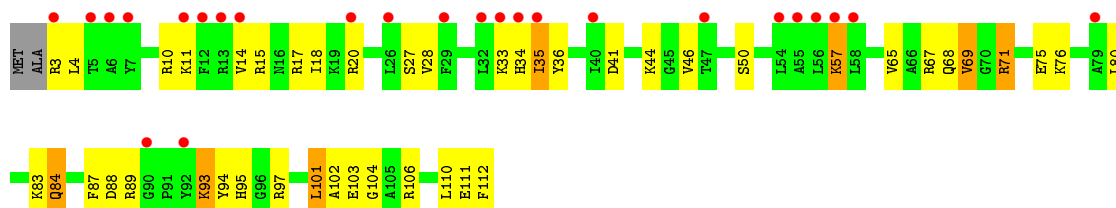




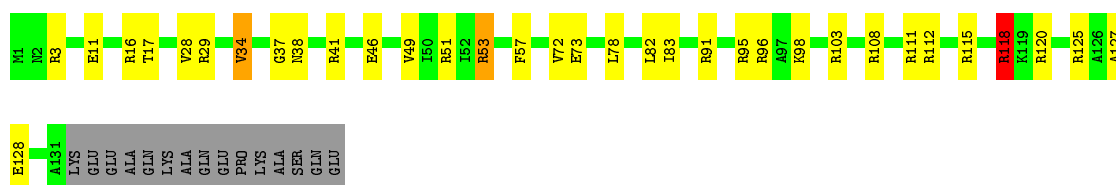
- Molecule 39: 50S ribosomal protein L18



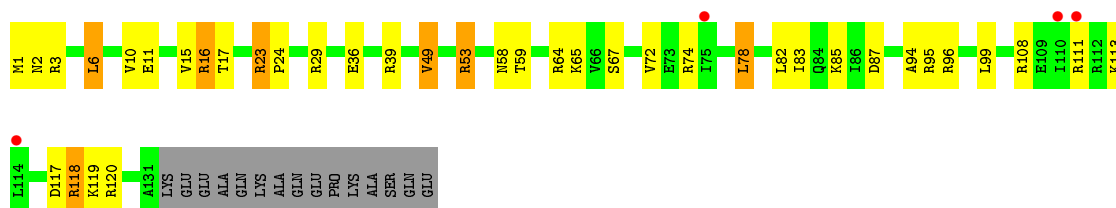
- Molecule 39: 50S ribosomal protein L18



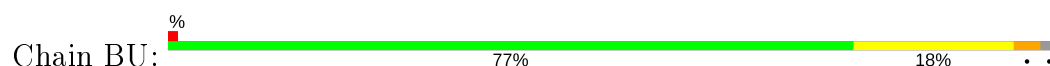
- Molecule 40: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L19

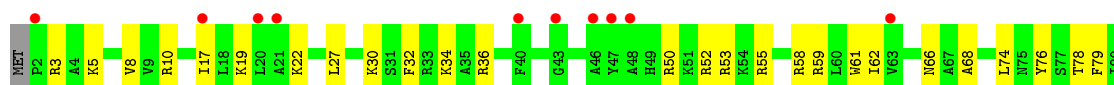


- Molecule 41: 50S ribosomal protein L20

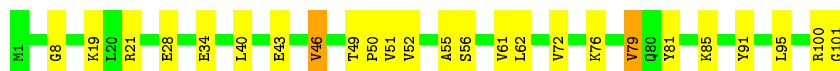
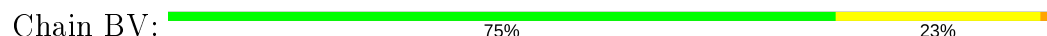




- Molecule 41: 50S ribosomal protein L20



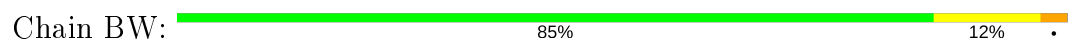
- Molecule 42: 50S ribosomal protein L21



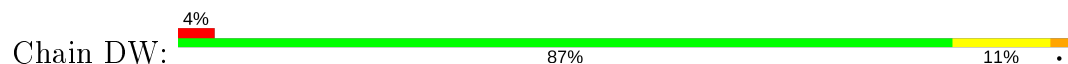
- Molecule 42: 50S ribosomal protein L21



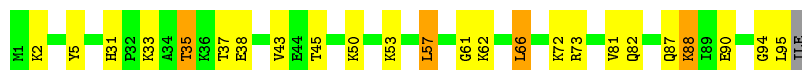
- Molecule 43: 50S ribosomal protein L22



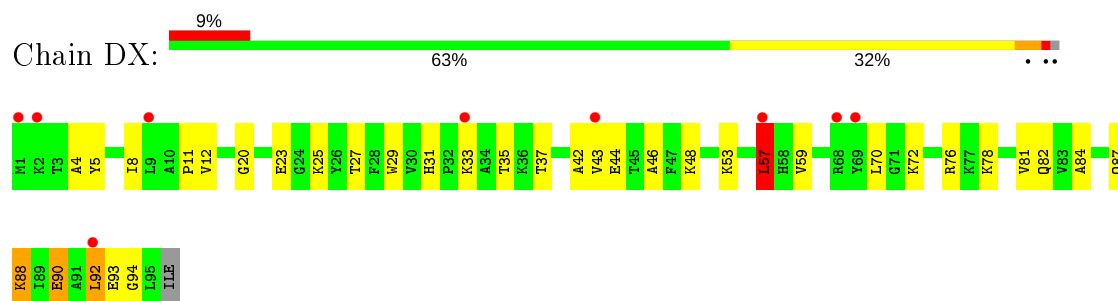
- Molecule 43: 50S ribosomal protein L22



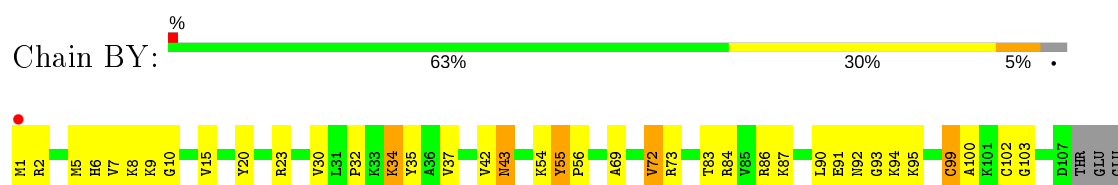
- Molecule 44: 50S ribosomal protein L23



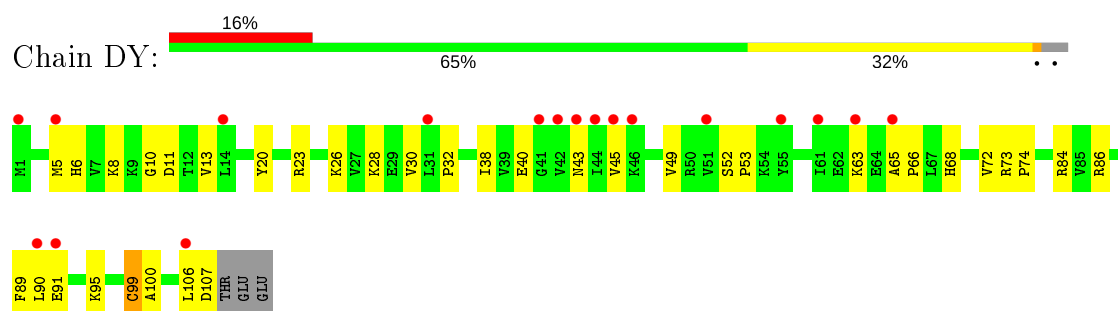
- Molecule 44: 50S ribosomal protein L23



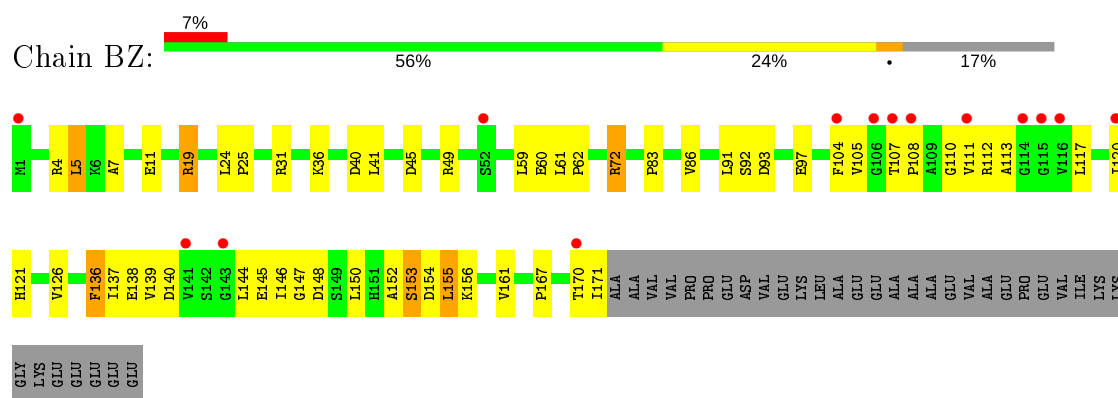
- Molecule 45: 50S ribosomal protein L24



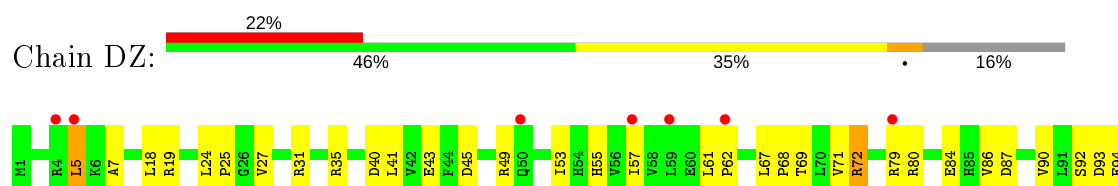
- Molecule 45: 50S ribosomal protein L24

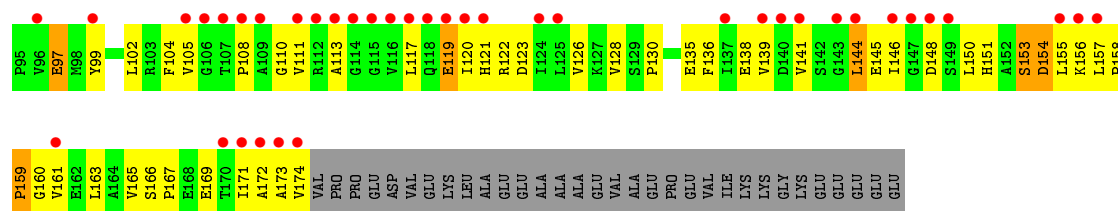


- Molecule 46: 50S ribosomal protein L25

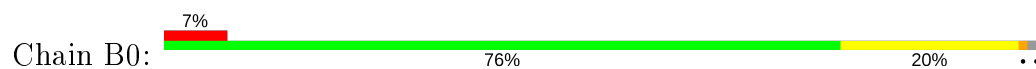


- Molecule 46: 50S ribosomal protein L25

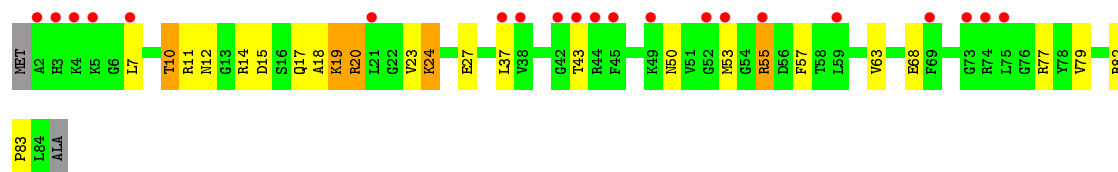




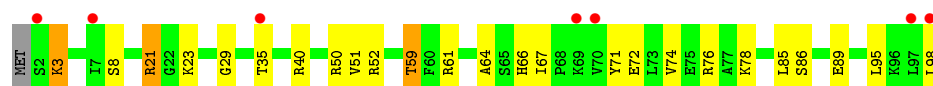
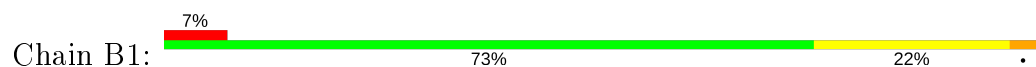
- Molecule 47: 50S ribosomal protein L27



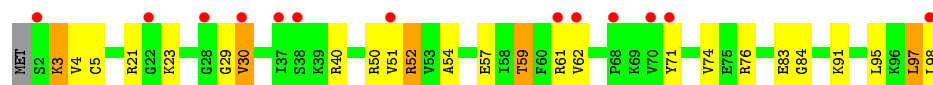
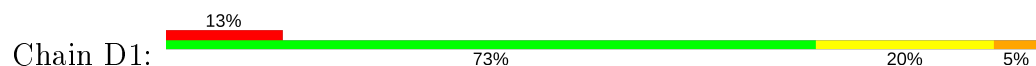
- Molecule 47: 50S ribosomal protein L27



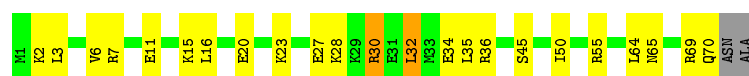
- Molecule 48: 50S ribosomal protein L28



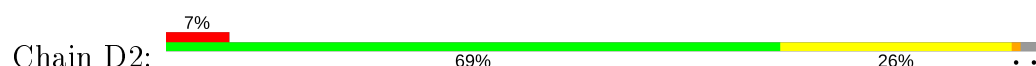
- Molecule 48: 50S ribosomal protein L28

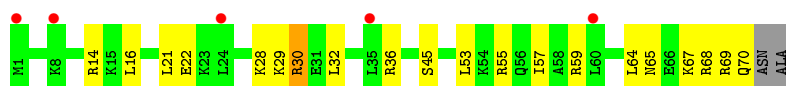


- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29

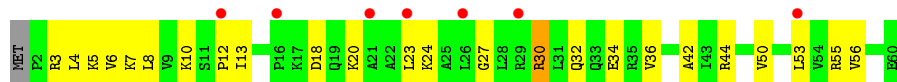




- Molecule 50: 50S ribosomal protein L30



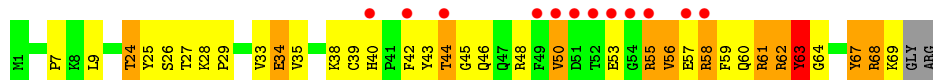
- Molecule 50: 50S ribosomal protein L30



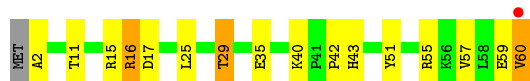
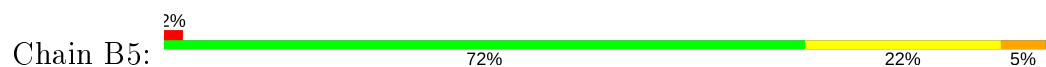
- Molecule 51: 50S ribosomal protein L31



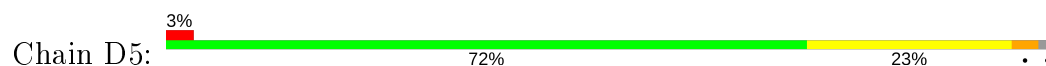
- Molecule 51: 50S ribosomal protein L31



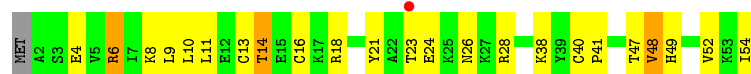
- Molecule 52: 50S ribosomal protein L32



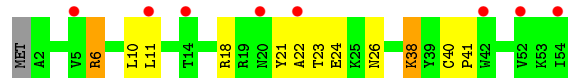
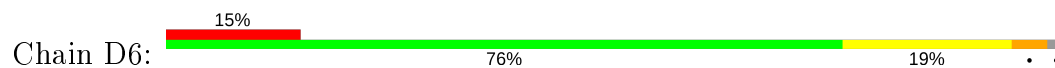
- Molecule 52: 50S ribosomal protein L32



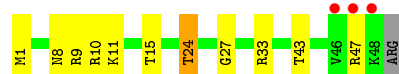
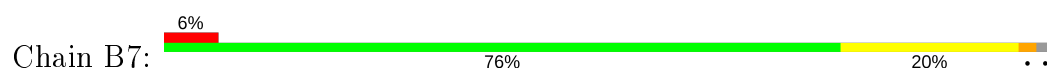
- Molecule 53: 50S ribosomal protein L33



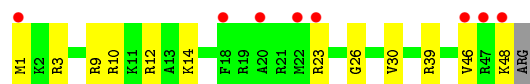
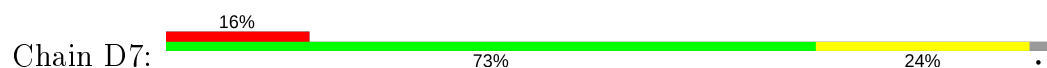
- Molecule 53: 50S ribosomal protein L33



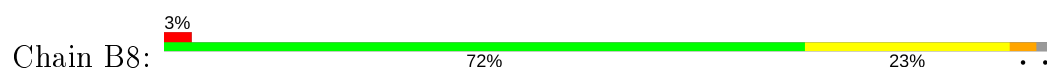
- Molecule 54: 50S ribosomal protein L34



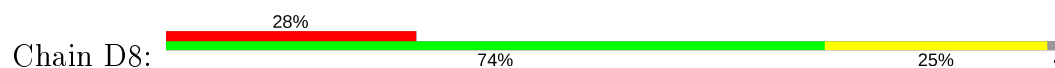
- Molecule 54: 50S ribosomal protein L34



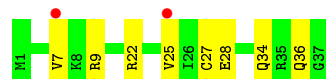
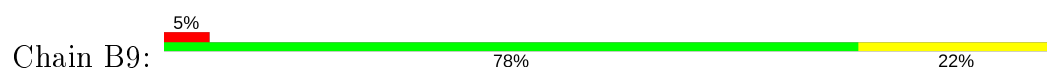
- Molecule 55: 50S ribosomal protein L35



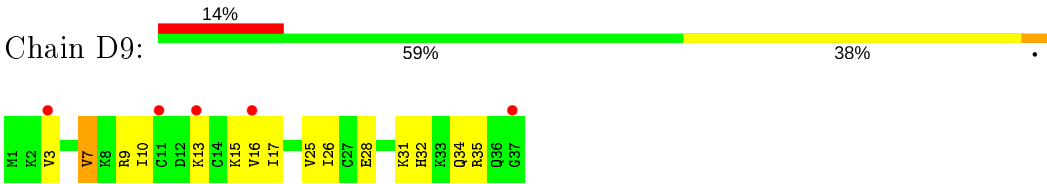
- Molecule 55: 50S ribosomal protein L35



- 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, α , β , γ	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 255.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (255.92-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.280 0.233 , 0.280	Depositor DCC
R_{free} test set	90444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297141	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, 31M, MIA, SF4, MG, 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	0.37	0/36049	0.91	42/56261 (0.1%)
1	CA	0.40	6/36170 (0.0%)	1.00	88/56452 (0.2%)
2	AB	0.31	0/1881	0.60	0/2542
2	CB	0.33	0/1860	0.65	1/2518 (0.0%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.32	0/1566	0.61	0/2119
4	AD	0.29	0/1689	0.58	2/2267 (0.1%)
4	CD	0.30	0/1704	0.54	0/2284
5	AE	0.30	0/1145	0.55	0/1543
5	CE	0.31	0/1149	0.62	1/1548 (0.1%)
6	AF	0.28	0/819	0.49	0/1111
6	CF	0.31	0/829	0.52	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.28	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.50	0/1494
8	CH	0.27	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.59	0/1346
9	CI	0.30	0/997	0.57	0/1343
10	AJ	0.28	0/722	0.59	0/982
10	CJ	0.31	0/727	0.59	0/988
11	AK	0.28	0/844	0.60	1/1145 (0.1%)
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.30	0/946	0.52	0/1274
12	CL	0.30	0/946	0.55	0/1274
13	AM	0.28	0/969	0.61	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.55	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.28	0/697	0.52	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.56	0/746
18	CR	0.28	0/560	0.56	0/746
19	AS	0.29	0/667	0.58	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.28	0/730	0.58	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.26	0/203	0.52	0/266
21	CU	0.35	0/203	0.52	0/266
22	AV	0.41	0/310	0.94	0/480
22	CV	0.45	0/282	1.06	1/437 (0.2%)
23	AW	0.47	0/1577	1.18	6/2454 (0.2%)
23	CW	0.59	0/1531	1.46	25/2379 (1.1%)
24	AX	0.51	0/1725	1.17	14/2689 (0.5%)
24	CX	0.44	0/1725	1.12	10/2689 (0.4%)
25	AY	0.62	0/1602	1.43	22/2493 (0.9%)
25	CY	0.64	0/1579	1.46	32/2455 (1.3%)
26	BA	0.48	2/68013 (0.0%)	0.95	84/106165 (0.1%)
26	DA	0.42	1/67542 (0.0%)	0.94	72/105428 (0.1%)
27	BB	0.41	0/2878	0.88	0/4490
27	DB	0.44	0/2878	0.94	0/4490
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2186	0.55	0/2944
29	BE	0.36	0/1592	0.57	0/2149
29	DE	0.34	0/1592	0.60	1/2149 (0.0%)
30	BF	0.35	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.58	0/2188
31	BG	0.31	0/1450	0.54	0/1959
31	DG	0.33	0/1449	0.57	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.30	0/1356	0.52	0/1834
33	BI	0.29	0/1100	0.60	0/1501
33	DI	0.28	0/1076	0.57	0/1471
34	BN	0.32	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.54	0/1543
35	BO	0.34	0/943	0.58	1/1269 (0.1%)
35	DO	0.31	0/943	0.51	0/1269
36	BP	0.34	0/1152	0.58	0/1533
36	DP	0.31	0/1152	0.59	0/1533
37	BQ	0.34	0/1143	0.53	0/1527
37	DQ	0.31	0/1143	0.52	0/1527
38	BR	0.35	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.52	0/1312
39	BS	0.31	0/887	0.63	2/1180 (0.2%)
39	DS	0.29	0/880	0.61	0/1172
40	BT	0.33	0/1105	0.59	1/1477 (0.1%)
40	DT	0.29	0/1097	0.56	0/1468
41	BU	0.37	0/977	0.56	0/1301
41	DU	0.31	0/977	0.50	0/1301
42	BV	0.39	0/782	0.58	0/1049
42	DV	0.32	0/782	0.64	2/1049 (0.2%)
43	BW	0.38	0/897	0.57	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.39	0/764	0.59	1/1025 (0.1%)
44	DX	0.32	0/764	0.56	1/1025 (0.1%)
45	BY	0.34	0/819	0.57	0/1095
45	DY	0.31	0/819	0.55	0/1095
46	BZ	0.31	0/1379	0.61	0/1873
46	DZ	0.29	0/1390	0.57	0/1890
47	B0	0.35	0/662	0.57	0/881
47	D0	0.29	0/662	0.49	0/881
48	B1	0.34	0/762	0.56	0/1014
48	D1	0.32	0/762	0.54	0/1014
49	B2	0.32	0/590	0.56	0/781
49	D2	0.27	0/590	0.46	0/781
50	B3	0.36	0/474	0.58	0/635
50	D3	0.27	0/469	0.50	0/630
51	B4	0.35	0/571	0.71	0/768
51	D4	0.34	0/545	0.70	0/737
52	B5	0.38	0/469	0.60	0/635
52	D5	0.33	0/469	0.52	0/635
53	B6	0.36	0/460	0.51	0/613
53	D6	0.30	0/456	0.48	0/608
54	B7	0.39	0/426	0.55	0/561
54	D7	0.33	0/426	0.59	0/561
55	B8	0.36	0/519	0.58	0/684
55	D8	0.32	0/525	0.52	0/691
56	B9	0.35	0/310	0.51	0/407
56	D9	0.31	0/310	0.56	0/407
All	All	0.40	9/316594 (0.0%)	0.88	410/473970 (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	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-11.01	1.28	1.37
1	CA	1154	G	C6-N1	-10.68	1.32	1.39
1	CA	1119	C	N3-C4	-9.86	1.27	1.33
1	CA	1154	G	N7-C5	-7.17	1.34	1.39
26	BA	330	A	N9-C4	-6.79	1.33	1.37

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	32.18	138.21	118.90
1	CA	1154	G	N3-C2-N2	24.48	137.03	119.90
1	CA	1154	G	C5-C6-O6	24.01	143.00	128.60
1	CA	1154	G	N1-C2-N2	-21.95	96.45	116.20
1	CA	1119	C	N3-C2-O2	-20.26	107.72	121.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	495	0
1	CA	32312	0	16307	663	0
2	AB	1846	0	1867	92	0
2	CB	1825	0	1828	102	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	61	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	33	0
6	AF	806	0	793	24	0
6	CF	816	0	808	18	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	42	0
9	AI	983	0	986	47	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	14	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	39	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	20	0
15	CO	728	0	760	31	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	17	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	42	0
20	AT	728	0	798	32	0
20	CT	727	0	796	25	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	10	0
22	AV	277	0	140	2	0
22	CV	252	0	130	7	0
23	AW	1607	0	839	55	0
23	CW	1560	0	803	55	0
24	AX	1625	0	828	34	0
24	CX	1625	0	828	33	0
25	AY	1581	0	805	96	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	669	0
26	DA	60311	0	30409	876	0
27	BB	2573	0	1306	19	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	51	0
28	DD	2136	0	2218	61	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	45	0
30	BF	1584	0	1625	47	0
30	DF	1580	0	1619	50	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	66	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	41	0
33	DI	1061	0	1080	25	0
34	BN	1117	0	1183	17	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	20	0
35	DO	933	0	996	29	0
36	BP	1135	0	1212	38	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	31	0
37	DQ	1122	0	1179	35	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	27	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	17	0
41	DU	959	0	1019	38	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	25	0
43	BW	886	0	939	12	0
43	DW	886	0	940	9	0
44	BX	750	0	814	16	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	26	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	61	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	18	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	12	0
51	B4	558	0	544	22	0
51	D4	532	0	503	31	0
52	B5	455	0	465	11	0
52	D5	455	0	465	12	0
53	B6	453	0	473	13	0
53	D6	449	0	469	9	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	21	0
55	D8	517	0	582	10	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0
61	DX	3	0	0	0	0
61	DY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	297141	0	196251	5228	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 11.

The worst 5 of 5228 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)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12

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%)	14 (6%)	7 (3%)	4	3
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	4	3
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	29	40
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	15	22
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	40
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	5	5
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	30
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	19	27
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	1
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	0
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	10
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	10
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	12	16
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	13	17
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	1
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	4	3
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	34	46
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	22	30
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	40
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	15	22
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	29	40
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	15	22
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	34
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	9	11
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	25	34
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	25	34
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	7	7
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	30
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	30
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	30
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	15
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	30
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	24
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	24
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (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%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	22
43	BW	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
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	34
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	14	19
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	19
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%)	53 (79%)	11 (16%)	3 (4%)	2	1
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	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%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	7
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
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	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	22	30

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU

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Mol	Chain	Res	Type
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	BD	275	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	163 (85%)	29 (15%)	3	2
2	CB	187/220 (85%)	149 (80%)	38 (20%)	1	1
3	AC	143/188 (76%)	121 (85%)	22 (15%)	2	2
3	CC	140/188 (74%)	124 (89%)	16 (11%)	5	5
4	AD	170/181 (94%)	152 (89%)	18 (11%)	6	7
4	CD	173/181 (96%)	152 (88%)	21 (12%)	5	4
5	AE	113/123 (92%)	105 (93%)	8 (7%)	14	19
5	CE	114/123 (93%)	101 (89%)	13 (11%)	5	5
6	AF	83/90 (92%)	76 (92%)	7 (8%)	11	13
6	CF	85/90 (94%)	80 (94%)	5 (6%)	19	25
7	AG	119/127 (94%)	108 (91%)	11 (9%)	9	11
7	CG	120/127 (94%)	109 (91%)	11 (9%)	9	11
8	AH	114/119 (96%)	105 (92%)	9 (8%)	12	15
8	CH	114/119 (96%)	107 (94%)	7 (6%)	18	24
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	2
9	CI	89/99 (90%)	76 (85%)	13 (15%)	3	2
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	5	4
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	10	12
11	AK	82/99 (83%)	77 (94%)	5 (6%)	18	24
11	CK	83/99 (84%)	76 (92%)	7 (8%)	11	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	93 (96%)	4 (4%)	30	41
12	CL	97/109 (89%)	93 (96%)	4 (4%)	30	41
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5	5
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	3
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	3
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	2
15	AO	78/80 (98%)	64 (82%)	14 (18%)	2	1
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5	5
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	3
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7	7
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	9
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	18
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	13
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5	5
19	AS	69/80 (86%)	64 (93%)	5 (7%)	14	18
19	CS	67/80 (84%)	63 (94%)	4 (6%)	19	25
20	AT	70/82 (85%)	62 (89%)	8 (11%)	5	5
20	CT	70/82 (85%)	62 (89%)	8 (11%)	5	5
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	2
21	CU	18/22 (82%)	17 (94%)	1 (6%)	21	28
28	BD	215/218 (99%)	195 (91%)	20 (9%)	9	10
28	DD	215/218 (99%)	193 (90%)	22 (10%)	7	8
29	BE	164/166 (99%)	146 (89%)	18 (11%)	6	6
29	DE	164/166 (99%)	145 (88%)	19 (12%)	5	5
30	BF	160/166 (96%)	149 (93%)	11 (7%)	15	20
30	DF	159/166 (96%)	144 (91%)	15 (9%)	8	10
31	BG	143/156 (92%)	128 (90%)	15 (10%)	7	7
31	DG	142/156 (91%)	122 (86%)	20 (14%)	3	3
32	BH	144/148 (97%)	126 (88%)	18 (12%)	4	4
32	DH	144/148 (97%)	126 (88%)	18 (12%)	4	4
33	BI	110/124 (89%)	86 (78%)	24 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	88 (85%)	16 (15%)	2	2
34	BN	118/119 (99%)	103 (87%)	15 (13%)	4	4
34	DN	118/119 (99%)	106 (90%)	12 (10%)	7	8
35	BO	100/100 (100%)	93 (93%)	7 (7%)	15	19
35	DO	100/100 (100%)	93 (93%)	7 (7%)	15	19
36	BP	115/116 (99%)	98 (85%)	17 (15%)	3	2
36	DP	115/116 (99%)	100 (87%)	15 (13%)	4	3
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	3
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	6
38	BR	101/101 (100%)	82 (81%)	19 (19%)	1	1
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	1
39	BS	87/88 (99%)	81 (93%)	6 (7%)	15	20
39	DS	85/88 (97%)	75 (88%)	10 (12%)	5	5
40	BT	115/127 (91%)	106 (92%)	9 (8%)	12	16
40	DT	113/127 (89%)	103 (91%)	10 (9%)	10	12
41	BU	93/94 (99%)	84 (90%)	9 (10%)	8	9
41	DU	93/94 (99%)	85 (91%)	8 (9%)	10	13
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	2
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	2
43	BW	90/92 (98%)	83 (92%)	7 (8%)	12	16
43	DW	90/92 (98%)	83 (92%)	7 (8%)	12	16
44	BX	77/78 (99%)	71 (92%)	6 (8%)	12	16
44	DX	77/78 (99%)	71 (92%)	6 (8%)	12	16
45	BY	85/91 (93%)	75 (88%)	10 (12%)	5	5
45	DY	85/91 (93%)	79 (93%)	6 (7%)	14	19
46	BZ	145/179 (81%)	133 (92%)	12 (8%)	11	14
46	DZ	145/179 (81%)	129 (89%)	16 (11%)	6	6
47	B0	65/67 (97%)	62 (95%)	3 (5%)	27	36
47	D0	65/67 (97%)	60 (92%)	5 (8%)	13	16
48	B1	80/83 (96%)	73 (91%)	7 (9%)	10	12
48	D1	80/83 (96%)	71 (89%)	9 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	57 (88%)	8 (12%)	4	4
49	D2	65/67 (97%)	59 (91%)	6 (9%)	9	11
50	B3	51/52 (98%)	46 (90%)	5 (10%)	8	9
50	D3	50/52 (96%)	44 (88%)	6 (12%)	5	5
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	1
51	D4	53/63 (84%)	43 (81%)	10 (19%)	1	1
52	B5	50/52 (96%)	45 (90%)	5 (10%)	7	8
52	D5	50/52 (96%)	46 (92%)	4 (8%)	12	15
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	3
53	D6	50/52 (96%)	48 (96%)	2 (4%)	31	43
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14	18
54	D7	41/42 (98%)	38 (93%)	3 (7%)	14	18
55	B8	53/55 (96%)	49 (92%)	4 (8%)	13	17
55	D8	54/55 (98%)	51 (94%)	3 (6%)	21	28
56	B9	34/34 (100%)	34 (100%)	0	100	100
56	D9	34/34 (100%)	32 (94%)	2 (6%)	19	25
All	All	9320/10066 (93%)	8304 (89%)	1016 (11%)	6	6

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	82	ARG
4	CD	31	CYS
44	DX	57	LEU
49	B2	64	LEU
2	CB	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
40	BT	123	GLN
3	CC	28	GLN
40	DT	123	GLN
44	BX	31	HIS
51	B4	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	304 (20%)	25 (1%)
1	CA	1501/1521 (98%)	316 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	70/76 (92%)	30 (42%)	2 (2%)
23	CW	67/76 (88%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	71/76 (93%)	35 (49%)	4 (5%)
25	CY	69/76 (90%)	32 (46%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	552 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9286/9620 (96%)	1824 (19%)	126 (1%)

5 of 1824 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2126	A
1	CA	509	A
26	DA	1992	G
26	BA	2183	C
26	BA	2756	U

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

38 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	5MU	CW	54	23	15,22,23	1.08	1 (6%)	16,32,35	1.92	1 (6%)
24	5MC	AX	32	24	15,22,23	1.35	1 (6%)	19,32,35	1.36	3 (15%)
23	MIA	AW	37	23	24,31,32	2.19	4 (16%)	26,44,47	2.60	10 (38%)
25	PSU	CY	55	25	17,21,22	1.46	4 (23%)	20,30,33	3.47	7 (35%)
23	4SU	AW	8	23	14,21,22	1.26	1 (7%)	15,30,33	1.43	2 (13%)
23	PSU	CW	39	23	17,21,22	1.64	3 (17%)	20,30,33	3.37	6 (30%)
25	MIA	CY	37	25	18,24,32	1.16	2 (11%)	18,35,47	1.25	3 (16%)
24	5MC	CX	32	24	15,22,23	1.30	1 (6%)	19,32,35	1.34	3 (15%)
23	PSU	AW	32	23	17,21,22	1.53	2 (11%)	20,30,33	3.22	6 (30%)
23	PSU	CW	32	23	17,21,22	1.58	3 (17%)	20,30,33	3.09	5 (25%)
25	7MG	CY	46	25	22,26,27	1.80	4 (18%)	28,39,42	2.76	10 (35%)
23	31M	CW	76	23	38,44,45	1.41	5 (13%)	38,61,64	1.23	3 (7%)
25	4SU	AY	8	25	14,21,22	1.31	2 (14%)	15,30,33	1.61	2 (13%)
23	PSU	AW	55	23	17,21,22	1.54	2 (11%)	20,30,33	3.34	6 (30%)
24	PSU	AX	55	24,57	17,21,22	1.66	3 (17%)	20,30,33	3.16	7 (35%)
25	PSU	AY	55	25	17,21,22	1.81	3 (17%)	20,30,33	3.00	8 (40%)
25	PSU	CY	32	25	17,21,22	1.47	3 (17%)	20,30,33	3.22	7 (35%)
23	PSU	CW	55	23	17,21,22	1.42	2 (11%)	20,30,33	3.17	6 (30%)
24	5MU	CX	54	24	15,22,23	1.10	1 (6%)	16,32,35	1.70	2 (12%)
24	4SU	CX	8	24	14,21,22	1.25	2 (14%)	15,30,33	2.36	2 (13%)
25	PSU	AY	32	25	17,21,22	1.45	2 (11%)	20,30,33	3.18	7 (35%)
24	4SU	AX	8	24	14,21,22	1.50	2 (14%)	15,30,33	2.68	2 (13%)
23	MIA	CW	37	23	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
23	5MU	AW	54	23	15,22,23	1.04	1 (6%)	16,32,35	2.02	2 (12%)
23	7MG	AW	46	23	22,26,27	1.78	4 (18%)	28,39,42	2.85	9 (32%)
24	PSU	CX	55	24	17,21,22	1.54	3 (17%)	20,30,33	3.11	6 (30%)
23	7MG	CW	46	23	22,26,27	1.81	4 (18%)	28,39,42	2.62	8 (28%)
25	PSU	CY	39	25	17,21,22	1.66	4 (23%)	20,30,33	2.88	6 (30%)
23	PSU	AW	39	23	17,21,22	1.63	3 (17%)	20,30,33	3.32	6 (30%)
25	MIA	AY	37	25	18,24,32	1.14	2 (11%)	18,35,47	1.22	2 (11%)
23	31M	AW	76	23	38,44,45	1.40	5 (13%)	38,61,64	1.39	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	AY	54	25	15,22,23	1.15	1 (6%)	16,32,35	1.81	2 (12%)
25	4SU	CY	8	25	14,21,22	1.32	1 (7%)	15,30,33	1.17	1 (6%)
25	5MU	CY	54	25	15,22,23	1.05	2 (13%)	16,32,35	1.85	2 (12%)
25	PSU	AY	39	25	17,21,22	1.58	4 (23%)	20,30,33	3.80	5 (25%)
25	7MG	AY	46	25	22,26,27	1.72	3 (13%)	28,39,42	3.02	9 (32%)
24	5MU	AX	54	24,57	15,22,23	1.07	1 (6%)	16,32,35	1.94	2 (12%)
23	4SU	CW	8	23	14,21,22	1.27	1 (7%)	15,30,33	1.32	2 (13%)

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	5MU	CW	54	23	-	0/5/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/5/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
25	PSU	CY	55	25	-	1/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/5/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/3/25/34	0/3/3/3
24	5MC	CX	32	24	-	0/5/25/26	0/2/2/2
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	5/7/37/38	0/3/3/3
23	31M	CW	76	23	-	11/27/49/50	0/4/4/4
25	4SU	AY	8	25	-	1/5/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24,57	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	1/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	1/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/5/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
25	PSU	AY	32	25	-	1/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/5/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	5MU	AW	54	23	-	0/5/25/26	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
25	PSU	CY	39	25	-	2/7/25/26	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
23	31M	AW	76	23	-	9/27/49/50	0/4/4/4
25	5MU	AY	54	25	-	2/5/25/26	0/2/2/2
25	4SU	CY	8	25	-	2/5/25/26	0/2/2/2
25	5MU	CY	54	25	-	2/5/25/26	0/2/2/2
25	PSU	AY	39	25	-	2/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3
24	5MU	AX	54	24,57	-	0/5/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/5/25/26	0/2/2/2

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	7.24	1.53	1.32
23	AW	37	MIA	C2-S10	-6.30	1.70	1.75
25	AY	55	PSU	C5-C1'	-5.84	1.47	1.52
25	CY	46	7MG	C6-C5	5.43	1.48	1.41
23	CW	46	7MG	C6-C5	5.07	1.48	1.41

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	46	7MG	N3-C4-N9	10.62	140.54	126.91
25	AY	39	PSU	C4-N3-C2	9.65	123.29	115.14
23	AW	46	7MG	N3-C4-N9	9.26	138.81	126.91
24	AX	8	4SU	C2-N3-C4	9.26	128.58	115.15
25	AY	39	PSU	N1-C2-N3	-9.18	121.13	128.43

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
25	CY	37	MIA	C3'-C4'-C5'-O5'
25	CY	46	7MG	O4'-C4'-C5'-O5'
23	CW	76	31M	C3'-C4'-C5'-O5'
23	CW	76	31M	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	32	5MC	3	0
23	AW	37	MIA	1	0
25	CY	55	PSU	4	0
23	AW	8	4SU	1	0
23	CW	39	PSU	3	0
25	CY	37	MIA	2	0
24	CX	32	5MC	2	0
25	CY	46	7MG	1	0
23	CW	76	31M	7	0
25	AY	8	4SU	1	0
24	AX	55	PSU	1	0
25	AY	55	PSU	4	0
23	CW	55	PSU	1	0
24	CX	54	5MU	2	0
24	CX	8	4SU	2	0
25	AY	32	PSU	2	0
24	AX	8	4SU	2	0
23	AW	46	7MG	1	0
23	CW	46	7MG	1	0
25	CY	39	PSU	4	0
23	AW	39	PSU	1	0
25	AY	37	MIA	3	0
23	AW	76	31M	4	0
25	AY	54	5MU	2	0
25	CY	8	4SU	5	0
25	AY	39	PSU	4	0
25	AY	46	7MG	3	0
23	CW	8	4SU	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2093 ligands modelled in this entry, 2091 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	302	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	302	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.35	28 (1%) 66 73	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.38	63 (4%) 36 42	44, 74, 94, 109	0
2	AB	231/256 (90%)	0.77	30 (12%) 3 4	72, 82, 90, 94	0
2	CB	231/256 (90%)	1.43	52 (22%) 0 0	73, 84, 90, 95	0
3	AC	206/239 (86%)	0.96	33 (16%) 1 2	68, 79, 87, 94	0
3	CC	206/239 (86%)	1.84	76 (36%) 0 0	71, 81, 89, 94	0
4	AD	208/209 (99%)	0.97	27 (12%) 3 4	57, 72, 81, 90	0
4	CD	208/209 (99%)	0.80	16 (7%) 13 17	58, 71, 80, 91	0
5	AE	148/162 (91%)	1.01	17 (11%) 4 6	58, 71, 80, 85	0
5	CE	148/162 (91%)	1.21	29 (19%) 1 1	60, 73, 81, 86	0
6	AF	100/101 (99%)	0.56	5 (5%) 28 34	56, 69, 78, 82	0
6	CF	100/101 (99%)	0.43	5 (5%) 28 34	57, 70, 78, 82	0
7	AG	155/156 (99%)	0.84	10 (6%) 18 22	65, 75, 83, 91	0
7	CG	155/156 (99%)	1.13	24 (15%) 2 2	66, 76, 84, 92	0
8	AH	137/138 (99%)	0.96	25 (18%) 1 1	62, 72, 79, 87	0
8	CH	137/138 (99%)	1.09	27 (19%) 1 1	64, 74, 80, 87	0
9	AI	127/128 (99%)	1.11	25 (19%) 1 1	65, 80, 86, 89	0
9	CI	127/128 (99%)	2.49	72 (56%) 0 0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	1.18	19 (19%) 1 1	64, 82, 90, 93	0
10	CJ	96/105 (91%)	1.72	35 (36%) 0 0	67, 84, 91, 93	0
11	AK	114/129 (88%)	0.83	8 (7%) 16 19	48, 70, 79, 84	0
11	CK	114/129 (88%)	0.76	8 (7%) 16 19	51, 71, 79, 84	0
12	AL	122/132 (92%)	0.77	5 (4%) 37 44	50, 65, 73, 78	0
12	CL	122/132 (92%)	1.17	24 (19%) 1 1	53, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.70	9 (7%) 15 18	55, 70, 81, 89	0
13	CM	122/126 (96%)	2.06	53 (43%) 0 0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.20	9 (15%) 2 2	67, 74, 83, 84	0
14	CN	60/61 (98%)	3.00	38 (63%) 0 0	69, 77, 84, 88	0
15	AO	88/89 (98%)	0.67	6 (6%) 17 20	56, 67, 80, 81	0
15	CO	88/89 (98%)	0.92	8 (9%) 9 11	59, 69, 80, 83	0
16	AP	82/88 (93%)	1.57	24 (29%) 0 0	57, 71, 80, 84	0
16	CP	82/88 (93%)	0.97	7 (8%) 10 12	58, 70, 80, 84	0
17	AQ	99/105 (94%)	0.81	11 (11%) 5 7	59, 71, 80, 84	0
17	CQ	99/105 (94%)	1.29	25 (25%) 0 0	61, 71, 81, 85	0
18	AR	68/88 (77%)	0.75	5 (7%) 14 18	59, 68, 81, 83	0
18	CR	68/88 (77%)	0.60	3 (4%) 34 41	61, 70, 80, 84	0
19	AS	83/93 (89%)	0.60	3 (3%) 42 49	71, 80, 86, 95	0
19	CS	83/93 (89%)	1.93	31 (37%) 0 0	74, 82, 89, 96	0
20	AT	96/106 (90%)	0.94	14 (14%) 2 3	57, 71, 81, 85	0
20	CT	96/106 (90%)	1.15	15 (15%) 2 2	58, 70, 82, 85	0
21	AU	23/27 (85%)	1.65	7 (30%) 0 0	67, 74, 77, 81	0
21	CU	23/27 (85%)	2.78	15 (65%) 0 0	71, 75, 80, 84	0
22	AV	13/24 (54%)	2.86	7 (53%) 0 0	58, 81, 96, 99	0
22	CV	12/24 (50%)	3.67	8 (66%) 0 0	63, 84, 93, 94	0
23	AW	66/76 (86%)	1.96	25 (37%) 0 0	68, 96, 103, 105	0
23	CW	64/76 (84%)	3.61	52 (81%) 0 0	73, 97, 103, 106	0
24	AX	72/77 (93%)	0.44	1 (1%) 75 81	39, 68, 87, 91	0
24	CX	72/77 (93%)	0.73	4 (5%) 24 29	53, 82, 93, 97	0
25	AY	67/76 (88%)	1.42	21 (31%) 0 0	44, 97, 102, 105	0
25	CY	66/76 (86%)	2.35	32 (48%) 0 0	47, 97, 102, 105	0
26	BA	2819/2915 (96%)	0.67	29 (1%) 82 86	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.18	65 (2%) 60 67	30, 49, 90, 108	0
27	BB	120/121 (99%)	0.55	0 100 100	40, 64, 73, 86	0
27	DB	120/121 (99%)	0.20	5 (4%) 36 42	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.81	7 (2%) 57 63	27, 43, 58, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.69	14 (5%) 28 33	29, 45, 61, 81	0
29	BE	204/206 (99%)	0.79	7 (3%) 45 52	25, 48, 66, 80	0
29	DE	204/206 (99%)	0.57	4 (1%) 65 72	29, 52, 67, 81	0
30	BF	203/210 (96%)	0.75	1 (0%) 91 94	26, 53, 76, 87	0
30	DF	203/210 (96%)	0.57	7 (3%) 45 52	30, 58, 77, 87	0
31	BG	181/182 (99%)	0.81	10 (5%) 25 30	51, 69, 81, 88	0
31	DG	181/182 (99%)	1.26	40 (22%) 0 0	56, 73, 82, 90	0
32	BH	174/180 (96%)	0.75	4 (2%) 60 67	51, 65, 75, 88	0
32	DH	174/180 (96%)	1.09	34 (19%) 1 1	55, 70, 78, 88	0
33	BI	146/148 (98%)	0.56	5 (3%) 45 52	50, 74, 82, 87	0
33	DI	146/148 (98%)	0.60	13 (8%) 9 11	52, 75, 82, 86	0
34	BN	140/140 (100%)	0.90	3 (2%) 63 70	32, 50, 67, 76	0
34	DN	140/140 (100%)	0.68	8 (5%) 23 28	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.58	0 100 100	30, 43, 59, 70	0
35	DO	122/122 (100%)	0.75	3 (2%) 57 63	45, 59, 73, 78	0
36	BP	149/150 (99%)	0.82	3 (2%) 65 72	26, 55, 75, 83	0
36	DP	149/150 (99%)	0.95	22 (14%) 2 2	30, 59, 77, 85	0
37	BQ	141/141 (100%)	0.83	1 (0%) 87 90	36, 52, 67, 80	0
37	DQ	141/141 (100%)	1.25	26 (18%) 1 1	41, 57, 70, 82	0
38	BR	118/118 (100%)	0.68	0 100 100	25, 36, 54, 59	0
38	DR	118/118 (100%)	0.64	2 (1%) 70 76	41, 54, 65, 72	0
39	BS	110/112 (98%)	0.50	1 (0%) 84 88	38, 51, 65, 72	0
39	DS	110/112 (98%)	1.22	25 (22%) 0 0	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.51	0 100 100	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.66	4 (3%) 49 56	48, 63, 79, 85	0
41	BU	116/118 (98%)	0.80	1 (0%) 84 88	18, 33, 49, 59	0
41	DU	116/118 (98%)	0.82	10 (8%) 10 12	42, 61, 78, 84	0
42	BV	101/101 (100%)	0.55	0 100 100	21, 41, 58, 67	0
42	DV	101/101 (100%)	0.63	4 (3%) 38 45	41, 71, 83, 91	0
43	BW	112/113 (99%)	0.73	0 100 100	23, 34, 54, 79	0
43	DW	112/113 (99%)	0.69	5 (4%) 33 40	39, 50, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.56	0	100 100	23, 38, 61, 84	0
44	DX	95/96 (98%)	0.97	9 (9%)	8 10	43, 60, 76, 79	0
45	BY	107/110 (97%)	0.51	1 (0%)	84 88	32, 50, 69, 83	0
45	DY	107/110 (97%)	1.19	18 (16%)	1 1	57, 71, 81, 88	0
46	BZ	171/206 (83%)	0.70	14 (8%)	11 14	39, 64, 91, 95	0
46	DZ	174/206 (84%)	1.53	46 (26%)	0 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	0.88	6 (7%)	15 18	27, 39, 61, 73	0
47	D0	83/85 (97%)	1.49	21 (25%)	0 0	47, 66, 75, 82	0
48	B1	97/98 (98%)	0.80	7 (7%)	15 18	30, 48, 70, 76	0
48	D1	97/98 (98%)	0.95	13 (13%)	3 4	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.57	0	100 100	34, 50, 64, 79	0
49	D2	70/72 (97%)	0.66	5 (7%)	16 19	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.63	0	100 100	24, 37, 63, 71	0
50	D3	59/60 (98%)	0.96	7 (11%)	4 5	49, 64, 79, 85	0
51	B4	69/71 (97%)	0.48	5 (7%)	15 18	54, 73, 87, 92	0
51	D4	69/71 (97%)	1.13	12 (17%)	1 1	74, 88, 94, 99	0
52	B5	59/60 (98%)	0.63	1 (1%)	70 76	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.55	2 (3%)	45 52	36, 51, 67, 73	0
53	B6	53/54 (98%)	0.60	1 (1%)	66 73	31, 44, 61, 68	0
53	D6	53/54 (98%)	1.10	8 (15%)	2 2	52, 63, 76, 79	0
54	B7	48/49 (97%)	1.03	3 (6%)	20 23	21, 30, 62, 76	0
54	D7	48/49 (97%)	1.31	8 (16%)	1 1	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.74	2 (3%)	49 56	25, 36, 45, 60	0
55	D8	64/65 (98%)	1.51	18 (28%)	0 0	46, 58, 66, 72	0
56	B9	37/37 (100%)	1.07	2 (5%)	25 30	31, 49, 73, 74	0
56	D9	37/37 (100%)	1.27	5 (13%)	3 4	46, 57, 73, 76	0
All	All	20897/21748 (96%)	0.73	1673 (8%)	12 15	18, 64, 89, 109	0

The worst 5 of 1673 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	12.7
2	CB	165	VAL	12.6

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Mol	Chain	Res	Type	RSRZ
13	AM	124	PRO	11.3
23	CW	71	G	10.9
7	CG	83	ALA	10.6

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	7MG	CY	46	24/25	0.48	0.37	86,105,111,137	0
25	MIA	CY	37	22/30	0.61	0.38	72,95,113,138	0
25	5MU	CY	54	21/22	0.63	0.53	78,94,109,140	0
23	7MG	CW	46	24/25	0.66	0.27	79,96,109,133	0
25	PSU	CY	55	20/21	0.67	0.49	94,102,110,124	0
25	4SU	CY	8	20/21	0.68	0.22	93,103,113,128	0
23	4SU	CW	8	20/21	0.69	0.30	81,98,120,127	0
25	PSU	AY	55	20/21	0.70	0.29	93,101,108,122	0
23	7MG	AW	46	24/25	0.72	0.23	84,99,117,133	0
25	5MU	AY	54	21/22	0.73	0.26	80,96,105,131	0
25	7MG	AY	46	24/25	0.76	0.27	75,101,111,123	0
25	PSU	AY	39	20/21	0.76	0.30	78,90,117,123	0
25	PSU	CY	39	20/21	0.77	0.30	79,90,116,130	0
25	4SU	AY	8	20/21	0.78	0.16	82,96,103,118	0
23	PSU	CW	55	20/21	0.79	0.30	79,89,99,104	0
25	PSU	CY	32	20/21	0.79	0.21	80,92,101,107	0
25	MIA	AY	37	22/30	0.80	0.22	77,90,111,119	0
23	4SU	AW	8	20/21	0.81	0.20	86,95,112,128	0
25	PSU	AY	32	20/21	0.83	0.24	78,93,100,106	0
23	PSU	AW	55	20/21	0.84	0.27	77,90,98,104	0
23	MIA	CW	37	22/30	0.84	0.32	75,85,92,100	0
23	5MU	CW	54	21/22	0.84	0.24	74,88,99,101	0
23	PSU	CW	39	20/21	0.87	0.42	78,84,97,98	0
23	PSU	AW	32	20/21	0.88	0.25	77,83,92,98	0
23	PSU	CW	32	20/21	0.88	0.45	81,87,94,103	0
24	PSU	CX	55	20/21	0.89	0.15	70,80,91,96	0
23	31M	CW	76	41/42	0.89	0.41	50,63,73,88	20
23	5MU	AW	54	21/22	0.91	0.20	65,82,91,93	0
24	4SU	CX	8	20/21	0.91	0.17	77,87,95,97	0
24	5MU	CX	54	21/22	0.92	0.22	70,81,89,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	PSU	AW	39	20/21	0.93	0.23	73,82,95,97	0
23	MIA	AW	37	29/30	0.94	0.26	59,71,81,86	0
24	4SU	AX	8	20/21	0.94	0.18	54,66,82,89	0
23	31M	AW	76	41/42	0.94	0.33	37,54,66,83	9
24	5MC	AX	32	21/22	0.95	0.21	43,53,62,78	0
24	5MU	AX	54	21/22	0.95	0.20	49,68,79,84	0
24	PSU	AX	55	20/21	0.95	0.21	50,63,73,83	0
24	5MC	CX	32	21/22	0.96	0.21	63,76,86,88	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3730	1/1	0.31	0.19	71,71,71,71	0
57	MG	BA	3427	1/1	0.41	0.20	61,61,61,61	0
57	MG	BA	3670	1/1	0.43	0.26	61,61,61,61	0
57	MG	DA	3448	1/1	0.43	0.20	70,70,70,70	0
57	MG	DA	3403	1/1	0.45	0.14	57,57,57,57	0
57	MG	BA	3721	1/1	0.46	0.32	82,82,82,82	0
57	MG	DA	3651	1/1	0.48	0.53	75,75,75,75	0
57	MG	DA	3530	1/1	0.51	0.13	74,74,74,74	0
57	MG	DA	3329	1/1	0.54	0.13	54,54,54,54	0
57	MG	AW	3004	1/1	0.57	0.14	49,49,49,49	0
57	MG	DA	3563	1/1	0.57	0.15	74,74,74,74	0
57	MG	CT	3001	1/1	0.58	0.12	56,56,56,56	0
57	MG	DR	5001	1/1	0.58	0.24	70,70,70,70	0
57	MG	BA	3636	1/1	0.58	0.14	64,64,64,64	0
57	MG	DA	3259	1/1	0.58	0.21	43,43,43,43	0
57	MG	BB	215	1/1	0.59	0.18	73,73,73,73	0
57	MG	DA	3673	1/1	0.60	0.14	69,69,69,69	0
57	MG	CA	3070	1/1	0.61	0.15	63,63,63,63	0
57	MG	DA	3320	1/1	0.61	0.15	55,55,55,55	0
57	MG	CA	3088	1/1	0.62	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3616	1/1	0.62	0.21	65,65,65,65	0
57	MG	BA	3568	1/1	0.63	0.10	59,59,59,59	0
57	MG	AA	3004	1/1	0.63	0.15	67,67,67,67	0
57	MG	DA	3566	1/1	0.64	0.12	69,69,69,69	0
57	MG	DA	3213	1/1	0.64	0.32	63,63,63,63	0
57	MG	BA	3470	1/1	0.65	0.13	62,62,62,62	0
57	MG	D8	5001	1/1	0.65	0.23	66,66,66,66	0
57	MG	DA	3532	1/1	0.66	0.24	69,69,69,69	0
57	MG	CA	3051	1/1	0.66	0.19	81,81,81,81	0
57	MG	DA	3413	1/1	0.66	0.23	48,48,48,48	0
57	MG	DA	3518	1/1	0.66	0.24	54,54,54,54	0
57	MG	AA	3153	1/1	0.66	0.18	74,74,74,74	0
57	MG	DA	3256	1/1	0.67	0.19	62,62,62,62	0
57	MG	CX	3002	1/1	0.67	0.14	70,70,70,70	0
57	MG	AX	3014	1/1	0.67	0.19	72,72,72,72	0
57	MG	DA	3244	1/1	0.69	0.11	71,71,71,71	0
57	MG	DA	3076	1/1	0.69	0.14	58,58,58,58	0
57	MG	DB	3011	1/1	0.69	0.14	72,72,72,72	0
57	MG	BA	3678	1/1	0.70	0.08	65,65,65,65	0
57	MG	DA	3125	1/1	0.71	0.26	70,70,70,70	0
57	MG	DA	3633	1/1	0.71	0.12	58,58,58,58	0
57	MG	CA	3018	1/1	0.72	0.16	69,69,69,69	0
57	MG	BA	3070	1/1	0.72	0.37	59,59,59,59	0
57	MG	BA	3003	1/1	0.72	0.19	60,60,60,60	0
57	MG	DA	3316	1/1	0.72	0.11	45,45,45,45	0
57	MG	BA	3053	1/1	0.72	0.21	54,54,54,54	0
57	MG	AA	3103	1/1	0.73	0.24	73,73,73,73	0
57	MG	DA	3546	1/1	0.73	0.11	71,71,71,71	0
57	MG	BA	3257	1/1	0.73	0.23	53,53,53,53	0
57	MG	BA	3540	1/1	0.73	0.23	37,37,37,37	0
57	MG	DA	3060	1/1	0.74	0.15	64,64,64,64	0
57	MG	DA	3616	1/1	0.74	0.11	71,71,71,71	0
57	MG	DD	303	1/1	0.74	0.62	87,87,87,87	0
57	MG	AA	3169	1/1	0.74	0.13	62,62,62,62	0
57	MG	BA	3300	1/1	0.74	0.25	57,57,57,57	0
57	MG	AA	3206	1/1	0.74	0.19	64,64,64,64	0
57	MG	BA	3401	1/1	0.75	0.16	35,35,35,35	0
57	MG	BB	209	1/1	0.75	0.32	65,65,65,65	0
57	MG	B4	502	1/1	0.75	0.14	71,71,71,71	0
57	MG	BA	3641	1/1	0.75	0.21	68,68,68,68	0
57	MG	DA	3608	1/1	0.75	0.13	68,68,68,68	0
57	MG	BA	3503	1/1	0.75	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3538	1/1	0.75	0.15	40,40,40,40	0
57	MG	BA	3704	1/1	0.76	0.14	77,77,77,77	0
57	MG	DA	3252	1/1	0.76	0.08	37,37,37,37	0
57	MG	BA	3602	1/1	0.76	0.16	53,53,53,53	0
57	MG	BF	308	1/1	0.76	0.20	46,46,46,46	0
57	MG	DB	3008	1/1	0.76	0.20	67,67,67,67	0
57	MG	DA	3531	1/1	0.76	0.18	61,61,61,61	0
57	MG	DA	3635	1/1	0.76	0.11	38,38,38,38	0
57	MG	BA	3362	1/1	0.76	0.20	41,41,41,41	0
57	MG	AA	3013	1/1	0.76	0.17	69,69,69,69	0
57	MG	BA	3353	1/1	0.76	0.12	50,50,50,50	0
57	MG	BA	3095	1/1	0.76	0.24	51,51,51,51	0
57	MG	BA	3225	1/1	0.76	0.16	61,61,61,61	0
57	MG	BF	304	1/1	0.76	0.18	45,45,45,45	0
57	MG	DA	3642	1/1	0.76	0.28	54,54,54,54	0
57	MG	DA	3620	1/1	0.76	0.12	68,68,68,68	0
57	MG	CJ	5001	1/1	0.76	0.08	73,73,73,73	0
57	MG	BA	3560	1/1	0.77	0.14	56,56,56,56	0
57	MG	DA	3262	1/1	0.77	0.10	65,65,65,65	0
57	MG	BA	3615	1/1	0.77	0.21	68,68,68,68	0
57	MG	BB	214	1/1	0.77	0.18	49,49,49,49	0
57	MG	BA	3733	1/1	0.77	0.11	58,58,58,58	0
57	MG	DA	3383	1/1	0.77	0.21	54,54,54,54	0
57	MG	DA	3205	1/1	0.77	0.10	56,56,56,56	0
57	MG	DA	3234	1/1	0.77	0.21	63,63,63,63	0
57	MG	AA	3084	1/1	0.78	0.24	51,51,51,51	0
57	MG	BA	3421	1/1	0.78	0.17	32,32,32,32	0
57	MG	DA	3585	1/1	0.78	0.12	43,43,43,43	0
57	MG	BA	3716	1/1	0.78	0.12	65,65,65,65	0
57	MG	BA	3771	1/1	0.78	0.29	50,50,50,50	0
57	MG	DA	3610	1/1	0.78	0.22	64,64,64,64	0
57	MG	DA	3218	1/1	0.78	0.13	59,59,59,59	0
57	MG	DA	3554	1/1	0.78	0.10	62,62,62,62	0
57	MG	CA	3017	1/1	0.78	0.19	53,53,53,53	0
57	MG	BA	3638	1/1	0.79	0.14	63,63,63,63	0
57	MG	CA	3013	1/1	0.79	0.13	69,69,69,69	0
57	MG	DA	3212	1/1	0.79	0.15	45,45,45,45	0
57	MG	BA	3724	1/1	0.79	0.18	62,62,62,62	0
57	MG	AE	202	1/1	0.79	0.12	80,80,80,80	0
57	MG	CA	3024	1/1	0.79	0.10	74,74,74,74	0
57	MG	DA	3335	1/1	0.79	0.16	47,47,47,47	0
59	ZN	D4	501	1/1	0.79	0.07	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3607	1/1	0.79	0.14	65,65,65,65	0
57	MG	BA	3114	1/1	0.79	0.18	53,53,53,53	0
57	MG	DP	201	1/1	0.79	0.29	70,70,70,70	0
57	MG	DA	3417	1/1	0.79	0.11	52,52,52,52	0
57	MG	BA	3757	1/1	0.80	0.20	76,76,76,76	0
57	MG	CA	3064	1/1	0.80	0.17	60,60,60,60	0
57	MG	BA	3052	1/1	0.80	0.16	56,56,56,56	0
57	MG	AA	3069	1/1	0.80	0.19	68,68,68,68	0
57	MG	DA	3222	1/1	0.80	0.14	57,57,57,57	0
57	MG	BA	3020	1/1	0.80	0.22	53,53,53,53	0
57	MG	DA	3078	1/1	0.80	0.19	57,57,57,57	0
57	MG	BA	3781	1/1	0.80	0.20	41,41,41,41	0
57	MG	AA	3160	1/1	0.80	0.21	59,59,59,59	0
57	MG	CA	3166	1/1	0.80	0.14	66,66,66,66	0
57	MG	BA	3728	1/1	0.80	0.33	48,48,48,48	0
57	MG	DA	3340	1/1	0.80	0.18	58,58,58,58	0
57	MG	DA	3025	1/1	0.80	0.16	54,54,54,54	0
57	MG	AX	3011	1/1	0.80	0.20	78,78,78,78	0
57	MG	CA	3152	1/1	0.80	0.20	76,76,76,76	0
57	MG	DG	3001	1/1	0.81	0.09	55,55,55,55	0
57	MG	AA	3183	1/1	0.81	0.15	65,65,65,65	0
57	MG	DA	3082	1/1	0.81	0.14	47,47,47,47	0
57	MG	BB	218	1/1	0.81	0.22	77,77,77,77	0
57	MG	AA	3138	1/1	0.81	0.18	71,71,71,71	0
57	MG	DA	3321	1/1	0.81	0.08	48,48,48,48	0
57	MG	BA	3316	1/1	0.81	0.12	66,66,66,66	0
57	MG	DA	3118	1/1	0.81	0.15	77,77,77,77	0
57	MG	BA	3066	1/1	0.81	0.19	49,49,49,49	0
57	MG	DA	3451	1/1	0.81	0.16	55,55,55,55	0
57	MG	AA	3170	1/1	0.81	0.13	75,75,75,75	0
57	MG	CX	3003	1/1	0.81	0.22	54,54,54,54	0
57	MG	DA	3669	1/1	0.81	0.25	55,55,55,55	0
57	MG	AA	3091	1/1	0.81	0.14	60,60,60,60	0
57	MG	BA	3172	1/1	0.81	0.19	46,46,46,46	0
57	MG	BA	3463	1/1	0.81	0.20	48,48,48,48	0
57	MG	DA	3402	1/1	0.81	0.10	66,66,66,66	0
57	MG	BA	3693	1/1	0.81	0.19	56,56,56,56	0
57	MG	CA	3146	1/1	0.81	0.19	66,66,66,66	0
57	MG	AW	3001	1/1	0.81	0.11	60,60,60,60	0
57	MG	DA	3408	1/1	0.81	0.08	58,58,58,58	0
57	MG	BA	3715	1/1	0.81	0.14	63,63,63,63	0
57	MG	DA	3589	1/1	0.81	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3630	1/1	0.82	0.19	61,61,61,61	0
57	MG	BA	3342	1/1	0.82	0.10	46,46,46,46	0
57	MG	DA	3553	1/1	0.82	0.10	49,49,49,49	0
57	MG	BA	3707	1/1	0.82	0.24	44,44,44,44	0
57	MG	DA	3513	1/1	0.82	0.16	52,52,52,52	0
57	MG	CA	3107	1/1	0.82	0.20	80,80,80,80	0
57	MG	BA	3695	1/1	0.82	0.18	67,67,67,67	0
57	MG	DA	3333	1/1	0.82	0.13	41,41,41,41	0
57	MG	DA	3487	1/1	0.82	0.21	62,62,62,62	0
57	MG	BA	3709	1/1	0.82	0.20	62,62,62,62	0
57	MG	DA	3394	1/1	0.82	0.18	65,65,65,65	0
57	MG	DA	3406	1/1	0.82	0.11	51,51,51,51	0
57	MG	DA	3342	1/1	0.82	0.11	42,42,42,42	0
57	MG	BA	3761	1/1	0.82	0.16	59,59,59,59	0
57	MG	BA	3242	1/1	0.82	0.21	55,55,55,55	0
57	MG	DA	3582	1/1	0.82	0.07	56,56,56,56	0
57	MG	DA	3276	1/1	0.82	0.12	49,49,49,49	0
57	MG	CA	3109	1/1	0.82	0.13	67,67,67,67	0
57	MG	BA	3317	1/1	0.82	0.18	53,53,53,53	0
57	MG	BA	3473	1/1	0.82	0.19	56,56,56,56	0
57	MG	DA	3308	1/1	0.82	0.15	61,61,61,61	0
57	MG	DA	3628	1/1	0.82	0.24	76,76,76,76	0
57	MG	BA	3273	1/1	0.82	0.22	54,54,54,54	0
57	MG	BA	3335	1/1	0.82	0.23	52,52,52,52	0
57	MG	BA	3760	1/1	0.82	0.19	44,44,44,44	0
57	MG	CA	3149	1/1	0.82	0.14	52,52,52,52	0
57	MG	BA	3418	1/1	0.82	0.17	30,30,30,30	0
57	MG	BA	3587	1/1	0.83	0.17	36,36,36,36	0
57	MG	BA	3788	1/1	0.83	0.15	51,51,51,51	0
57	MG	BA	3372	1/1	0.83	0.16	28,28,28,28	0
57	MG	AA	3002	1/1	0.83	0.15	71,71,71,71	0
57	MG	AA	3023	1/1	0.83	0.13	74,74,74,74	0
57	MG	BA	3154	1/1	0.83	0.23	47,47,47,47	0
57	MG	CA	3058	1/1	0.83	0.13	68,68,68,68	0
57	MG	CA	3009	1/1	0.83	0.11	64,64,64,64	0
57	MG	B5	101	1/1	0.83	0.24	51,51,51,51	0
57	MG	BA	3759	1/1	0.83	0.18	33,33,33,33	0
57	MG	AA	3189	1/1	0.83	0.12	65,65,65,65	0
57	MG	DA	3268	1/1	0.83	0.17	51,51,51,51	0
57	MG	DA	3385	1/1	0.83	0.11	52,52,52,52	0
57	MG	AA	3020	1/1	0.83	0.13	76,76,76,76	0
57	MG	AA	3008	1/1	0.83	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3075	1/1	0.83	0.29	59,59,59,59	0
57	MG	DA	3544	1/1	0.83	0.12	65,65,65,65	0
57	MG	AA	3127	1/1	0.83	0.16	65,65,65,65	0
57	MG	CA	3087	1/1	0.83	0.19	67,67,67,67	0
57	MG	DA	3446	1/1	0.83	0.11	45,45,45,45	0
57	MG	BA	3769	1/1	0.83	0.18	52,52,52,52	0
57	MG	DA	3422	1/1	0.83	0.08	46,46,46,46	0
57	MG	BA	3669	1/1	0.83	0.09	62,62,62,62	0
57	MG	BA	3434	1/1	0.83	0.13	55,55,55,55	0
57	MG	AA	3017	1/1	0.83	0.18	71,71,71,71	0
57	MG	BA	3802	1/1	0.83	0.47	54,54,54,54	0
57	MG	AA	3139	1/1	0.83	0.14	59,59,59,59	0
57	MG	BA	3594	1/1	0.83	0.12	40,40,40,40	0
57	MG	BA	3446	1/1	0.83	0.17	40,40,40,40	0
57	MG	AA	3005	1/1	0.84	0.14	62,62,62,62	0
57	MG	DA	3421	1/1	0.84	0.13	50,50,50,50	0
57	MG	BA	3438	1/1	0.84	0.14	60,60,60,60	0
57	MG	DA	3646	1/1	0.84	0.14	59,59,59,59	0
57	MG	CA	3066	1/1	0.84	0.14	66,66,66,66	0
57	MG	DA	3044	1/1	0.84	0.10	62,62,62,62	0
57	MG	AA	3025	1/1	0.84	0.24	62,62,62,62	0
57	MG	DA	3431	1/1	0.84	0.23	50,50,50,50	0
57	MG	BA	3512	1/1	0.84	0.18	52,52,52,52	0
57	MG	DA	3450	1/1	0.84	0.10	40,40,40,40	0
57	MG	DA	3414	1/1	0.84	0.13	43,43,43,43	0
57	MG	DA	3071	1/1	0.84	0.13	59,59,59,59	0
57	MG	BA	3179	1/1	0.84	0.17	50,50,50,50	0
57	MG	BA	3480	1/1	0.84	0.20	35,35,35,35	0
57	MG	DA	3247	1/1	0.84	0.09	45,45,45,45	0
57	MG	DA	3147	1/1	0.84	0.15	56,56,56,56	0
57	MG	BA	3391	1/1	0.84	0.24	63,63,63,63	0
57	MG	BA	3764	1/1	0.84	0.17	51,51,51,51	0
57	MG	DA	3088	1/1	0.84	0.18	47,47,47,47	0
57	MG	DA	3430	1/1	0.84	0.11	37,37,37,37	0
57	MG	DA	3122	1/1	0.84	0.11	49,49,49,49	0
57	MG	CV	101	1/1	0.84	0.13	72,72,72,72	0
57	MG	CA	3098	1/1	0.84	0.09	65,65,65,65	0
57	MG	DA	3476	1/1	0.84	0.14	62,62,62,62	0
57	MG	CA	3021	1/1	0.84	0.14	61,61,61,61	0
57	MG	BA	3018	1/1	0.84	0.20	56,56,56,56	0
57	MG	BA	3794	1/1	0.84	0.26	51,51,51,51	0
57	MG	BA	3404	1/1	0.84	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3253	1/1	0.84	0.23	55,55,55,55	0
57	MG	DA	3468	1/1	0.84	0.27	66,66,66,66	0
57	MG	DA	3497	1/1	0.84	0.11	55,55,55,55	0
57	MG	BA	3129	1/1	0.84	0.28	58,58,58,58	0
57	MG	CA	3140	1/1	0.84	0.15	67,67,67,67	0
57	MG	CA	3116	1/1	0.84	0.22	68,68,68,68	0
57	MG	BA	3546	1/1	0.85	0.19	40,40,40,40	0
57	MG	BA	3754	1/1	0.85	0.18	48,48,48,48	0
57	MG	CA	3052	1/1	0.85	0.21	72,72,72,72	0
57	MG	DA	3362	1/1	0.85	0.21	44,44,44,44	0
57	MG	AA	3079	1/1	0.85	0.13	68,68,68,68	0
57	MG	D0	101	1/1	0.85	0.08	71,71,71,71	0
57	MG	BA	3755	1/1	0.85	0.15	55,55,55,55	0
57	MG	DA	3425	1/1	0.85	0.12	61,61,61,61	0
57	MG	BA	3432	1/1	0.85	0.14	58,58,58,58	0
57	MG	BA	3231	1/1	0.85	0.32	63,63,63,63	0
57	MG	AA	3034	1/1	0.85	0.11	47,47,47,47	0
57	MG	BA	3293	1/1	0.85	0.26	50,50,50,50	0
57	MG	BA	3296	1/1	0.85	0.18	53,53,53,53	0
57	MG	AA	3166	1/1	0.85	0.14	69,69,69,69	0
57	MG	BA	3443	1/1	0.85	0.23	37,37,37,37	0
57	MG	CA	3141	1/1	0.85	0.04	92,92,92,92	0
57	MG	AA	3196	1/1	0.85	0.21	74,74,74,74	0
57	MG	DU	3002	1/1	0.85	0.40	55,55,55,55	0
57	MG	DA	3661	1/1	0.85	0.16	62,62,62,62	0
57	MG	AA	3073	1/1	0.85	0.10	56,56,56,56	0
57	MG	BA	3453	1/1	0.85	0.32	45,45,45,45	0
57	MG	AA	3041	1/1	0.85	0.21	46,46,46,46	0
57	MG	BA	3301	1/1	0.85	0.13	60,60,60,60	0
57	MG	BA	3718	1/1	0.85	0.11	71,71,71,71	0
57	MG	AA	3184	1/1	0.85	0.12	60,60,60,60	0
57	MG	DA	3498	1/1	0.85	0.08	51,51,51,51	0
57	MG	BA	3456	1/1	0.85	0.18	49,49,49,49	0
57	MG	BA	3506	1/1	0.85	0.10	58,58,58,58	0
57	MG	AA	3001	1/1	0.85	0.14	61,61,61,61	0
57	MG	BB	220	1/1	0.85	0.13	57,57,57,57	0
57	MG	DA	3069	1/1	0.85	0.23	57,57,57,57	0
57	MG	AA	3033	1/1	0.85	0.14	59,59,59,59	0
57	MG	DA	3571	1/1	0.85	0.12	56,56,56,56	0
57	MG	B2	3001	1/1	0.85	0.21	56,56,56,56	0
57	MG	DA	3410	1/1	0.85	0.13	53,53,53,53	0
57	MG	DA	3139	1/1	0.85	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3657	1/1	0.85	0.10	63,63,63,63	0
57	MG	CA	3016	1/1	0.85	0.11	57,57,57,57	0
57	MG	CA	3158	1/1	0.85	0.13	67,67,67,67	0
57	MG	DA	3178	1/1	0.85	0.22	50,50,50,50	0
57	MG	DA	3415	1/1	0.85	0.11	68,68,68,68	0
57	MG	BA	3681	1/1	0.85	0.08	66,66,66,66	0
57	MG	BA	3305	1/1	0.85	0.09	62,62,62,62	0
57	MG	DE	303	1/1	0.85	0.12	54,54,54,54	0
57	MG	DA	3180	1/1	0.85	0.20	42,42,42,42	0
57	MG	AA	3047	1/1	0.85	0.17	63,63,63,63	0
57	MG	BA	3530	1/1	0.86	0.22	49,49,49,49	0
57	MG	DA	3495	1/1	0.86	0.11	47,47,47,47	0
57	MG	BA	3284	1/1	0.86	0.27	43,43,43,43	0
57	MG	DA	3462	1/1	0.86	0.20	42,42,42,42	0
57	MG	AA	3177	1/1	0.86	0.08	66,66,66,66	0
57	MG	DA	3658	1/1	0.86	0.12	62,62,62,62	0
57	MG	BA	3426	1/1	0.86	0.20	37,37,37,37	0
57	MG	BA	3308	1/1	0.86	0.19	43,43,43,43	0
57	MG	DA	3641	1/1	0.86	0.20	69,69,69,69	0
57	MG	DA	3360	1/1	0.86	0.16	46,46,46,46	0
57	MG	BB	202	1/1	0.86	0.28	59,59,59,59	0
57	MG	CA	3073	1/1	0.86	0.14	57,57,57,57	0
57	MG	DA	3592	1/1	0.86	0.07	51,51,51,51	0
57	MG	CA	3033	1/1	0.86	0.19	71,71,71,71	0
57	MG	BA	3598	1/1	0.86	0.14	63,63,63,63	0
57	MG	BA	3680	1/1	0.86	0.11	68,68,68,68	0
57	MG	DA	3309	1/1	0.86	0.09	51,51,51,51	0
57	MG	DA	3440	1/1	0.86	0.09	61,61,61,61	0
57	MG	BA	3213	1/1	0.86	0.26	40,40,40,40	0
57	MG	CA	3097	1/1	0.86	0.15	69,69,69,69	0
57	MG	DA	3484	1/1	0.86	0.12	62,62,62,62	0
57	MG	DA	3523	1/1	0.86	0.10	59,59,59,59	0
57	MG	BA	3165	1/1	0.86	0.17	45,45,45,45	0
57	MG	DA	3667	1/1	0.86	0.12	50,50,50,50	0
57	MG	CE	3001	1/1	0.86	0.10	79,79,79,79	0
57	MG	AA	3214	1/1	0.86	0.17	73,73,73,73	0
57	MG	AA	3192	1/1	0.86	0.14	71,71,71,71	0
57	MG	BE	305	1/1	0.86	0.17	43,43,43,43	0
57	MG	DA	3528	1/1	0.86	0.15	62,62,62,62	0
57	MG	DA	3138	1/1	0.86	0.13	55,55,55,55	0
57	MG	DB	3012	1/1	0.86	0.33	61,61,61,61	0
57	MG	BA	3447	1/1	0.86	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3185	1/1	0.86	0.11	68,68,68,68	0
57	MG	BA	3601	1/1	0.86	0.12	55,55,55,55	0
57	MG	AA	3054	1/1	0.86	0.13	53,53,53,53	0
57	MG	BA	3180	1/1	0.86	0.17	47,47,47,47	0
57	MG	DA	3035	1/1	0.86	0.20	52,52,52,52	0
57	MG	BA	3274	1/1	0.86	0.14	49,49,49,49	0
57	MG	DA	3312	1/1	0.86	0.10	54,54,54,54	0
57	MG	CA	3115	1/1	0.86	0.09	63,63,63,63	0
57	MG	AA	3065	1/1	0.86	0.20	63,63,63,63	0
57	MG	DA	3654	1/1	0.86	0.12	56,56,56,56	0
57	MG	DA	3062	1/1	0.86	0.20	63,63,63,63	0
57	MG	DA	3577	1/1	0.86	0.14	58,58,58,58	0
57	MG	BA	3486	1/1	0.86	0.13	57,57,57,57	0
57	MG	DA	3575	1/1	0.87	0.14	64,64,64,64	0
57	MG	BA	3419	1/1	0.87	0.23	37,37,37,37	0
57	MG	DA	3437	1/1	0.87	0.16	52,52,52,52	0
57	MG	DA	3676	1/1	0.87	0.33	67,67,67,67	0
57	MG	BA	3513	1/1	0.87	0.15	59,59,59,59	0
57	MG	CA	3027	1/1	0.87	0.20	64,64,64,64	0
57	MG	BA	3732	1/1	0.87	0.26	51,51,51,51	0
57	MG	DA	3148	1/1	0.87	0.12	54,54,54,54	0
57	MG	DA	3356	1/1	0.87	0.10	36,36,36,36	0
57	MG	BA	3147	1/1	0.87	0.16	45,45,45,45	0
57	MG	AA	3089	1/1	0.87	0.15	60,60,60,60	0
57	MG	BA	3658	1/1	0.87	0.26	61,61,61,61	0
57	MG	BA	3742	1/1	0.87	0.24	65,65,65,65	0
57	MG	DA	3110	1/1	0.87	0.31	58,58,58,58	0
57	MG	DF	3001	1/1	0.87	0.20	44,44,44,44	0
57	MG	DA	3242	1/1	0.87	0.11	52,52,52,52	0
57	MG	DA	3659	1/1	0.87	0.14	48,48,48,48	0
57	MG	DA	3632	1/1	0.87	0.15	36,36,36,36	0
57	MG	DA	3400	1/1	0.87	0.12	54,54,54,54	0
57	MG	DA	3140	1/1	0.87	0.15	58,58,58,58	0
57	MG	BX	3002	1/1	0.87	0.19	46,46,46,46	0
57	MG	AA	3031	1/1	0.87	0.23	70,70,70,70	0
57	MG	BA	3548	1/1	0.87	0.17	40,40,40,40	0
57	MG	BA	3637	1/1	0.87	0.11	39,39,39,39	0
57	MG	DA	3007	1/1	0.87	0.14	50,50,50,50	0
57	MG	BA	3584	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	3217	1/1	0.87	0.14	38,38,38,38	0
57	MG	CA	3138	1/1	0.87	0.19	80,80,80,80	0
57	MG	DA	3240	1/1	0.87	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3038	1/1	0.87	0.33	68,68,68,68	0
57	MG	AA	3124	1/1	0.87	0.09	47,47,47,47	0
57	MG	BA	3258	1/1	0.87	0.13	44,44,44,44	0
57	MG	AA	3197	1/1	0.87	0.26	70,70,70,70	0
57	MG	BA	3780	1/1	0.87	0.11	62,62,62,62	0
57	MG	CA	3124	1/1	0.87	0.12	59,59,59,59	0
57	MG	DQ	3004	1/1	0.87	0.28	54,54,54,54	0
57	MG	DA	3521	1/1	0.87	0.13	58,58,58,58	0
57	MG	DA	3339	1/1	0.87	0.15	61,61,61,61	0
57	MG	BA	3583	1/1	0.87	0.21	45,45,45,45	0
57	MG	BA	3001	1/1	0.87	0.14	53,53,53,53	0
57	MG	BA	3386	1/1	0.87	0.16	53,53,53,53	0
57	MG	BA	3206	1/1	0.87	0.23	49,49,49,49	0
57	MG	BA	3071	1/1	0.87	0.35	59,59,59,59	0
57	MG	DA	3061	1/1	0.87	0.13	48,48,48,48	0
57	MG	BA	3074	1/1	0.87	0.21	46,46,46,46	0
57	MG	DA	3283	1/1	0.87	0.11	51,51,51,51	0
57	MG	AA	3045	1/1	0.87	0.12	58,58,58,58	0
57	MG	BA	3684	1/1	0.87	0.12	68,68,68,68	0
57	MG	CA	3168	1/1	0.87	0.11	56,56,56,56	0
57	MG	BA	3318	1/1	0.87	0.12	41,41,41,41	0
57	MG	CA	3090	1/1	0.87	0.10	67,67,67,67	0
57	MG	BA	3545	1/1	0.87	0.14	65,65,65,65	0
57	MG	DA	3002	1/1	0.87	0.10	48,48,48,48	0
57	MG	BB	211	1/1	0.87	0.10	51,51,51,51	0
57	MG	AA	3121	1/1	0.87	0.12	70,70,70,70	0
57	MG	AA	3190	1/1	0.87	0.10	58,58,58,58	0
57	MG	AA	3049	1/1	0.87	0.21	64,64,64,64	0
57	MG	DA	3361	1/1	0.87	0.12	44,44,44,44	0
57	MG	DA	3558	1/1	0.87	0.17	61,61,61,61	0
57	MG	BA	3128	1/1	0.87	0.14	69,69,69,69	0
57	MG	AA	3051	1/1	0.87	0.23	73,73,73,73	0
57	MG	BA	3710	1/1	0.88	0.17	57,57,57,57	0
57	MG	DA	3606	1/1	0.88	0.10	71,71,71,71	0
57	MG	BA	3267	1/1	0.88	0.19	65,65,65,65	0
57	MG	BA	3033	1/1	0.88	0.29	53,53,53,53	0
57	MG	AA	3019	1/1	0.88	0.11	66,66,66,66	0
57	MG	DA	3527	1/1	0.88	0.12	60,60,60,60	0
57	MG	DA	3567	1/1	0.88	0.27	62,62,62,62	0
57	MG	B7	105	1/1	0.88	0.16	56,56,56,56	0
57	MG	BA	3030	1/1	0.88	0.18	46,46,46,46	0
57	MG	BA	3740	1/1	0.88	0.16	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3526	1/1	0.88	0.17	44,44,44,44	0
57	MG	BA	3619	1/1	0.88	0.20	58,58,58,58	0
57	MG	BA	3673	1/1	0.88	0.17	55,55,55,55	0
57	MG	DA	3208	1/1	0.88	0.36	58,58,58,58	0
57	MG	BA	3624	1/1	0.88	0.10	68,68,68,68	0
57	MG	BA	3430	1/1	0.88	0.16	37,37,37,37	0
57	MG	DA	3380	1/1	0.88	0.07	55,55,55,55	0
57	MG	BA	3578	1/1	0.88	0.09	46,46,46,46	0
57	MG	CA	3157	1/1	0.88	0.11	58,58,58,58	0
57	MG	DA	3288	1/1	0.88	0.14	52,52,52,52	0
57	MG	DA	3591	1/1	0.88	0.17	55,55,55,55	0
57	MG	AA	3026	1/1	0.88	0.13	70,70,70,70	0
57	MG	DA	3334	1/1	0.88	0.15	52,52,52,52	0
57	MG	DA	3323	1/1	0.88	0.11	50,50,50,50	0
57	MG	AA	3107	1/1	0.88	0.18	64,64,64,64	0
57	MG	DA	3609	1/1	0.88	0.10	46,46,46,46	0
57	MG	BA	3057	1/1	0.88	0.20	34,34,34,34	0
57	MG	CA	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3162	1/1	0.88	0.15	38,38,38,38	0
57	MG	BA	3297	1/1	0.88	0.14	43,43,43,43	0
57	MG	BA	3002	1/1	0.88	0.10	50,50,50,50	0
57	MG	DA	3274	1/1	0.88	0.15	58,58,58,58	0
57	MG	AA	3072	1/1	0.88	0.12	66,66,66,66	0
57	MG	DA	3388	1/1	0.88	0.15	53,53,53,53	0
57	MG	BA	3566	1/1	0.88	0.21	67,67,67,67	0
57	MG	DA	3056	1/1	0.88	0.09	51,51,51,51	0
57	MG	DB	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3266	1/1	0.88	0.19	39,39,39,39	0
57	MG	BA	3006	1/1	0.88	0.19	48,48,48,48	0
57	MG	BA	3514	1/1	0.88	0.23	48,48,48,48	0
57	MG	DA	3590	1/1	0.88	0.10	51,51,51,51	0
57	MG	BA	3442	1/1	0.88	0.17	44,44,44,44	0
57	MG	DA	3603	1/1	0.88	0.06	41,41,41,41	0
57	MG	BA	3333	1/1	0.88	0.20	38,38,38,38	0
57	MG	BA	3072	1/1	0.88	0.14	47,47,47,47	0
57	MG	DA	3093	1/1	0.88	0.09	62,62,62,62	0
57	MG	DA	3636	1/1	0.88	0.32	63,63,63,63	0
57	MG	BA	3532	1/1	0.88	0.15	52,52,52,52	0
57	MG	DA	3469	1/1	0.88	0.28	44,44,44,44	0
57	MG	BA	3471	1/1	0.88	0.27	53,53,53,53	0
57	MG	AA	3046	1/1	0.88	0.22	55,55,55,55	0
57	MG	AX	3002	1/1	0.88	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3679	1/1	0.88	0.12	62,62,62,62	0
57	MG	AA	3145	1/1	0.88	0.12	66,66,66,66	0
57	MG	BA	3502	1/1	0.88	0.12	56,56,56,56	0
57	MG	DA	3618	1/1	0.88	0.12	53,53,53,53	0
57	MG	BA	3409	1/1	0.88	0.16	30,30,30,30	0
57	MG	AX	3010	1/1	0.88	0.21	59,59,59,59	0
57	MG	CA	3163	1/1	0.88	0.09	63,63,63,63	0
57	MG	DA	3614	1/1	0.88	0.07	65,65,65,65	0
57	MG	AA	3200	1/1	0.88	0.08	73,73,73,73	0
57	MG	AA	3128	1/1	0.88	0.08	57,57,57,57	0
57	MG	CA	3039	1/1	0.88	0.11	68,68,68,68	0
57	MG	DA	3216	1/1	0.88	0.22	56,56,56,56	0
57	MG	DA	3572	1/1	0.88	0.06	62,62,62,62	0
57	MG	DA	3526	1/1	0.88	0.11	48,48,48,48	0
57	MG	BA	3117	1/1	0.88	0.20	59,59,59,59	0
57	MG	DA	3092	1/1	0.88	0.18	45,45,45,45	0
57	MG	DA	3367	1/1	0.88	0.14	61,61,61,61	0
57	MG	BA	3275	1/1	0.88	0.17	58,58,58,58	0
57	MG	AA	3094	1/1	0.88	0.17	59,59,59,59	0
57	MG	BA	3185	1/1	0.88	0.19	57,57,57,57	0
57	MG	BA	3212	1/1	0.88	0.24	54,54,54,54	0
57	MG	BA	3337	1/1	0.88	0.17	58,58,58,58	0
57	MG	DB	3002	1/1	0.88	0.17	65,65,65,65	0
57	MG	BA	3122	1/1	0.88	0.15	41,41,41,41	0
57	MG	DA	3332	1/1	0.89	0.11	53,53,53,53	0
57	MG	BA	3397	1/1	0.89	0.15	30,30,30,30	0
57	MG	CA	3020	1/1	0.89	0.11	56,56,56,56	0
57	MG	CA	3159	1/1	0.89	0.18	70,70,70,70	0
57	MG	DA	3371	1/1	0.89	0.13	58,58,58,58	0
57	MG	DA	3355	1/1	0.89	0.12	58,58,58,58	0
57	MG	CA	3076	1/1	0.89	0.14	57,57,57,57	0
57	MG	DA	3638	1/1	0.89	0.10	51,51,51,51	0
57	MG	DX	101	1/1	0.89	0.12	51,51,51,51	0
57	MG	CA	3156	1/1	0.89	0.10	73,73,73,73	0
57	MG	DA	3248	1/1	0.89	0.12	56,56,56,56	0
57	MG	CA	3062	1/1	0.89	0.17	64,64,64,64	0
57	MG	CA	3022	1/1	0.89	0.20	78,78,78,78	0
57	MG	BA	3008	1/1	0.89	0.17	47,47,47,47	0
57	MG	CA	3128	1/1	0.89	0.15	65,65,65,65	0
57	MG	DA	3275	1/1	0.89	0.17	42,42,42,42	0
57	MG	BV	203	1/1	0.89	0.19	38,38,38,38	0
57	MG	CA	3041	1/1	0.89	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3402	1/1	0.89	0.14	40,40,40,40	0
57	MG	AA	3176	1/1	0.89	0.10	67,67,67,67	0
57	MG	BA	3023	1/1	0.89	0.22	36,36,36,36	0
57	MG	BA	3596	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3499	1/1	0.89	0.10	58,58,58,58	0
57	MG	DA	3311	1/1	0.89	0.17	54,54,54,54	0
57	MG	DA	3420	1/1	0.89	0.24	60,60,60,60	0
57	MG	BQ	3005	1/1	0.89	0.13	49,49,49,49	0
57	MG	DA	3444	1/1	0.89	0.06	44,44,44,44	0
57	MG	DA	3481	1/1	0.89	0.41	55,55,55,55	0
57	MG	BA	3314	1/1	0.89	0.13	58,58,58,58	0
57	MG	AM	201	1/1	0.89	0.16	51,51,51,51	0
57	MG	AA	3064	1/1	0.89	0.24	60,60,60,60	0
57	MG	DA	3151	1/1	0.89	0.09	55,55,55,55	0
57	MG	AA	3108	1/1	0.89	0.28	67,67,67,67	0
57	MG	DA	3564	1/1	0.89	0.16	61,61,61,61	0
57	MG	DA	3593	1/1	0.89	0.11	40,40,40,40	0
57	MG	DA	3124	1/1	0.89	0.15	57,57,57,57	0
57	MG	DA	3106	1/1	0.89	0.13	52,52,52,52	0
57	MG	DA	3470	1/1	0.89	0.19	45,45,45,45	0
57	MG	BA	3106	1/1	0.89	0.22	42,42,42,42	0
57	MG	BA	3324	1/1	0.89	0.17	45,45,45,45	0
57	MG	DA	3206	1/1	0.89	0.13	50,50,50,50	0
57	MG	DA	3492	1/1	0.89	0.12	55,55,55,55	0
57	MG	DA	3223	1/1	0.89	0.15	50,50,50,50	0
57	MG	BA	3810	1/1	0.89	0.18	41,41,41,41	0
57	MG	BA	3745	1/1	0.89	0.08	75,75,75,75	0
57	MG	BA	3573	1/1	0.89	0.16	51,51,51,51	0
57	MG	DA	3095	1/1	0.89	0.15	58,58,58,58	0
57	MG	BA	3444	1/1	0.89	0.21	29,29,29,29	0
57	MG	BA	3092	1/1	0.89	0.16	37,37,37,37	0
57	MG	DA	3077	1/1	0.89	0.23	61,61,61,61	0
57	MG	BA	3590	1/1	0.89	0.16	50,50,50,50	0
57	MG	CA	3061	1/1	0.89	0.28	66,66,66,66	0
57	MG	AA	3210	1/1	0.89	0.27	59,59,59,59	0
57	MG	DA	3313	1/1	0.89	0.16	47,47,47,47	0
57	MG	BA	3131	1/1	0.89	0.11	58,58,58,58	0
57	MG	DA	3090	1/1	0.89	0.10	52,52,52,52	0
57	MG	DA	3098	1/1	0.89	0.17	53,53,53,53	0
57	MG	BA	3361	1/1	0.89	0.13	49,49,49,49	0
57	MG	AA	3102	1/1	0.89	0.25	59,59,59,59	0
57	MG	DA	3626	1/1	0.89	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3298	1/1	0.89	0.16	51,51,51,51	0
57	MG	BA	3749	1/1	0.89	0.12	56,56,56,56	0
57	MG	BA	3125	1/1	0.89	0.17	47,47,47,47	0
57	MG	BA	3790	1/1	0.89	0.18	34,34,34,34	0
57	MG	BA	3032	1/1	0.89	0.20	47,47,47,47	0
57	MG	BU	201	1/1	0.89	0.15	43,43,43,43	0
57	MG	BA	3431	1/1	0.89	0.17	59,59,59,59	0
57	MG	AA	3093	1/1	0.89	0.12	66,66,66,66	0
57	MG	BA	3703	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3622	1/1	0.89	0.19	48,48,48,48	0
57	MG	BA	3058	1/1	0.89	0.15	49,49,49,49	0
57	MG	DA	3066	1/1	0.89	0.10	42,42,42,42	0
57	MG	CA	3044	1/1	0.89	0.23	62,62,62,62	0
57	MG	DA	3605	1/1	0.89	0.12	58,58,58,58	0
57	MG	CA	3036	1/1	0.89	0.14	66,66,66,66	0
57	MG	BA	3640	1/1	0.89	0.17	53,53,53,53	0
57	MG	BA	3741	1/1	0.89	0.74	64,64,64,64	0
57	MG	CA	3081	1/1	0.89	0.09	46,46,46,46	0
57	MG	BA	3618	1/1	0.89	0.14	65,65,65,65	0
57	MG	AA	3209	1/1	0.89	0.08	59,59,59,59	0
57	MG	BZ	3001	1/1	0.89	0.29	55,55,55,55	0
57	MG	BA	3315	1/1	0.89	0.19	31,31,31,31	0
57	MG	BA	3445	1/1	0.89	0.30	63,63,63,63	0
57	MG	BA	3793	1/1	0.89	0.13	40,40,40,40	0
57	MG	BA	3109	1/1	0.89	0.18	51,51,51,51	0
57	MG	DA	3621	1/1	0.89	0.08	44,44,44,44	0
57	MG	BE	301	1/1	0.89	0.14	35,35,35,35	0
57	MG	BA	3697	1/1	0.89	0.17	61,61,61,61	0
57	MG	CA	3004	1/1	0.89	0.25	66,66,66,66	0
57	MG	BA	3399	1/1	0.89	0.20	45,45,45,45	0
57	MG	AA	3042	1/1	0.89	0.09	57,57,57,57	0
57	MG	DP	202	1/1	0.89	0.11	53,53,53,53	0
57	MG	BA	3192	1/1	0.90	0.28	46,46,46,46	0
57	MG	DA	3141	1/1	0.90	0.27	61,61,61,61	0
57	MG	CA	3054	1/1	0.90	0.30	69,69,69,69	0
57	MG	DA	3214	1/1	0.90	0.24	59,59,59,59	0
57	MG	DA	3126	1/1	0.90	0.08	55,55,55,55	0
57	MG	AA	3142	1/1	0.90	0.11	41,41,41,41	0
59	ZN	DY	501	1/1	0.90	0.15	96,96,96,96	0
57	MG	BA	3047	1/1	0.90	0.22	60,60,60,60	0
57	MG	BA	3312	1/1	0.90	0.18	32,32,32,32	0
57	MG	DA	3666	1/1	0.90	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3465	1/1	0.90	0.12	46,46,46,46	0
57	MG	BA	3465	1/1	0.90	0.18	43,43,43,43	0
57	MG	BA	3276	1/1	0.90	0.31	54,54,54,54	0
57	MG	BA	3411	1/1	0.90	0.19	33,33,33,33	0
57	MG	BA	3811	1/1	0.90	0.14	65,65,65,65	0
57	MG	DA	3132	1/1	0.90	0.23	52,52,52,52	0
57	MG	DA	3070	1/1	0.90	0.13	58,58,58,58	0
57	MG	BA	3581	1/1	0.90	0.19	30,30,30,30	0
57	MG	AA	3100	1/1	0.90	0.12	65,65,65,65	0
57	MG	BA	3634	1/1	0.90	0.14	62,62,62,62	0
57	MG	BA	3623	1/1	0.90	0.26	55,55,55,55	0
57	MG	AA	3135	1/1	0.90	0.24	65,65,65,65	0
57	MG	CA	3038	1/1	0.90	0.14	58,58,58,58	0
57	MG	DA	3280	1/1	0.90	0.16	33,33,33,33	0
57	MG	DA	3301	1/1	0.90	0.19	52,52,52,52	0
57	MG	BA	3394	1/1	0.90	0.18	40,40,40,40	0
57	MG	BA	3541	1/1	0.90	0.16	38,38,38,38	0
57	MG	AA	3036	1/1	0.90	0.17	61,61,61,61	0
57	MG	BA	3648	1/1	0.90	0.11	65,65,65,65	0
57	MG	DA	3033	1/1	0.90	0.10	42,42,42,42	0
57	MG	DA	3378	1/1	0.90	0.13	57,57,57,57	0
57	MG	AA	3058	1/1	0.90	0.28	59,59,59,59	0
57	MG	CA	3130	1/1	0.90	0.09	57,57,57,57	0
57	MG	DB	3001	1/1	0.90	0.17	64,64,64,64	0
57	MG	BA	3700	1/1	0.90	0.16	61,61,61,61	0
57	MG	CA	3002	1/1	0.90	0.12	63,63,63,63	0
57	MG	DA	3452	1/1	0.90	0.16	51,51,51,51	0
57	MG	DA	3209	1/1	0.90	0.24	53,53,53,53	0
57	MG	DA	3677	1/1	0.90	0.47	52,52,52,52	0
57	MG	BA	3686	1/1	0.90	0.25	60,60,60,60	0
57	MG	BA	3177	1/1	0.90	0.19	46,46,46,46	0
57	MG	AX	3016	1/1	0.90	0.10	56,56,56,56	0
57	MG	AA	3204	1/1	0.90	0.13	53,53,53,53	0
57	MG	CA	3006	1/1	0.90	0.14	64,64,64,64	0
57	MG	AA	3194	1/1	0.90	0.11	56,56,56,56	0
57	MG	BA	3429	1/1	0.90	0.10	65,65,65,65	0
57	MG	DA	3401	1/1	0.90	0.10	38,38,38,38	0
57	MG	DA	3499	1/1	0.90	0.10	53,53,53,53	0
57	MG	DA	3502	1/1	0.90	0.10	55,55,55,55	0
57	MG	DA	3615	1/1	0.90	0.09	65,65,65,65	0
57	MG	DB	3004	1/1	0.90	0.15	55,55,55,55	0
57	MG	BA	3612	1/1	0.90	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3185	1/1	0.90	0.12	82,82,82,82	0
57	MG	BN	3004	1/1	0.90	0.12	60,60,60,60	0
57	MG	DA	3556	1/1	0.90	0.11	67,67,67,67	0
57	MG	BA	3104	1/1	0.90	0.13	42,42,42,42	0
57	MG	BA	3461	1/1	0.90	0.10	62,62,62,62	0
57	MG	BA	3664	1/1	0.90	0.16	55,55,55,55	0
57	MG	CA	3057	1/1	0.90	0.18	76,76,76,76	0
57	MG	DA	3337	1/1	0.90	0.13	41,41,41,41	0
57	MG	DA	3424	1/1	0.90	0.09	61,61,61,61	0
57	MG	BA	3702	1/1	0.90	0.27	51,51,51,51	0
57	MG	DA	3119	1/1	0.90	0.22	39,39,39,39	0
57	MG	BA	3666	1/1	0.90	0.19	50,50,50,50	0
57	MG	AA	3146	1/1	0.90	0.13	66,66,66,66	0
57	MG	BA	3199	1/1	0.90	0.15	46,46,46,46	0
57	MG	DA	3547	1/1	0.90	0.14	54,54,54,54	0
57	MG	AA	3143	1/1	0.90	0.08	60,60,60,60	0
57	MG	DA	3103	1/1	0.90	0.10	58,58,58,58	0
57	MG	BA	3550	1/1	0.90	0.19	36,36,36,36	0
57	MG	BA	3195	1/1	0.90	0.11	46,46,46,46	0
57	MG	DA	3270	1/1	0.90	0.10	46,46,46,46	0
57	MG	DA	3524	1/1	0.90	0.17	61,61,61,61	0
57	MG	DA	3314	1/1	0.90	0.12	43,43,43,43	0
57	MG	AA	3187	1/1	0.90	0.13	62,62,62,62	0
57	MG	DA	3463	1/1	0.90	0.14	55,55,55,55	0
57	MG	DA	3215	1/1	0.90	0.13	59,59,59,59	0
57	MG	DA	3271	1/1	0.90	0.15	48,48,48,48	0
57	MG	DA	3245	1/1	0.90	0.12	54,54,54,54	0
57	MG	BD	309	1/1	0.90	0.32	57,57,57,57	0
57	MG	BA	3659	1/1	0.90	0.19	61,61,61,61	0
57	MG	AA	3117	1/1	0.90	0.12	79,79,79,79	0
57	MG	DA	3328	1/1	0.90	0.08	47,47,47,47	0
57	MG	AA	3059	1/1	0.90	0.12	78,78,78,78	0
57	MG	DA	3221	1/1	0.90	0.27	52,52,52,52	0
57	MG	CA	3026	1/1	0.90	0.20	63,63,63,63	0
57	MG	DA	3018	1/1	0.90	0.20	62,62,62,62	0
57	MG	AA	3211	1/1	0.90	0.12	47,47,47,47	0
57	MG	DA	3146	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3599	1/1	0.90	0.21	43,43,43,43	0
57	MG	BA	3485	1/1	0.90	0.09	42,42,42,42	0
57	MG	DA	3129	1/1	0.90	0.12	46,46,46,46	0
57	MG	BB	210	1/1	0.90	0.07	61,61,61,61	0
57	MG	BA	3351	1/1	0.90	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3133	1/1	0.90	0.22	50,50,50,50	0
57	MG	DA	3051	1/1	0.90	0.11	48,48,48,48	0
57	MG	BA	3501	1/1	0.90	0.23	71,71,71,71	0
57	MG	AA	3057	1/1	0.90	0.22	64,64,64,64	0
57	MG	BA	3478	1/1	0.91	0.19	58,58,58,58	0
57	MG	BA	3304	1/1	0.91	0.15	67,67,67,67	0
57	MG	AX	3007	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3285	1/1	0.91	0.27	50,50,50,50	0
57	MG	BA	3073	1/1	0.91	0.22	61,61,61,61	0
57	MG	DA	3120	1/1	0.91	0.13	49,49,49,49	0
57	MG	DA	3134	1/1	0.91	0.21	41,41,41,41	0
57	MG	BA	3746	1/1	0.91	0.11	51,51,51,51	0
57	MG	BA	3396	1/1	0.91	0.15	50,50,50,50	0
57	MG	BA	3061	1/1	0.91	0.23	29,29,29,29	0
57	MG	BA	3226	1/1	0.91	0.27	47,47,47,47	0
57	MG	BA	3508	1/1	0.91	0.20	51,51,51,51	0
57	MG	BA	3150	1/1	0.91	0.17	55,55,55,55	0
57	MG	BA	3366	1/1	0.91	0.12	57,57,57,57	0
57	MG	DA	3239	1/1	0.91	0.24	56,56,56,56	0
57	MG	B7	104	1/1	0.91	0.27	48,48,48,48	0
57	MG	DA	3622	1/1	0.91	0.21	61,61,61,61	0
57	MG	DA	3279	1/1	0.91	0.12	56,56,56,56	0
57	MG	B1	101	1/1	0.91	0.50	51,51,51,51	0
57	MG	DA	3236	1/1	0.91	0.26	47,47,47,47	0
57	MG	CA	3046	1/1	0.91	0.09	69,69,69,69	0
57	MG	CA	3012	1/1	0.91	0.21	60,60,60,60	0
57	MG	AA	3066	1/1	0.91	0.31	60,60,60,60	0
57	MG	BA	3668	1/1	0.91	0.17	53,53,53,53	0
57	MG	BA	3321	1/1	0.91	0.24	55,55,55,55	0
57	MG	DA	3405	1/1	0.91	0.16	46,46,46,46	0
57	MG	DA	3085	1/1	0.91	0.08	53,53,53,53	0
57	MG	BA	3621	1/1	0.91	0.17	53,53,53,53	0
57	MG	BO	202	1/1	0.91	0.09	65,65,65,65	0
57	MG	AA	3131	1/1	0.91	0.15	71,71,71,71	0
57	MG	CA	3075	1/1	0.91	0.18	59,59,59,59	0
57	MG	CW	3001	1/1	0.91	0.22	67,67,67,67	0
57	MG	BA	3507	1/1	0.91	0.20	49,49,49,49	0
57	MG	AA	3198	1/1	0.91	0.13	61,61,61,61	0
57	MG	CA	3153	1/1	0.91	0.16	70,70,70,70	0
57	MG	DA	3049	1/1	0.91	0.27	52,52,52,52	0
57	MG	DD	309	1/1	0.91	0.20	59,59,59,59	0
57	MG	AA	3080	1/1	0.91	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3121	1/1	0.91	0.21	64,64,64,64	0
57	MG	BA	3606	1/1	0.91	0.14	61,61,61,61	0
57	MG	BD	302	1/1	0.91	0.27	50,50,50,50	0
57	MG	BA	3575	1/1	0.91	0.12	48,48,48,48	0
57	MG	BA	3005	1/1	0.91	0.16	30,30,30,30	0
57	MG	DA	3550	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3561	1/1	0.91	0.12	45,45,45,45	0
57	MG	DA	3170	1/1	0.91	0.12	53,53,53,53	0
57	MG	AN	502	1/1	0.91	0.29	63,63,63,63	0
57	MG	BA	3303	1/1	0.91	0.17	36,36,36,36	0
57	MG	DA	3317	1/1	0.91	0.12	44,44,44,44	0
57	MG	DA	3130	1/1	0.91	0.18	52,52,52,52	0
57	MG	DA	3165	1/1	0.91	0.24	57,57,57,57	0
57	MG	BO	201	1/1	0.91	0.19	50,50,50,50	0
57	MG	BA	3007	1/1	0.91	0.19	55,55,55,55	0
57	MG	AA	3133	1/1	0.91	0.16	56,56,56,56	0
57	MG	CA	3100	1/1	0.91	0.09	52,52,52,52	0
57	MG	BN	3002	1/1	0.91	0.16	39,39,39,39	0
57	MG	DA	3243	1/1	0.91	0.12	55,55,55,55	0
57	MG	CA	3118	1/1	0.91	0.19	68,68,68,68	0
57	MG	DA	3038	1/1	0.91	0.16	47,47,47,47	0
57	MG	DA	3004	1/1	0.91	0.17	40,40,40,40	0
57	MG	BA	3750	1/1	0.91	0.17	27,27,27,27	0
57	MG	DA	3588	1/1	0.91	0.30	65,65,65,65	0
57	MG	DA	3643	1/1	0.91	0.13	61,61,61,61	0
57	MG	AA	3188	1/1	0.91	0.08	69,69,69,69	0
57	MG	BA	3229	1/1	0.91	0.22	54,54,54,54	0
57	MG	BA	3143	1/1	0.91	0.26	45,45,45,45	0
57	MG	BA	3654	1/1	0.91	0.20	57,57,57,57	0
57	MG	BA	3495	1/1	0.91	0.13	37,37,37,37	0
57	MG	CA	3028	1/1	0.91	0.13	41,41,41,41	0
57	MG	BA	3423	1/1	0.91	0.18	44,44,44,44	0
57	MG	DA	3407	1/1	0.91	0.04	66,66,66,66	0
57	MG	BA	3024	1/1	0.91	0.19	49,49,49,49	0
57	MG	CA	3129	1/1	0.91	0.09	43,43,43,43	0
57	MG	BA	3562	1/1	0.91	0.14	37,37,37,37	0
57	MG	DA	3604	1/1	0.91	0.18	59,59,59,59	0
57	MG	DA	3429	1/1	0.91	0.14	41,41,41,41	0
57	MG	BA	3019	1/1	0.91	0.15	42,42,42,42	0
57	MG	BA	3466	1/1	0.91	0.17	49,49,49,49	0
57	MG	BB	206	1/1	0.91	0.30	47,47,47,47	0
57	MG	DA	3011	1/1	0.91	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3210	1/1	0.91	0.33	49,49,49,49	0
57	MG	BA	3126	1/1	0.91	0.16	54,54,54,54	0
57	MG	BA	3650	1/1	0.91	0.12	52,52,52,52	0
57	MG	DA	3494	1/1	0.91	0.12	47,47,47,47	0
57	MG	BA	3400	1/1	0.91	0.21	33,33,33,33	0
57	MG	CA	3055	1/1	0.91	0.09	69,69,69,69	0
57	MG	CA	3160	1/1	0.91	0.17	62,62,62,62	0
57	MG	BA	3227	1/1	0.91	0.24	57,57,57,57	0
57	MG	AA	3028	1/1	0.91	0.22	76,76,76,76	0
57	MG	BA	3631	1/1	0.91	0.18	42,42,42,42	0
57	MG	AA	3063	1/1	0.91	0.10	35,35,35,35	0
57	MG	BA	3405	1/1	0.91	0.19	63,63,63,63	0
57	MG	BA	3269	1/1	0.91	0.16	53,53,53,53	0
57	MG	DA	3653	1/1	0.91	0.14	52,52,52,52	0
57	MG	DA	3097	1/1	0.91	0.21	33,33,33,33	0
57	MG	BA	3252	1/1	0.91	0.41	60,60,60,60	0
57	MG	BA	3120	1/1	0.91	0.21	55,55,55,55	0
57	MG	BA	3683	1/1	0.91	0.15	73,73,73,73	0
57	MG	CA	3011	1/1	0.91	0.23	61,61,61,61	0
57	MG	CA	3111	1/1	0.91	0.16	64,64,64,64	0
57	MG	BA	3433	1/1	0.91	0.20	32,32,32,32	0
57	MG	CA	3144	1/1	0.91	0.19	71,71,71,71	0
57	MG	AA	3021	1/1	0.91	0.14	63,63,63,63	0
57	MG	AA	3003	1/1	0.91	0.30	72,72,72,72	0
57	MG	DA	3538	1/1	0.91	0.11	58,58,58,58	0
57	MG	AA	3162	1/1	0.91	0.07	66,66,66,66	0
57	MG	AA	3030	1/1	0.91	0.18	60,60,60,60	0
57	MG	CA	3091	1/1	0.91	0.12	55,55,55,55	0
57	MG	AX	3003	1/1	0.91	0.13	71,71,71,71	0
57	MG	DA	3116	1/1	0.91	0.48	52,52,52,52	0
57	MG	BA	3413	1/1	0.91	0.13	47,47,47,47	0
57	MG	CA	3150	1/1	0.91	0.21	56,56,56,56	0
57	MG	CA	3007	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3164	1/1	0.91	0.21	48,48,48,48	0
57	MG	BA	3255	1/1	0.91	0.15	47,47,47,47	0
57	MG	BX	3003	1/1	0.92	0.17	35,35,35,35	0
57	MG	DA	3050	1/1	0.92	0.17	59,59,59,59	0
57	MG	AA	3119	1/1	0.92	0.12	51,51,51,51	0
57	MG	BA	3290	1/1	0.92	0.28	40,40,40,40	0
57	MG	AA	3061	1/1	0.92	0.34	55,55,55,55	0
57	MG	BA	3385	1/1	0.92	0.16	59,59,59,59	0
57	MG	D3	3001	1/1	0.92	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3767	1/1	0.92	0.12	73,73,73,73	0
57	MG	DA	3398	1/1	0.92	0.14	45,45,45,45	0
57	MG	DA	3083	1/1	0.92	0.18	40,40,40,40	0
57	MG	BA	3779	1/1	0.92	0.29	66,66,66,66	0
57	MG	AA	3097	1/1	0.92	0.34	56,56,56,56	0
57	MG	BA	3407	1/1	0.92	0.15	47,47,47,47	0
57	MG	DA	3586	1/1	0.92	0.16	60,60,60,60	0
57	MG	DA	3137	1/1	0.92	0.23	54,54,54,54	0
57	MG	BA	3388	1/1	0.92	0.19	48,48,48,48	0
57	MG	BX	3001	1/1	0.92	0.82	48,48,48,48	0
57	MG	DA	3135	1/1	0.92	0.12	38,38,38,38	0
57	MG	BA	3412	1/1	0.92	0.23	40,40,40,40	0
57	MG	BA	3043	1/1	0.92	0.15	48,48,48,48	0
57	MG	BA	3734	1/1	0.92	0.16	52,52,52,52	0
57	MG	CA	3074	1/1	0.92	0.23	64,64,64,64	0
57	MG	DA	3668	1/1	0.92	0.39	60,60,60,60	0
57	MG	BA	3477	1/1	0.92	0.18	61,61,61,61	0
57	MG	DA	3576	1/1	0.92	0.09	53,53,53,53	0
57	MG	BA	3240	1/1	0.92	0.40	47,47,47,47	0
57	MG	BA	3292	1/1	0.92	0.15	48,48,48,48	0
57	MG	B6	102	1/1	0.92	0.11	68,68,68,68	0
57	MG	CA	3059	1/1	0.92	0.25	72,72,72,72	0
57	MG	AA	3171	1/1	0.92	0.10	51,51,51,51	0
57	MG	DA	3128	1/1	0.92	0.15	58,58,58,58	0
57	MG	DA	3219	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3100	1/1	0.92	0.16	43,43,43,43	0
57	MG	DA	3001	1/1	0.92	0.17	60,60,60,60	0
57	MG	DV	3003	1/1	0.92	0.10	65,65,65,65	0
57	MG	BA	3100	1/1	0.92	0.17	39,39,39,39	0
57	MG	BA	3310	1/1	0.92	0.24	58,58,58,58	0
57	MG	BA	3207	1/1	0.92	0.24	54,54,54,54	0
57	MG	BA	3651	1/1	0.92	0.19	45,45,45,45	0
57	MG	DA	3423	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3671	1/1	0.92	0.16	63,63,63,63	0
57	MG	BA	3812	1/1	0.92	0.28	47,47,47,47	0
57	MG	DA	3263	1/1	0.92	0.13	41,41,41,41	0
57	MG	BA	3346	1/1	0.92	0.10	27,27,27,27	0
57	MG	BA	3271	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3554	1/1	0.92	0.13	51,51,51,51	0
57	MG	BA	3628	1/1	0.92	0.25	49,49,49,49	0
57	MG	DA	3543	1/1	0.92	0.08	53,53,53,53	0
57	MG	BA	3136	1/1	0.92	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3456	1/1	0.92	0.07	50,50,50,50	0
57	MG	DA	3473	1/1	0.92	0.12	50,50,50,50	0
57	MG	AA	3109	1/1	0.92	0.14	62,62,62,62	0
57	MG	BA	3717	1/1	0.92	0.16	50,50,50,50	0
57	MG	AX	3008	1/1	0.92	0.19	70,70,70,70	0
57	MG	BF	302	1/1	0.92	0.18	46,46,46,46	0
57	MG	BA	3714	1/1	0.92	0.11	57,57,57,57	0
57	MG	CA	3120	1/1	0.92	0.18	64,64,64,64	0
57	MG	BA	3022	1/1	0.92	0.19	60,60,60,60	0
57	MG	BY	502	1/1	0.92	0.25	40,40,40,40	0
57	MG	AA	3022	1/1	0.92	0.10	71,71,71,71	0
57	MG	AX	3009	1/1	0.92	0.18	64,64,64,64	0
57	MG	BA	3542	1/1	0.92	0.18	45,45,45,45	0
57	MG	DA	3325	1/1	0.92	0.12	35,35,35,35	0
57	MG	BA	3652	1/1	0.92	0.15	67,67,67,67	0
57	MG	AA	3037	1/1	0.92	0.22	55,55,55,55	0
57	MG	BA	3357	1/1	0.92	0.23	25,25,25,25	0
57	MG	BA	3369	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3347	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3799	1/1	0.92	0.06	49,49,49,49	0
57	MG	DA	3112	1/1	0.92	0.16	59,59,59,59	0
57	MG	BA	3708	1/1	0.92	0.21	50,50,50,50	0
57	MG	DA	3382	1/1	0.92	0.07	48,48,48,48	0
57	MG	BA	3424	1/1	0.92	0.25	39,39,39,39	0
57	MG	AA	3122	1/1	0.92	0.11	56,56,56,56	0
57	MG	DA	3354	1/1	0.92	0.19	44,44,44,44	0
57	MG	BA	3459	1/1	0.92	0.19	48,48,48,48	0
57	MG	BA	3098	1/1	0.92	0.23	40,40,40,40	0
57	MG	DA	3063	1/1	0.92	0.22	54,54,54,54	0
57	MG	BA	3134	1/1	0.92	0.17	48,48,48,48	0
57	MG	AA	3115	1/1	0.92	0.09	79,79,79,79	0
57	MG	DA	3250	1/1	0.92	0.18	69,69,69,69	0
57	MG	BA	3101	1/1	0.92	0.19	53,53,53,53	0
57	MG	BA	3307	1/1	0.92	0.17	29,29,29,29	0
57	MG	BG	202	1/1	0.92	0.21	41,41,41,41	0
57	MG	DA	3478	1/1	0.92	0.12	59,59,59,59	0
57	MG	BA	3493	1/1	0.92	0.16	58,58,58,58	0
57	MG	DA	3153	1/1	0.92	0.19	47,47,47,47	0
57	MG	BA	3203	1/1	0.92	0.24	40,40,40,40	0
57	MG	CA	3008	1/1	0.92	0.27	51,51,51,51	0
57	MG	BE	307	1/1	0.92	0.15	62,62,62,62	0
57	MG	BA	3016	1/1	0.92	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3017	1/1	0.92	0.25	48,48,48,48	0
57	MG	DA	3173	1/1	0.92	0.12	53,53,53,53	0
57	MG	DA	3047	1/1	0.92	0.15	49,49,49,49	0
57	MG	BA	3151	1/1	0.92	0.26	52,52,52,52	0
57	MG	BA	3051	1/1	0.92	0.19	43,43,43,43	0
57	MG	DA	3079	1/1	0.92	0.17	55,55,55,55	0
57	MG	DA	3409	1/1	0.92	0.15	57,57,57,57	0
57	MG	BA	3675	1/1	0.92	0.19	67,67,67,67	0
57	MG	AA	3161	1/1	0.92	0.23	65,65,65,65	0
57	MG	DA	3505	1/1	0.92	0.08	56,56,56,56	0
57	MG	DD	304	1/1	0.92	0.38	52,52,52,52	0
57	MG	DA	3164	1/1	0.92	0.12	51,51,51,51	0
57	MG	AA	3163	1/1	0.92	0.18	56,56,56,56	0
57	MG	BA	3239	1/1	0.92	0.34	48,48,48,48	0
57	MG	BA	3182	1/1	0.92	0.14	55,55,55,55	0
57	MG	DA	3391	1/1	0.92	0.09	45,45,45,45	0
57	MG	BA	3127	1/1	0.92	0.29	57,57,57,57	0
57	MG	DA	3091	1/1	0.92	0.10	48,48,48,48	0
57	MG	DA	3503	1/1	0.92	0.14	52,52,52,52	0
57	MG	BA	3099	1/1	0.92	0.22	41,41,41,41	0
57	MG	DA	3392	1/1	0.92	0.19	70,70,70,70	0
57	MG	DA	3595	1/1	0.92	0.17	59,59,59,59	0
57	MG	AA	3202	1/1	0.92	0.14	57,57,57,57	0
57	MG	DA	3267	1/1	0.92	0.16	49,49,49,49	0
57	MG	BA	3535	1/1	0.92	0.19	31,31,31,31	0
57	MG	CA	3135	1/1	0.92	0.15	63,63,63,63	0
57	MG	DA	3273	1/1	0.92	0.11	47,47,47,47	0
57	MG	BA	3138	1/1	0.92	0.34	42,42,42,42	0
57	MG	DA	3327	1/1	0.92	0.12	57,57,57,57	0
57	MG	DA	3194	1/1	0.92	0.10	56,56,56,56	0
57	MG	DA	3162	1/1	0.92	0.36	50,50,50,50	0
57	MG	BA	3145	1/1	0.92	0.10	44,44,44,44	0
57	MG	BA	3662	1/1	0.92	0.10	61,61,61,61	0
57	MG	BA	3387	1/1	0.92	0.15	54,54,54,54	0
57	MG	AA	3191	1/1	0.92	0.21	47,47,47,47	0
57	MG	DA	3251	1/1	0.92	0.17	62,62,62,62	0
57	MG	BA	3403	1/1	0.92	0.08	54,54,54,54	0
57	MG	B0	102	1/1	0.92	0.22	48,48,48,48	0
57	MG	DA	3637	1/1	0.92	0.59	58,58,58,58	0
57	MG	BA	3322	1/1	0.92	0.17	52,52,52,52	0
57	MG	CA	3095	1/1	0.92	0.14	64,64,64,64	0
57	MG	CA	3112	1/1	0.92	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3201	1/1	0.92	0.13	52,52,52,52	0
57	MG	AY	3003	1/1	0.92	0.30	53,53,53,53	0
57	MG	BA	3797	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3048	1/1	0.92	0.06	53,53,53,53	0
57	MG	BB	219	1/1	0.92	0.11	67,67,67,67	0
57	MG	CA	3014	1/1	0.92	0.21	58,58,58,58	0
57	MG	BA	3722	1/1	0.92	0.19	47,47,47,47	0
57	MG	AA	3070	1/1	0.92	0.18	52,52,52,52	0
57	MG	BA	3515	1/1	0.92	0.12	53,53,53,53	0
57	MG	BA	3455	1/1	0.92	0.16	64,64,64,64	0
57	MG	DA	3227	1/1	0.93	0.28	41,41,41,41	0
57	MG	BA	3173	1/1	0.93	0.15	48,48,48,48	0
57	MG	BE	308	1/1	0.93	0.17	40,40,40,40	0
57	MG	AA	3101	1/1	0.93	0.16	43,43,43,43	0
57	MG	BA	3320	1/1	0.93	0.22	48,48,48,48	0
57	MG	CA	3102	1/1	0.93	0.08	68,68,68,68	0
57	MG	AA	3027	1/1	0.93	0.15	50,50,50,50	0
57	MG	BB	201	1/1	0.93	0.17	55,55,55,55	0
57	MG	DW	3003	1/1	0.93	0.09	72,72,72,72	0
57	MG	BA	3014	1/1	0.93	0.29	42,42,42,42	0
57	MG	AA	3130	1/1	0.93	0.08	56,56,56,56	0
57	MG	BA	3713	1/1	0.93	0.18	33,33,33,33	0
57	MG	BA	3118	1/1	0.93	0.17	48,48,48,48	0
57	MG	BA	3706	1/1	0.93	0.11	53,53,53,53	0
57	MG	BA	3021	1/1	0.93	0.19	49,49,49,49	0
57	MG	DA	3536	1/1	0.93	0.11	48,48,48,48	0
57	MG	DA	3009	1/1	0.93	0.15	48,48,48,48	0
57	MG	CA	3170	1/1	0.93	0.18	58,58,58,58	0
57	MG	BA	3291	1/1	0.93	0.21	33,33,33,33	0
57	MG	DA	3652	1/1	0.93	0.39	67,67,67,67	0
57	MG	BA	3119	1/1	0.93	0.13	45,45,45,45	0
57	MG	BA	3580	1/1	0.93	0.13	55,55,55,55	0
57	MG	BA	3078	1/1	0.93	0.24	51,51,51,51	0
57	MG	DA	3013	1/1	0.93	0.09	40,40,40,40	0
57	MG	BA	3537	1/1	0.93	0.16	45,45,45,45	0
57	MG	DA	3074	1/1	0.93	0.13	37,37,37,37	0
57	MG	DA	3246	1/1	0.93	0.14	43,43,43,43	0
57	MG	CA	3142	1/1	0.93	0.13	69,69,69,69	0
57	MG	CA	3086	1/1	0.93	0.13	64,64,64,64	0
57	MG	DA	3482	1/1	0.93	0.10	50,50,50,50	0
57	MG	BA	3149	1/1	0.93	0.18	40,40,40,40	0
57	MG	AA	3060	1/1	0.93	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3012	1/1	0.93	0.16	46,46,46,46	0
57	MG	DA	3540	1/1	0.93	0.17	42,42,42,42	0
57	MG	AA	3155	1/1	0.93	0.24	48,48,48,48	0
57	MG	DA	3545	1/1	0.93	0.13	35,35,35,35	0
57	MG	AA	3141	1/1	0.93	0.23	61,61,61,61	0
57	MG	BA	3302	1/1	0.93	0.12	69,69,69,69	0
57	MG	AA	3095	1/1	0.93	0.29	60,60,60,60	0
57	MG	AA	3178	1/1	0.93	0.15	59,59,59,59	0
57	MG	DA	3358	1/1	0.93	0.14	45,45,45,45	0
57	MG	DA	3211	1/1	0.93	0.14	48,48,48,48	0
57	MG	AA	3136	1/1	0.93	0.10	70,70,70,70	0
57	MG	BP	202	1/1	0.93	0.21	36,36,36,36	0
57	MG	DV	3001	1/1	0.93	0.23	70,70,70,70	0
57	MG	BA	3075	1/1	0.93	0.24	45,45,45,45	0
57	MG	DA	3551	1/1	0.93	0.08	55,55,55,55	0
57	MG	BA	3800	1/1	0.93	0.23	38,38,38,38	0
57	MG	AA	3193	1/1	0.93	0.08	72,72,72,72	0
57	MG	DA	3163	1/1	0.93	0.15	49,49,49,49	0
57	MG	BA	3161	1/1	0.93	0.17	52,52,52,52	0
57	MG	BA	3464	1/1	0.93	0.14	45,45,45,45	0
57	MG	DA	3064	1/1	0.93	0.20	49,49,49,49	0
57	MG	BA	3604	1/1	0.93	0.15	36,36,36,36	0
57	MG	DA	3549	1/1	0.93	0.10	57,57,57,57	0
57	MG	DA	3029	1/1	0.93	0.35	49,49,49,49	0
57	MG	BA	3639	1/1	0.93	0.46	48,48,48,48	0
57	MG	DA	3045	1/1	0.93	0.29	51,51,51,51	0
57	MG	BA	3576	1/1	0.93	0.07	57,57,57,57	0
57	MG	BU	202	1/1	0.93	0.29	40,40,40,40	0
57	MG	BA	3505	1/1	0.93	0.12	55,55,55,55	0
57	MG	AE	201	1/1	0.93	0.15	59,59,59,59	0
57	MG	DA	3578	1/1	0.93	0.18	59,59,59,59	0
57	MG	DA	3149	1/1	0.93	0.06	56,56,56,56	0
57	MG	BA	3201	1/1	0.93	0.20	62,62,62,62	0
57	MG	DA	3397	1/1	0.93	0.09	57,57,57,57	0
57	MG	CA	3060	1/1	0.93	0.08	65,65,65,65	0
57	MG	AA	3181	1/1	0.93	0.16	51,51,51,51	0
57	MG	DA	3514	1/1	0.93	0.13	42,42,42,42	0
57	MG	BA	3328	1/1	0.93	0.27	40,40,40,40	0
57	MG	BA	3250	1/1	0.93	0.68	42,42,42,42	0
57	MG	DA	3670	1/1	0.93	0.42	60,60,60,60	0
57	MG	BA	3533	1/1	0.93	0.10	59,59,59,59	0
57	MG	DA	3351	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3650	1/1	0.93	0.12	67,67,67,67	0
57	MG	BA	3690	1/1	0.93	0.18	58,58,58,58	0
57	MG	DA	3006	1/1	0.93	0.10	38,38,38,38	0
57	MG	BA	3277	1/1	0.93	0.65	47,47,47,47	0
57	MG	DA	3291	1/1	0.93	0.20	44,44,44,44	0
57	MG	BV	204	1/1	0.93	0.21	49,49,49,49	0
57	MG	DA	3131	1/1	0.93	0.21	46,46,46,46	0
57	MG	BA	3055	1/1	0.93	0.21	45,45,45,45	0
57	MG	DA	3041	1/1	0.93	0.09	38,38,38,38	0
57	MG	AA	3007	1/1	0.93	0.13	57,57,57,57	0
57	MG	BA	3295	1/1	0.93	0.19	38,38,38,38	0
57	MG	DA	3381	1/1	0.93	0.17	56,56,56,56	0
57	MG	DA	3065	1/1	0.93	0.18	43,43,43,43	0
57	MG	DA	3432	1/1	0.93	0.12	37,37,37,37	0
57	MG	BA	3642	1/1	0.93	0.12	48,48,48,48	0
57	MG	BA	3406	1/1	0.93	0.10	50,50,50,50	0
57	MG	DA	3672	1/1	0.93	0.16	71,71,71,71	0
57	MG	AA	3055	1/1	0.93	0.21	57,57,57,57	0
57	MG	DA	3426	1/1	0.93	0.22	49,49,49,49	0
57	MG	CA	3117	1/1	0.93	0.10	71,71,71,71	0
57	MG	AA	3029	1/1	0.93	0.22	53,53,53,53	0
57	MG	DA	3617	1/1	0.93	0.07	56,56,56,56	0
57	MG	BA	3519	1/1	0.93	0.08	55,55,55,55	0
57	MG	BA	3228	1/1	0.93	0.25	59,59,59,59	0
57	MG	AA	3149	1/1	0.93	0.10	46,46,46,46	0
57	MG	AA	3076	1/1	0.93	0.26	77,77,77,77	0
57	MG	AA	3088	1/1	0.93	0.27	65,65,65,65	0
57	MG	BA	3646	1/1	0.93	0.17	42,42,42,42	0
57	MG	BA	3807	1/1	0.93	0.17	47,47,47,47	0
57	MG	BN	3006	1/1	0.93	0.20	49,49,49,49	0
57	MG	CA	3165	1/1	0.93	0.11	45,45,45,45	0
57	MG	DA	3017	1/1	0.93	0.06	55,55,55,55	0
57	MG	DB	3005	1/1	0.93	0.08	59,59,59,59	0
57	MG	BA	3079	1/1	0.93	0.19	39,39,39,39	0
57	MG	DA	3108	1/1	0.93	0.07	52,52,52,52	0
57	MG	BA	3355	1/1	0.93	0.17	61,61,61,61	0
57	MG	AA	3085	1/1	0.93	0.18	48,48,48,48	0
57	MG	BA	3585	1/1	0.93	0.09	46,46,46,46	0
57	MG	AA	3071	1/1	0.93	0.22	53,53,53,53	0
57	MG	AA	3067	1/1	0.93	0.26	57,57,57,57	0
57	MG	BA	3765	1/1	0.93	0.22	48,48,48,48	0
57	MG	DA	3127	1/1	0.93	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3200	1/1	0.93	0.15	67,67,67,67	0
57	MG	BA	3341	1/1	0.93	0.12	51,51,51,51	0
57	MG	DA	3438	1/1	0.93	0.20	47,47,47,47	0
57	MG	CA	3164	1/1	0.93	0.16	60,60,60,60	0
57	MG	BA	3282	1/1	0.93	0.16	39,39,39,39	0
57	MG	DA	3255	1/1	0.93	0.09	51,51,51,51	0
57	MG	CA	3078	1/1	0.93	0.14	44,44,44,44	0
57	MG	BA	3190	1/1	0.93	0.20	52,52,52,52	0
57	MG	AA	3096	1/1	0.93	0.22	63,63,63,63	0
57	MG	BA	3773	1/1	0.93	0.25	52,52,52,52	0
57	MG	DA	3625	1/1	0.93	0.07	69,69,69,69	0
57	MG	BA	3035	1/1	0.93	0.26	39,39,39,39	0
57	MG	DA	3447	1/1	0.93	0.15	58,58,58,58	0
57	MG	BA	3688	1/1	0.93	0.16	46,46,46,46	0
57	MG	DA	3675	1/1	0.93	0.13	52,52,52,52	0
57	MG	DA	3201	1/1	0.93	0.14	61,61,61,61	0
57	MG	DA	3284	1/1	0.93	0.12	47,47,47,47	0
57	MG	DA	3517	1/1	0.93	0.05	51,51,51,51	0
57	MG	BA	3261	1/1	0.93	0.11	61,61,61,61	0
57	MG	DA	3631	1/1	0.93	0.12	57,57,57,57	0
57	MG	BA	3524	1/1	0.93	0.13	42,42,42,42	0
57	MG	BA	3223	1/1	0.93	0.13	41,41,41,41	0
57	MG	BA	3077	1/1	0.93	0.17	49,49,49,49	0
57	MG	DA	3237	1/1	0.93	0.14	56,56,56,56	0
57	MG	B7	102	1/1	0.93	0.16	47,47,47,47	0
57	MG	DA	3036	1/1	0.93	0.14	48,48,48,48	0
57	MG	B9	502	1/1	0.93	0.19	48,48,48,48	0
57	MG	BA	3186	1/1	0.93	0.45	45,45,45,45	0
57	MG	DA	3121	1/1	0.93	0.07	44,44,44,44	0
57	MG	AA	3078	1/1	0.93	0.27	66,66,66,66	0
57	MG	CA	3040	1/1	0.93	0.11	51,51,51,51	0
57	MG	AA	3140	1/1	0.93	0.15	53,53,53,53	0
57	MG	BA	3768	1/1	0.93	0.12	47,47,47,47	0
57	MG	BA	3656	1/1	0.93	0.27	53,53,53,53	0
57	MG	DA	3627	1/1	0.93	0.17	63,63,63,63	0
57	MG	BA	3555	1/1	0.93	0.14	29,29,29,29	0
57	MG	AN	503	1/1	0.93	0.15	54,54,54,54	0
57	MG	BA	3457	1/1	0.93	0.19	32,32,32,32	0
57	MG	AA	3056	1/1	0.93	0.13	61,61,61,61	0
57	MG	BA	3319	1/1	0.93	0.19	46,46,46,46	0
57	MG	BA	3595	1/1	0.93	0.09	51,51,51,51	0
57	MG	CA	3082	1/1	0.93	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3265	1/1	0.93	0.21	54,54,54,54	0
57	MG	BA	3758	1/1	0.93	0.11	45,45,45,45	0
57	MG	CA	3114	1/1	0.93	0.04	57,57,57,57	0
57	MG	BA	3531	1/1	0.93	0.21	26,26,26,26	0
57	MG	DA	3152	1/1	0.93	0.20	51,51,51,51	0
57	MG	BA	3439	1/1	0.93	0.13	33,33,33,33	0
57	MG	DA	3557	1/1	0.93	0.15	51,51,51,51	0
57	MG	DA	3107	1/1	0.93	0.13	51,51,51,51	0
57	MG	AA	3152	1/1	0.93	0.10	62,62,62,62	0
57	MG	DA	3032	1/1	0.93	0.15	48,48,48,48	0
57	MG	DA	3396	1/1	0.93	0.10	40,40,40,40	0
57	MG	AE	203	1/1	0.93	0.18	63,63,63,63	0
57	MG	DA	3612	1/1	0.94	0.09	62,62,62,62	0
57	MG	CA	3145	1/1	0.94	0.14	66,66,66,66	0
57	MG	CA	3083	1/1	0.94	0.10	79,79,79,79	0
57	MG	BA	3520	1/1	0.94	0.16	61,61,61,61	0
57	MG	BA	3504	1/1	0.94	0.13	56,56,56,56	0
57	MG	BA	3096	1/1	0.94	0.23	54,54,54,54	0
57	MG	BA	3511	1/1	0.94	0.14	30,30,30,30	0
57	MG	BA	3738	1/1	0.94	0.15	43,43,43,43	0
57	MG	BA	3220	1/1	0.94	0.22	29,29,29,29	0
57	MG	BE	303	1/1	0.94	0.20	51,51,51,51	0
57	MG	BA	3183	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3329	1/1	0.94	0.19	60,60,60,60	0
57	MG	BA	3655	1/1	0.94	0.14	50,50,50,50	0
57	MG	DA	3067	1/1	0.94	0.26	57,57,57,57	0
57	MG	BA	3065	1/1	0.94	0.19	60,60,60,60	0
57	MG	DA	3533	1/1	0.94	0.11	43,43,43,43	0
57	MG	DA	3114	1/1	0.94	0.15	55,55,55,55	0
57	MG	BA	3785	1/1	0.94	0.23	59,59,59,59	0
57	MG	DA	3104	1/1	0.94	0.29	53,53,53,53	0
57	MG	BA	3805	1/1	0.94	0.12	44,44,44,44	0
57	MG	BA	3064	1/1	0.94	0.13	43,43,43,43	0
57	MG	AY	3002	1/1	0.94	0.24	56,56,56,56	0
57	MG	BA	3536	1/1	0.94	0.27	49,49,49,49	0
57	MG	BA	3155	1/1	0.94	0.27	44,44,44,44	0
57	MG	BA	3009	1/1	0.94	0.17	28,28,28,28	0
57	MG	CA	3037	1/1	0.94	0.14	73,73,73,73	0
57	MG	DA	3249	1/1	0.94	0.14	45,45,45,45	0
57	MG	DA	3331	1/1	0.94	0.17	37,37,37,37	0
57	MG	BA	3543	1/1	0.94	0.23	37,37,37,37	0
57	MG	AA	3104	1/1	0.94	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3633	1/1	0.94	0.12	49,49,49,49	0
57	MG	BA	3747	1/1	0.94	0.20	52,52,52,52	0
57	MG	CA	3079	1/1	0.94	0.21	66,66,66,66	0
57	MG	BA	3448	1/1	0.94	0.24	32,32,32,32	0
57	MG	BA	3236	1/1	0.94	0.20	49,49,49,49	0
57	MG	DA	3024	1/1	0.94	0.21	59,59,59,59	0
57	MG	AA	3111	1/1	0.94	0.09	79,79,79,79	0
57	MG	CA	3025	1/1	0.94	0.14	51,51,51,51	0
57	MG	CA	3094	1/1	0.94	0.11	70,70,70,70	0
57	MG	AW	3003	1/1	0.94	0.13	72,72,72,72	0
57	MG	BA	3170	1/1	0.94	0.16	38,38,38,38	0
57	MG	DA	3516	1/1	0.94	0.07	67,67,67,67	0
57	MG	DA	3154	1/1	0.94	0.17	48,48,48,48	0
57	MG	DA	3054	1/1	0.94	0.23	48,48,48,48	0
57	MG	BA	3809	1/1	0.94	0.13	63,63,63,63	0
57	MG	CA	3126	1/1	0.94	0.11	67,67,67,67	0
57	MG	DA	3336	1/1	0.94	0.19	40,40,40,40	0
57	MG	CA	3010	1/1	0.94	0.17	56,56,56,56	0
57	MG	AA	3083	1/1	0.94	0.31	57,57,57,57	0
57	MG	BA	3306	1/1	0.94	0.17	37,37,37,37	0
57	MG	DA	3324	1/1	0.94	0.11	33,33,33,33	0
57	MG	BA	3663	1/1	0.94	0.19	41,41,41,41	0
57	MG	CA	3068	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3243	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3649	1/1	0.94	0.11	40,40,40,40	0
57	MG	DA	3434	1/1	0.94	0.11	39,39,39,39	0
57	MG	BA	3389	1/1	0.94	0.13	55,55,55,55	0
57	MG	BA	3157	1/1	0.94	0.24	45,45,45,45	0
57	MG	DA	3230	1/1	0.94	0.22	73,73,73,73	0
57	MG	DA	3656	1/1	0.94	0.13	58,58,58,58	0
57	MG	DA	3260	1/1	0.94	0.09	55,55,55,55	0
57	MG	DA	3623	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3511	1/1	0.94	0.16	49,49,49,49	0
57	MG	BA	3365	1/1	0.94	0.13	62,62,62,62	0
57	MG	AA	3132	1/1	0.94	0.19	55,55,55,55	0
57	MG	DA	3411	1/1	0.94	0.22	53,53,53,53	0
57	MG	AA	3175	1/1	0.94	0.18	63,63,63,63	0
57	MG	BA	3523	1/1	0.94	0.11	48,48,48,48	0
57	MG	DA	3573	1/1	0.94	0.12	43,43,43,43	0
57	MG	DA	3660	1/1	0.94	0.09	61,61,61,61	0
57	MG	AA	3009	1/1	0.94	0.18	57,57,57,57	0
57	MG	BA	3217	1/1	0.94	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3202	1/1	0.94	0.11	57,57,57,57	0
57	MG	AA	3016	1/1	0.94	0.09	63,63,63,63	0
57	MG	BA	3610	1/1	0.94	0.09	61,61,61,61	0
57	MG	AA	3075	1/1	0.94	0.11	49,49,49,49	0
57	MG	BA	3279	1/1	0.94	0.24	43,43,43,43	0
57	MG	AA	3014	1/1	0.94	0.21	32,32,32,32	0
57	MG	DA	3264	1/1	0.94	0.13	40,40,40,40	0
57	MG	DA	3254	1/1	0.94	0.07	52,52,52,52	0
57	MG	BA	3219	1/1	0.94	0.17	36,36,36,36	0
57	MG	BA	3522	1/1	0.94	0.09	52,52,52,52	0
57	MG	BA	3176	1/1	0.94	0.17	45,45,45,45	0
57	MG	BA	3323	1/1	0.94	0.20	30,30,30,30	0
57	MG	DA	3624	1/1	0.94	0.19	56,56,56,56	0
57	MG	BU	205	1/1	0.94	0.24	47,47,47,47	0
57	MG	BA	3340	1/1	0.94	0.14	39,39,39,39	0
57	MG	DD	306	1/1	0.94	0.28	39,39,39,39	0
57	MG	AA	3032	1/1	0.94	0.19	67,67,67,67	0
57	MG	CA	3108	1/1	0.94	0.31	68,68,68,68	0
57	MG	DA	3235	1/1	0.94	0.20	45,45,45,45	0
57	MG	DA	3587	1/1	0.94	0.12	56,56,56,56	0
57	MG	BA	3509	1/1	0.94	0.21	31,31,31,31	0
57	MG	BA	3415	1/1	0.94	0.16	28,28,28,28	0
57	MG	DD	302	1/1	0.94	0.15	42,42,42,42	0
57	MG	BA	3054	1/1	0.94	0.28	36,36,36,36	0
57	MG	DA	3053	1/1	0.94	0.10	47,47,47,47	0
57	MG	AA	3159	1/1	0.94	0.12	66,66,66,66	0
57	MG	DA	3043	1/1	0.94	0.15	38,38,38,38	0
57	MG	DA	3490	1/1	0.94	0.13	47,47,47,47	0
57	MG	BA	3084	1/1	0.94	0.22	38,38,38,38	0
57	MG	BA	3268	1/1	0.94	0.22	55,55,55,55	0
60	K	AX	3001	1/1	0.94	0.12	65,65,65,65	0
57	MG	AA	3068	1/1	0.94	0.14	69,69,69,69	0
57	MG	BA	3743	1/1	0.94	0.17	44,44,44,44	0
57	MG	CA	3161	1/1	0.94	0.09	56,56,56,56	0
57	MG	DA	3039	1/1	0.94	0.10	43,43,43,43	0
57	MG	BA	3350	1/1	0.94	0.20	28,28,28,28	0
57	MG	DA	3203	1/1	0.94	0.57	50,50,50,50	0
57	MG	BA	3166	1/1	0.94	0.14	38,38,38,38	0
57	MG	BA	3377	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3172	1/1	0.94	0.09	62,62,62,62	0
57	MG	DA	3158	1/1	0.94	0.16	60,60,60,60	0
57	MG	DA	3300	1/1	0.94	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3685	1/1	0.94	0.19	53,53,53,53	0
57	MG	CA	3030	1/1	0.94	0.22	57,57,57,57	0
57	MG	CA	3096	1/1	0.94	0.10	44,44,44,44	0
57	MG	BA	3672	1/1	0.94	0.20	43,43,43,43	0
57	MG	DQ	3003	1/1	0.94	0.15	51,51,51,51	0
57	MG	BA	3682	1/1	0.94	0.19	53,53,53,53	0
57	MG	DB	3009	1/1	0.94	0.18	59,59,59,59	0
57	MG	DA	3594	1/1	0.94	0.31	54,54,54,54	0
57	MG	BA	3452	1/1	0.94	0.16	55,55,55,55	0
57	MG	BA	3777	1/1	0.94	0.17	40,40,40,40	0
57	MG	DA	3302	1/1	0.94	0.28	70,70,70,70	0
57	MG	BA	3063	1/1	0.94	0.15	59,59,59,59	0
57	MG	CA	3053	1/1	0.94	0.15	41,41,41,41	0
57	MG	BA	3436	1/1	0.94	0.14	40,40,40,40	0
57	MG	BA	3294	1/1	0.94	0.23	61,61,61,61	0
57	MG	BA	3417	1/1	0.94	0.24	38,38,38,38	0
57	MG	DA	3229	1/1	0.94	0.22	50,50,50,50	0
57	MG	AA	3052	1/1	0.94	0.29	65,65,65,65	0
57	MG	CA	3139	1/1	0.94	0.14	62,62,62,62	0
57	MG	DA	3238	1/1	0.94	0.27	44,44,44,44	0
57	MG	BU	208	1/1	0.94	0.21	40,40,40,40	0
57	MG	DA	3232	1/1	0.94	0.13	62,62,62,62	0
57	MG	DA	3102	1/1	0.94	0.19	40,40,40,40	0
57	MG	BA	3748	1/1	0.94	0.15	29,29,29,29	0
57	MG	BA	3204	1/1	0.94	0.23	36,36,36,36	0
57	MG	CA	3077	1/1	0.94	0.08	66,66,66,66	0
57	MG	AA	3199	1/1	0.94	0.15	73,73,73,73	0
57	MG	AA	3123	1/1	0.94	0.26	51,51,51,51	0
57	MG	AA	3098	1/1	0.94	0.18	55,55,55,55	0
57	MG	BA	3739	1/1	0.94	0.22	40,40,40,40	0
57	MG	BA	3189	1/1	0.94	0.19	39,39,39,39	0
57	MG	BA	3344	1/1	0.94	0.12	66,66,66,66	0
57	MG	BA	3237	1/1	0.94	0.15	45,45,45,45	0
57	MG	CA	3110	1/1	0.94	0.09	65,65,65,65	0
57	MG	DA	3479	1/1	0.94	0.17	43,43,43,43	0
57	MG	CA	3125	1/1	0.94	0.08	63,63,63,63	0
57	MG	BA	3564	1/1	0.94	0.16	44,44,44,44	0
57	MG	CA	3035	1/1	0.94	0.09	59,59,59,59	0
57	MG	DA	3379	1/1	0.94	0.14	63,63,63,63	0
57	MG	DA	3188	1/1	0.94	0.19	48,48,48,48	0
57	MG	AA	3174	1/1	0.94	0.10	50,50,50,50	0
57	MG	BA	3352	1/1	0.94	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BR	201	1/1	0.94	0.26	57,57,57,57	0
57	MG	DA	3662	1/1	0.94	0.13	62,62,62,62	0
57	MG	AX	3004	1/1	0.94	0.15	64,64,64,64	0
57	MG	BA	3376	1/1	0.94	0.16	48,48,48,48	0
57	MG	DA	3179	1/1	0.94	0.12	52,52,52,52	0
57	MG	DA	3584	1/1	0.94	0.18	53,53,53,53	0
57	MG	CA	3119	1/1	0.94	0.16	64,64,64,64	0
57	MG	BQ	3003	1/1	0.94	0.27	49,49,49,49	0
57	MG	DA	3458	1/1	0.94	0.05	52,52,52,52	0
57	MG	DA	3427	1/1	0.94	0.14	45,45,45,45	0
57	MG	CA	3122	1/1	0.94	0.21	64,64,64,64	0
57	MG	DA	3634	1/1	0.94	0.14	60,60,60,60	0
57	MG	DB	3013	1/1	0.94	0.17	64,64,64,64	0
57	MG	BA	3196	1/1	0.94	0.25	38,38,38,38	0
57	MG	DA	3200	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3472	1/1	0.94	0.16	44,44,44,44	0
57	MG	BA	3801	1/1	0.94	0.31	50,50,50,50	0
57	MG	DA	3428	1/1	0.94	0.18	37,37,37,37	0
57	MG	DA	3419	1/1	0.94	0.11	32,32,32,32	0
57	MG	BA	3559	1/1	0.94	0.08	47,47,47,47	0
57	MG	DA	3368	1/1	0.94	0.24	50,50,50,50	0
57	MG	CF	3001	1/1	0.94	0.12	46,46,46,46	0
57	MG	DA	3655	1/1	0.94	0.11	64,64,64,64	0
57	MG	BA	3770	1/1	0.94	0.16	45,45,45,45	0
57	MG	DA	3195	1/1	0.94	0.09	43,43,43,43	0
57	MG	AA	3172	1/1	0.94	0.10	72,72,72,72	0
57	MG	BA	3516	1/1	0.94	0.19	52,52,52,52	0
57	MG	BA	3289	1/1	0.94	0.21	56,56,56,56	0
57	MG	BA	3803	1/1	0.94	0.23	44,44,44,44	0
57	MG	DA	3037	1/1	0.94	0.16	43,43,43,43	0
57	MG	DA	3210	1/1	0.94	0.17	53,53,53,53	0
57	MG	DA	3486	1/1	0.95	0.09	47,47,47,47	0
57	MG	DA	3196	1/1	0.95	0.22	49,49,49,49	0
57	MG	BA	3246	1/1	0.95	0.35	39,39,39,39	0
57	MG	DA	3507	1/1	0.95	0.14	43,43,43,43	0
57	MG	BA	3600	1/1	0.95	0.31	44,44,44,44	0
57	MG	AA	3050	1/1	0.95	0.15	33,33,33,33	0
57	MG	DA	3372	1/1	0.95	0.08	56,56,56,56	0
57	MG	DA	3287	1/1	0.95	0.10	41,41,41,41	0
57	MG	BQ	3001	1/1	0.95	0.22	45,45,45,45	0
57	MG	DA	3303	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3113	1/1	0.95	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3213	1/1	0.95	0.23	54,54,54,54	0
57	MG	AA	3116	1/1	0.95	0.11	55,55,55,55	0
57	MG	BA	3440	1/1	0.95	0.12	42,42,42,42	0
57	MG	DA	3073	1/1	0.95	0.09	42,42,42,42	0
57	MG	DA	3015	1/1	0.95	0.20	52,52,52,52	0
57	MG	AW	3002	1/1	0.95	0.22	53,53,53,53	0
57	MG	DA	3477	1/1	0.95	0.09	43,43,43,43	0
57	MG	CK	3001	1/1	0.95	0.17	45,45,45,45	0
57	MG	DA	3087	1/1	0.95	0.18	58,58,58,58	0
57	MG	BA	3015	1/1	0.95	0.16	32,32,32,32	0
57	MG	BA	3496	1/1	0.95	0.17	41,41,41,41	0
57	MG	DA	3389	1/1	0.95	0.14	46,46,46,46	0
57	MG	DA	3167	1/1	0.95	0.13	41,41,41,41	0
57	MG	CA	3063	1/1	0.95	0.23	58,58,58,58	0
57	MG	DA	3488	1/1	0.95	0.07	41,41,41,41	0
57	MG	DA	3290	1/1	0.95	0.15	59,59,59,59	0
57	MG	BA	3723	1/1	0.95	0.07	47,47,47,47	0
57	MG	BA	3539	1/1	0.95	0.20	52,52,52,52	0
57	MG	DA	3377	1/1	0.95	0.10	38,38,38,38	0
57	MG	BA	3087	1/1	0.95	0.24	42,42,42,42	0
57	MG	BD	301	1/1	0.95	0.23	40,40,40,40	0
57	MG	BA	3171	1/1	0.95	0.25	31,31,31,31	0
57	MG	DA	3439	1/1	0.95	0.23	42,42,42,42	0
57	MG	CA	3106	1/1	0.95	0.07	56,56,56,56	0
57	MG	BA	3026	1/1	0.95	0.15	41,41,41,41	0
57	MG	DA	3467	1/1	0.95	0.25	40,40,40,40	0
57	MG	BA	3194	1/1	0.95	0.18	47,47,47,47	0
57	MG	BA	3062	1/1	0.95	0.27	42,42,42,42	0
57	MG	DO	5001	1/1	0.95	0.13	59,59,59,59	0
57	MG	AX	3015	1/1	0.95	0.21	42,42,42,42	0
57	MG	DA	3598	1/1	0.95	0.08	61,61,61,61	0
57	MG	BA	3081	1/1	0.95	0.21	46,46,46,46	0
57	MG	DA	3226	1/1	0.95	0.38	45,45,45,45	0
57	MG	DA	3318	1/1	0.95	0.14	40,40,40,40	0
57	MG	DA	3600	1/1	0.95	0.35	70,70,70,70	0
57	MG	CA	3080	1/1	0.95	0.09	49,49,49,49	0
57	MG	BA	3798	1/1	0.95	0.20	28,28,28,28	0
57	MG	CA	3113	1/1	0.95	0.11	67,67,67,67	0
57	MG	DA	3475	1/1	0.95	0.16	51,51,51,51	0
57	MG	DA	3030	1/1	0.95	0.14	39,39,39,39	0
57	MG	CA	3136	1/1	0.95	0.14	72,72,72,72	0
57	MG	AA	3039	1/1	0.95	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3023	1/1	0.95	0.30	40,40,40,40	0
57	MG	CA	3032	1/1	0.95	0.24	62,62,62,62	0
57	MG	DA	3501	1/1	0.95	0.15	37,37,37,37	0
57	MG	BA	3027	1/1	0.95	0.11	26,26,26,26	0
57	MG	AA	3150	1/1	0.95	0.20	57,57,57,57	0
57	MG	BA	3354	1/1	0.95	0.10	48,48,48,48	0
57	MG	BA	3552	1/1	0.95	0.26	29,29,29,29	0
57	MG	BD	304	1/1	0.95	0.22	32,32,32,32	0
57	MG	BA	3712	1/1	0.95	0.18	53,53,53,53	0
57	MG	BA	3325	1/1	0.95	0.15	48,48,48,48	0
57	MG	DA	3583	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3667	1/1	0.95	0.15	61,61,61,61	0
57	MG	AA	3195	1/1	0.95	0.12	57,57,57,57	0
57	MG	B3	3001	1/1	0.95	0.12	34,34,34,34	0
57	MG	CX	3004	1/1	0.95	0.18	63,63,63,63	0
57	MG	BA	3205	1/1	0.95	0.27	50,50,50,50	0
57	MG	AY	3001	1/1	0.95	0.39	65,65,65,65	0
57	MG	DA	3207	1/1	0.95	0.30	63,63,63,63	0
57	MG	BA	3395	1/1	0.95	0.17	38,38,38,38	0
57	MG	BA	3359	1/1	0.95	0.30	62,62,62,62	0
57	MG	DA	3224	1/1	0.95	0.17	49,49,49,49	0
57	MG	BA	3557	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3383	1/1	0.95	0.12	53,53,53,53	0
57	MG	CA	3127	1/1	0.95	0.18	62,62,62,62	0
57	MG	BA	3215	1/1	0.95	0.27	36,36,36,36	0
57	MG	DA	3117	1/1	0.95	0.20	52,52,52,52	0
57	MG	BA	3031	1/1	0.95	0.19	52,52,52,52	0
57	MG	AA	3205	1/1	0.95	0.22	51,51,51,51	0
57	MG	DA	3645	1/1	0.95	0.07	45,45,45,45	0
57	MG	BA	3209	1/1	0.95	0.24	54,54,54,54	0
57	MG	DA	3272	1/1	0.95	0.10	41,41,41,41	0
57	MG	BA	3579	1/1	0.95	0.17	49,49,49,49	0
57	MG	BA	3617	1/1	0.95	0.16	51,51,51,51	0
57	MG	AA	3156	1/1	0.95	0.26	63,63,63,63	0
57	MG	BA	3783	1/1	0.95	0.12	56,56,56,56	0
57	MG	AA	3118	1/1	0.95	0.17	47,47,47,47	0
57	MG	AA	3106	1/1	0.95	0.10	57,57,57,57	0
57	MG	BA	3056	1/1	0.95	0.21	40,40,40,40	0
57	MG	BA	3381	1/1	0.95	0.16	46,46,46,46	0
57	MG	BA	3527	1/1	0.95	0.16	54,54,54,54	0
57	MG	DA	3519	1/1	0.95	0.18	63,63,63,63	0
57	MG	DA	3343	1/1	0.95	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3136	1/1	0.95	0.14	52,52,52,52	0
57	MG	DA	3304	1/1	0.95	0.06	48,48,48,48	0
57	MG	DA	3522	1/1	0.95	0.12	71,71,71,71	0
57	MG	BA	3808	1/1	0.95	0.16	42,42,42,42	0
57	MG	BA	3130	1/1	0.95	0.08	44,44,44,44	0
57	MG	BU	207	1/1	0.95	0.17	38,38,38,38	0
57	MG	BA	3796	1/1	0.95	0.25	45,45,45,45	0
57	MG	DA	3186	1/1	0.95	0.15	54,54,54,54	0
57	MG	DA	3541	1/1	0.95	0.14	44,44,44,44	0
57	MG	BA	3687	1/1	0.95	0.21	22,22,22,22	0
57	MG	DA	3570	1/1	0.95	0.13	31,31,31,31	0
57	MG	DQ	3002	1/1	0.95	0.10	51,51,51,51	0
57	MG	BA	3123	1/1	0.95	0.22	32,32,32,32	0
57	MG	BA	3632	1/1	0.95	0.07	50,50,50,50	0
57	MG	BA	3577	1/1	0.95	0.19	51,51,51,51	0
57	MG	BA	3090	1/1	0.95	0.31	53,53,53,53	0
57	MG	DA	3474	1/1	0.95	0.14	51,51,51,51	0
57	MG	BA	3635	1/1	0.95	0.13	58,58,58,58	0
57	MG	BQ	3004	1/1	0.95	0.27	42,42,42,42	0
57	MG	DA	3602	1/1	0.95	0.10	65,65,65,65	0
57	MG	DA	3483	1/1	0.95	0.32	55,55,55,55	0
57	MG	BA	3156	1/1	0.95	0.29	41,41,41,41	0
57	MG	DA	3539	1/1	0.95	0.12	53,53,53,53	0
57	MG	DA	3181	1/1	0.95	0.13	50,50,50,50	0
57	MG	DA	3277	1/1	0.95	0.11	55,55,55,55	0
57	MG	CA	3019	1/1	0.95	0.10	65,65,65,65	0
57	MG	AA	3035	1/1	0.95	0.21	56,56,56,56	0
57	MG	DA	3496	1/1	0.95	0.07	53,53,53,53	0
57	MG	BA	3775	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3484	1/1	0.95	0.13	54,54,54,54	0
57	MG	CA	3015	1/1	0.95	0.22	56,56,56,56	0
57	MG	CA	3104	1/1	0.95	0.12	68,68,68,68	0
57	MG	CA	3029	1/1	0.95	0.17	63,63,63,63	0
57	MG	BA	3398	1/1	0.95	0.21	32,32,32,32	0
57	MG	AA	3015	1/1	0.95	0.15	65,65,65,65	0
57	MG	DA	3611	1/1	0.95	0.14	48,48,48,48	0
57	MG	BA	3110	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3482	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3178	1/1	0.95	0.13	46,46,46,46	0
57	MG	DA	3548	1/1	0.95	0.06	60,60,60,60	0
57	MG	DA	3386	1/1	0.95	0.11	35,35,35,35	0
57	MG	DA	3418	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3295	1/1	0.95	0.21	44,44,44,44	0
57	MG	DA	3225	1/1	0.95	0.07	49,49,49,49	0
57	MG	BA	3249	1/1	0.95	0.13	49,49,49,49	0
57	MG	BA	3661	1/1	0.95	0.09	44,44,44,44	0
57	MG	AA	3129	1/1	0.95	0.11	47,47,47,47	0
57	MG	CA	3169	1/1	0.95	0.24	51,51,51,51	0
57	MG	AA	3165	1/1	0.95	0.20	54,54,54,54	0
57	MG	BA	3592	1/1	0.95	0.20	28,28,28,28	0
57	MG	BA	3567	1/1	0.95	0.15	34,34,34,34	0
57	MG	CA	3092	1/1	0.95	0.10	50,50,50,50	0
57	MG	DA	3174	1/1	0.95	0.13	44,44,44,44	0
57	MG	BA	3133	1/1	0.95	0.19	45,45,45,45	0
57	MG	DA	3485	1/1	0.95	0.12	52,52,52,52	0
57	MG	CA	3042	1/1	0.95	0.11	59,59,59,59	0
57	MG	BA	3146	1/1	0.95	0.17	40,40,40,40	0
57	MG	DA	3565	1/1	0.95	0.08	59,59,59,59	0
57	MG	BA	3795	1/1	0.95	0.15	35,35,35,35	0
57	MG	BA	3288	1/1	0.95	0.20	56,56,56,56	0
57	MG	AA	3010	1/1	0.95	0.17	52,52,52,52	0
57	MG	DA	3581	1/1	0.95	0.22	57,57,57,57	0
57	MG	CA	3031	1/1	0.95	0.10	68,68,68,68	0
57	MG	BA	3348	1/1	0.95	0.18	36,36,36,36	0
57	MG	DA	3375	1/1	0.95	0.16	39,39,39,39	0
57	MG	BA	3620	1/1	0.95	0.15	40,40,40,40	0
57	MG	AA	3081	1/1	0.95	0.11	48,48,48,48	0
57	MG	BA	3608	1/1	0.95	0.31	62,62,62,62	0
57	MG	AA	3157	1/1	0.95	0.17	45,45,45,45	0
57	MG	AA	3179	1/1	0.95	0.13	69,69,69,69	0
57	MG	BA	3175	1/1	0.95	0.20	20,20,20,20	0
57	MG	BA	3283	1/1	0.95	0.20	35,35,35,35	0
57	MG	DA	3183	1/1	0.95	0.15	38,38,38,38	0
57	MG	CA	3154	1/1	0.95	0.17	56,56,56,56	0
57	MG	DB	3006	1/1	0.95	0.14	57,57,57,57	0
57	MG	DA	3376	1/1	0.95	0.16	61,61,61,61	0
57	MG	BA	3570	1/1	0.95	0.16	42,42,42,42	0
57	MG	CA	3101	1/1	0.95	0.11	49,49,49,49	0
57	MG	AA	3167	1/1	0.95	0.10	57,57,57,57	0
59	ZN	B4	501	1/1	0.95	0.15	89,89,89,89	0
57	MG	BA	3626	1/1	0.95	0.25	44,44,44,44	0
57	MG	CA	3121	1/1	0.95	0.14	63,63,63,63	0
57	MG	DE	304	1/1	0.95	0.15	43,43,43,43	0
57	MG	BA	3571	1/1	0.95	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3151	1/1	0.95	0.27	59,59,59,59	0
57	MG	DA	3441	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3510	1/1	0.95	0.17	46,46,46,46	0
57	MG	DA	3674	1/1	0.95	0.15	37,37,37,37	0
57	MG	CD	301	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3551	1/1	0.95	0.19	36,36,36,36	0
57	MG	AA	3134	1/1	0.95	0.14	66,66,66,66	0
57	MG	BA	3593	1/1	0.95	0.22	38,38,38,38	0
57	MG	BA	3163	1/1	0.95	0.14	55,55,55,55	0
57	MG	DA	3640	1/1	0.95	0.19	43,43,43,43	0
57	MG	BP	201	1/1	0.95	0.28	41,41,41,41	0
57	MG	CA	3132	1/1	0.95	0.13	66,66,66,66	0
57	MG	BU	204	1/1	0.95	0.16	35,35,35,35	0
57	MG	DA	3510	1/1	0.95	0.25	49,49,49,49	0
57	MG	DA	3649	1/1	0.95	0.05	58,58,58,58	0
57	MG	BA	3218	1/1	0.95	0.20	47,47,47,47	0
57	MG	BP	205	1/1	0.95	0.18	65,65,65,65	0
57	MG	BA	3782	1/1	0.95	0.16	65,65,65,65	0
57	MG	DA	3568	1/1	0.95	0.08	52,52,52,52	0
57	MG	DA	3080	1/1	0.95	0.10	55,55,55,55	0
57	MG	AF	3001	1/1	0.95	0.26	44,44,44,44	0
57	MG	BA	3262	1/1	0.95	0.14	41,41,41,41	0
57	MG	BA	3751	1/1	0.95	0.17	26,26,26,26	0
57	MG	DA	3286	1/1	0.95	0.14	42,42,42,42	0
57	MG	DA	3562	1/1	0.95	0.12	64,64,64,64	0
57	MG	CA	3001	1/1	0.95	0.10	75,75,75,75	0
57	MG	BA	3500	1/1	0.95	0.14	56,56,56,56	0
57	MG	DA	3364	1/1	0.95	0.07	40,40,40,40	0
57	MG	AA	3144	1/1	0.95	0.14	46,46,46,46	0
57	MG	DY	502	1/1	0.95	0.13	50,50,50,50	0
57	MG	BA	3373	1/1	0.95	0.17	48,48,48,48	0
57	MG	DA	3433	1/1	0.95	0.18	46,46,46,46	0
57	MG	BA	3451	1/1	0.95	0.16	31,31,31,31	0
57	MG	DA	3348	1/1	0.95	0.10	34,34,34,34	0
57	MG	BE	306	1/1	0.95	0.20	26,26,26,26	0
57	MG	DA	3629	1/1	0.95	0.27	62,62,62,62	0
57	MG	DA	3359	1/1	0.95	0.13	47,47,47,47	0
57	MG	BA	3068	1/1	0.95	0.18	43,43,43,43	0
57	MG	BA	3647	1/1	0.95	0.09	56,56,56,56	0
57	MG	BW	201	1/1	0.95	0.31	44,44,44,44	0
57	MG	BA	3517	1/1	0.96	0.14	45,45,45,45	0
57	MG	BD	308	1/1	0.96	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3586	1/1	0.96	0.09	53,53,53,53	0
57	MG	AX	3012	1/1	0.96	0.17	59,59,59,59	0
57	MG	DA	3457	1/1	0.96	0.07	54,54,54,54	0
57	MG	DA	3068	1/1	0.96	0.10	58,58,58,58	0
57	MG	BA	3720	1/1	0.96	0.14	65,65,65,65	0
57	MG	AA	3114	1/1	0.96	0.17	59,59,59,59	0
57	MG	DA	3515	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3729	1/1	0.96	0.19	47,47,47,47	0
57	MG	DA	3639	1/1	0.96	0.48	59,59,59,59	0
57	MG	DA	3199	1/1	0.96	0.11	47,47,47,47	0
57	MG	BA	3614	1/1	0.96	0.11	63,63,63,63	0
57	MG	BA	3645	1/1	0.96	0.20	33,33,33,33	0
57	MG	BA	3211	1/1	0.96	0.15	55,55,55,55	0
57	MG	DA	3145	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3298	1/1	0.96	0.16	59,59,59,59	0
57	MG	DA	3123	1/1	0.96	0.20	56,56,56,56	0
57	MG	AX	3013	1/1	0.96	0.13	58,58,58,58	0
57	MG	AA	3044	1/1	0.96	0.25	60,60,60,60	0
57	MG	DA	3293	1/1	0.96	0.14	54,54,54,54	0
57	MG	AA	3006	1/1	0.96	0.12	52,52,52,52	0
57	MG	AA	3110	1/1	0.96	0.13	48,48,48,48	0
57	MG	DA	3353	1/1	0.96	0.16	42,42,42,42	0
57	MG	BA	3627	1/1	0.96	0.17	56,56,56,56	0
57	MG	DA	3504	1/1	0.96	0.07	47,47,47,47	0
57	MG	BQ	3002	1/1	0.96	0.23	43,43,43,43	0
57	MG	CA	3143	1/1	0.96	0.10	64,64,64,64	0
57	MG	BA	3382	1/1	0.96	0.09	63,63,63,63	0
57	MG	DA	3150	1/1	0.96	0.08	56,56,56,56	0
57	MG	DA	3559	1/1	0.96	0.12	43,43,43,43	0
57	MG	DA	3461	1/1	0.96	0.11	62,62,62,62	0
57	MG	DA	3443	1/1	0.96	0.10	54,54,54,54	0
57	MG	BA	3525	1/1	0.96	0.17	34,34,34,34	0
57	MG	BA	3264	1/1	0.96	0.22	58,58,58,58	0
57	MG	DA	3233	1/1	0.96	0.19	53,53,53,53	0
57	MG	BA	3256	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3108	1/1	0.96	0.32	44,44,44,44	0
57	MG	DA	3489	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3591	1/1	0.96	0.17	35,35,35,35	0
57	MG	BW	204	1/1	0.96	0.22	42,42,42,42	0
57	MG	BB	205	1/1	0.96	0.20	60,60,60,60	0
57	MG	BB	216	1/1	0.96	0.23	51,51,51,51	0
57	MG	BA	3224	1/1	0.96	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3319	1/1	0.96	0.12	41,41,41,41	0
57	MG	BA	3238	1/1	0.96	0.24	62,62,62,62	0
57	MG	DA	3387	1/1	0.96	0.10	42,42,42,42	0
57	MG	DA	3159	1/1	0.96	0.15	58,58,58,58	0
57	MG	BA	3529	1/1	0.96	0.20	56,56,56,56	0
57	MG	DA	3160	1/1	0.96	0.10	56,56,56,56	0
57	MG	BA	3088	1/1	0.96	0.35	48,48,48,48	0
57	MG	DA	3366	1/1	0.96	0.14	42,42,42,42	0
57	MG	CA	3067	1/1	0.96	0.31	61,61,61,61	0
57	MG	BP	204	1/1	0.96	0.06	46,46,46,46	0
57	MG	DA	3081	1/1	0.96	0.28	55,55,55,55	0
57	MG	BA	3437	1/1	0.96	0.14	36,36,36,36	0
57	MG	BE	304	1/1	0.96	0.19	42,42,42,42	0
57	MG	BA	3589	1/1	0.96	0.21	27,27,27,27	0
57	MG	DA	3055	1/1	0.96	0.17	49,49,49,49	0
57	MG	DA	3520	1/1	0.96	0.11	57,57,57,57	0
57	MG	DA	3537	1/1	0.96	0.08	44,44,44,44	0
57	MG	CA	3023	1/1	0.96	0.14	44,44,44,44	0
57	MG	BA	3692	1/1	0.96	0.15	40,40,40,40	0
57	MG	CA	3093	1/1	0.96	0.10	55,55,55,55	0
57	MG	DA	3350	1/1	0.96	0.12	51,51,51,51	0
57	MG	B3	3002	1/1	0.96	0.12	66,66,66,66	0
57	MG	DA	3241	1/1	0.96	0.13	45,45,45,45	0
57	MG	BA	3629	1/1	0.96	0.16	43,43,43,43	0
57	MG	BA	3528	1/1	0.96	0.18	56,56,56,56	0
57	MG	DA	3014	1/1	0.96	0.21	46,46,46,46	0
57	MG	BA	3272	1/1	0.96	0.61	48,48,48,48	0
57	MG	BA	3727	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3494	1/1	0.96	0.09	49,49,49,49	0
57	MG	DA	3176	1/1	0.96	0.19	41,41,41,41	0
57	MG	DW	3002	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3572	1/1	0.96	0.16	61,61,61,61	0
57	MG	BA	3460	1/1	0.96	0.10	62,62,62,62	0
57	MG	DA	3580	1/1	0.96	0.16	36,36,36,36	0
57	MG	BA	3491	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3153	1/1	0.96	0.31	47,47,47,47	0
57	MG	BA	3197	1/1	0.96	0.30	41,41,41,41	0
57	MG	BA	3244	1/1	0.96	0.22	53,53,53,53	0
57	MG	DA	3057	1/1	0.96	0.20	42,42,42,42	0
57	MG	BA	3547	1/1	0.96	0.23	39,39,39,39	0
57	MG	DA	3040	1/1	0.96	0.12	31,31,31,31	0
57	MG	DA	3220	1/1	0.96	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3299	1/1	0.96	0.20	55,55,55,55	0
57	MG	BA	3462	1/1	0.96	0.19	36,36,36,36	0
57	MG	DA	3193	1/1	0.96	0.13	57,57,57,57	0
57	MG	BA	3676	1/1	0.96	0.21	33,33,33,33	0
57	MG	BA	3012	1/1	0.96	0.20	39,39,39,39	0
57	MG	BW	203	1/1	0.96	0.20	44,44,44,44	0
57	MG	BA	3492	1/1	0.96	0.13	46,46,46,46	0
57	MG	BA	3804	1/1	0.96	0.42	53,53,53,53	0
57	MG	DA	3374	1/1	0.96	0.16	56,56,56,56	0
57	MG	BA	3251	1/1	0.96	0.19	44,44,44,44	0
57	MG	BB	213	1/1	0.96	0.19	60,60,60,60	0
57	MG	BA	3694	1/1	0.96	0.10	51,51,51,51	0
57	MG	DA	3156	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3091	1/1	0.96	0.40	56,56,56,56	0
57	MG	BA	3059	1/1	0.96	0.21	26,26,26,26	0
57	MG	DA	3059	1/1	0.96	0.26	43,43,43,43	0
57	MG	BA	3248	1/1	0.96	0.30	42,42,42,42	0
57	MG	DA	3109	1/1	0.96	0.15	40,40,40,40	0
57	MG	DA	3596	1/1	0.96	0.10	56,56,56,56	0
57	MG	DA	3395	1/1	0.96	0.12	47,47,47,47	0
57	MG	BA	3778	1/1	0.96	0.16	48,48,48,48	0
57	MG	BA	3665	1/1	0.96	0.16	49,49,49,49	0
57	MG	DA	3416	1/1	0.96	0.12	50,50,50,50	0
57	MG	DA	3454	1/1	0.96	0.16	56,56,56,56	0
57	MG	AA	3087	1/1	0.96	0.11	41,41,41,41	0
57	MG	BA	3191	1/1	0.96	0.18	43,43,43,43	0
57	MG	BA	3414	1/1	0.96	0.18	41,41,41,41	0
57	MG	BA	3691	1/1	0.96	0.16	55,55,55,55	0
57	MG	BA	3689	1/1	0.96	0.17	42,42,42,42	0
57	MG	BA	3208	1/1	0.96	0.16	44,44,44,44	0
57	MG	BA	3582	1/1	0.96	0.16	74,74,74,74	0
57	MG	BA	3336	1/1	0.96	0.15	64,64,64,64	0
57	MG	DA	3306	1/1	0.96	0.13	55,55,55,55	0
57	MG	DA	3341	1/1	0.96	0.13	51,51,51,51	0
57	MG	DA	3111	1/1	0.96	0.19	61,61,61,61	0
57	MG	DA	3169	1/1	0.96	0.24	47,47,47,47	0
57	MG	CA	3049	1/1	0.96	0.20	63,63,63,63	0
57	MG	BN	3001	1/1	0.96	0.31	53,53,53,53	0
57	MG	DA	3204	1/1	0.96	0.31	46,46,46,46	0
57	MG	BA	3469	1/1	0.96	0.15	49,49,49,49	0
57	MG	BF	303	1/1	0.96	0.54	49,49,49,49	0
57	MG	DA	3269	1/1	0.96	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DB	3007	1/1	0.96	0.20	58,58,58,58	0
57	MG	AA	3074	1/1	0.96	0.09	50,50,50,50	0
57	MG	BA	3763	1/1	0.96	0.19	24,24,24,24	0
57	MG	BG	203	1/1	0.96	0.16	42,42,42,42	0
57	MG	DA	3509	1/1	0.96	0.12	59,59,59,59	0
57	MG	BV	202	1/1	0.96	0.17	50,50,50,50	0
57	MG	BA	3488	1/1	0.96	0.19	60,60,60,60	0
57	MG	BB	207	1/1	0.96	0.22	54,54,54,54	0
57	MG	BA	3370	1/1	0.96	0.20	39,39,39,39	0
57	MG	BA	3711	1/1	0.96	0.19	54,54,54,54	0
57	MG	BA	3184	1/1	0.96	0.32	43,43,43,43	0
57	MG	DA	3619	1/1	0.96	0.11	69,69,69,69	0
57	MG	DA	3084	1/1	0.96	0.08	39,39,39,39	0
57	MG	DA	3282	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3648	1/1	0.96	0.14	57,57,57,57	0
57	MG	DA	3597	1/1	0.96	0.06	51,51,51,51	0
57	MG	BA	3107	1/1	0.96	0.16	53,53,53,53	0
57	MG	BA	3574	1/1	0.96	0.19	66,66,66,66	0
57	MG	BA	3613	1/1	0.96	0.41	42,42,42,42	0
57	MG	BA	3657	1/1	0.96	0.26	47,47,47,47	0
57	MG	BA	3699	1/1	0.96	0.23	35,35,35,35	0
57	MG	BA	3408	1/1	0.96	0.20	36,36,36,36	0
57	MG	DA	3022	1/1	0.96	0.27	51,51,51,51	0
57	MG	DA	3346	1/1	0.96	0.12	48,48,48,48	0
57	MG	DA	3365	1/1	0.96	0.08	36,36,36,36	0
57	MG	BA	3041	1/1	0.96	0.24	40,40,40,40	0
57	MG	BW	202	1/1	0.96	0.22	54,54,54,54	0
57	MG	DA	3012	1/1	0.96	0.12	33,33,33,33	0
57	MG	DE	302	1/1	0.96	0.17	33,33,33,33	0
57	MG	CA	3045	1/1	0.96	0.24	54,54,54,54	0
57	MG	DA	3493	1/1	0.96	0.30	66,66,66,66	0
57	MG	CA	3069	1/1	0.96	0.12	60,60,60,60	0
57	MG	B0	103	1/1	0.96	0.08	53,53,53,53	0
57	MG	BA	3132	1/1	0.96	0.14	40,40,40,40	0
57	MG	BA	3753	1/1	0.96	0.15	33,33,33,33	0
57	MG	AA	3048	1/1	0.96	0.22	57,57,57,57	0
57	MG	BA	3076	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3445	1/1	0.96	0.10	32,32,32,32	0
57	MG	DA	3253	1/1	0.96	0.13	45,45,45,45	0
57	MG	AA	3180	1/1	0.96	0.10	73,73,73,73	0
57	MG	DD	301	1/1	0.96	0.15	47,47,47,47	0
57	MG	BA	3356	1/1	0.96	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3349	1/1	0.96	0.09	56,56,56,56	0
57	MG	BA	3140	1/1	0.96	0.14	47,47,47,47	0
57	MG	CA	3056	1/1	0.96	0.10	64,64,64,64	0
57	MG	CA	3048	1/1	0.96	0.12	67,67,67,67	0
57	MG	AA	3011	1/1	0.96	0.34	57,57,57,57	0
57	MG	DA	3052	1/1	0.96	0.13	61,61,61,61	0
57	MG	BA	3660	1/1	0.96	0.11	61,61,61,61	0
57	MG	CA	3162	1/1	0.96	0.10	66,66,66,66	0
57	MG	BA	3696	1/1	0.96	0.14	33,33,33,33	0
57	MG	DA	3296	1/1	0.96	0.12	28,28,28,28	0
57	MG	DA	3464	1/1	0.96	0.10	46,46,46,46	0
57	MG	BA	3094	1/1	0.96	0.21	36,36,36,36	0
57	MG	AA	3173	1/1	0.96	0.15	54,54,54,54	0
57	MG	BA	3112	1/1	0.96	0.23	30,30,30,30	0
57	MG	BA	3701	1/1	0.96	0.15	43,43,43,43	0
57	MG	DA	3663	1/1	0.96	0.13	60,60,60,60	0
57	MG	BA	3468	1/1	0.96	0.17	62,62,62,62	0
57	MG	BV	205	1/1	0.96	0.09	38,38,38,38	0
57	MG	BA	3806	1/1	0.96	0.16	30,30,30,30	0
57	MG	AA	3043	1/1	0.96	0.23	51,51,51,51	0
57	MG	AA	3203	1/1	0.96	0.13	59,59,59,59	0
57	MG	BA	3160	1/1	0.96	0.32	55,55,55,55	0
57	MG	BA	3644	1/1	0.96	0.14	35,35,35,35	0
57	MG	BA	3603	1/1	0.96	0.13	53,53,53,53	0
57	MG	BA	3083	1/1	0.96	0.15	56,56,56,56	0
57	MG	AA	3212	1/1	0.96	0.13	42,42,42,42	0
57	MG	BA	3034	1/1	0.96	0.25	56,56,56,56	0
57	MG	AA	3113	1/1	0.96	0.12	58,58,58,58	0
57	MG	BA	3441	1/1	0.96	0.13	35,35,35,35	0
57	MG	AA	3151	1/1	0.96	0.14	45,45,45,45	0
57	MG	CA	3005	1/1	0.96	0.15	62,62,62,62	0
57	MG	BA	3169	1/1	0.96	0.17	45,45,45,45	0
57	MG	DA	3574	1/1	0.96	0.11	53,53,53,53	0
57	MG	DA	3101	1/1	0.96	0.16	49,49,49,49	0
57	MG	BA	3375	1/1	0.96	0.13	68,68,68,68	0
57	MG	DA	3569	1/1	0.96	0.23	49,49,49,49	0
57	MG	AX	3005	1/1	0.97	0.14	47,47,47,47	0
57	MG	CA	3050	1/1	0.97	0.20	61,61,61,61	0
57	MG	BF	301	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3776	1/1	0.97	0.20	43,43,43,43	0
57	MG	AA	3208	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3299	1/1	0.97	0.16	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3330	1/1	0.97	0.23	37,37,37,37	0
57	MG	BA	3752	1/1	0.97	0.19	32,32,32,32	0
57	MG	AA	3158	1/1	0.97	0.14	45,45,45,45	0
57	MG	BD	305	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3390	1/1	0.97	0.26	38,38,38,38	0
57	MG	BD	303	1/1	0.97	0.14	39,39,39,39	0
57	MG	BA	3113	1/1	0.97	0.25	53,53,53,53	0
57	MG	BF	306	1/1	0.97	0.28	31,31,31,31	0
57	MG	DA	3072	1/1	0.97	0.14	47,47,47,47	0
57	MG	BA	3222	1/1	0.97	0.18	37,37,37,37	0
57	MG	DA	3187	1/1	0.97	0.11	42,42,42,42	0
57	MG	BA	3428	1/1	0.97	0.19	46,46,46,46	0
57	MG	BF	307	1/1	0.97	0.24	37,37,37,37	0
57	MG	AA	3105	1/1	0.97	0.32	69,69,69,69	0
57	MG	DA	3168	1/1	0.97	0.29	45,45,45,45	0
57	MG	DA	3257	1/1	0.97	0.18	50,50,50,50	0
57	MG	BA	3311	1/1	0.97	0.27	48,48,48,48	0
57	MG	BG	201	1/1	0.97	0.20	58,58,58,58	0
57	MG	BA	3011	1/1	0.97	0.19	35,35,35,35	0
57	MG	BA	3731	1/1	0.97	0.30	37,37,37,37	0
57	MG	DA	3042	1/1	0.97	0.17	38,38,38,38	0
57	MG	BA	3379	1/1	0.97	0.18	31,31,31,31	0
57	MG	BA	3214	1/1	0.97	0.17	41,41,41,41	0
57	MG	BA	3653	1/1	0.97	0.21	39,39,39,39	0
57	MG	DA	3166	1/1	0.97	0.11	55,55,55,55	0
57	MG	BA	3674	1/1	0.97	0.15	63,63,63,63	0
57	MG	AA	3099	1/1	0.97	0.20	51,51,51,51	0
57	MG	DA	3466	1/1	0.97	0.11	41,41,41,41	0
57	MG	AA	3137	1/1	0.97	0.15	51,51,51,51	0
57	MG	DA	3369	1/1	0.97	0.15	28,28,28,28	0
57	MG	CA	3123	1/1	0.97	0.14	58,58,58,58	0
57	MG	BA	3481	1/1	0.97	0.18	41,41,41,41	0
60	K	CX	3001	1/1	0.97	0.19	82,82,82,82	0
57	MG	DA	3599	1/1	0.97	0.20	36,36,36,36	0
57	MG	BA	3549	1/1	0.97	0.29	39,39,39,39	0
57	MG	DA	3019	1/1	0.97	0.29	37,37,37,37	0
57	MG	BA	3089	1/1	0.97	0.17	19,19,19,19	0
57	MG	BA	3410	1/1	0.97	0.16	27,27,27,27	0
57	MG	BA	3029	1/1	0.97	0.48	37,37,37,37	0
57	MG	BE	302	1/1	0.97	0.23	39,39,39,39	0
57	MG	DA	3542	1/1	0.97	0.17	24,24,24,24	0
57	MG	DD	307	1/1	0.97	0.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3474	1/1	0.97	0.18	55,55,55,55	0
57	MG	AA	3112	1/1	0.97	0.17	63,63,63,63	0
57	MG	BA	3420	1/1	0.97	0.16	40,40,40,40	0
57	MG	BA	3630	1/1	0.97	0.14	58,58,58,58	0
57	MG	DA	3552	1/1	0.97	0.12	54,54,54,54	0
57	MG	DW	3004	1/1	0.97	0.22	52,52,52,52	0
57	MG	BA	3263	1/1	0.97	0.34	49,49,49,49	0
57	MG	AA	3147	1/1	0.97	0.10	70,70,70,70	0
57	MG	DA	3171	1/1	0.97	0.12	31,31,31,31	0
57	MG	DA	3191	1/1	0.97	0.17	37,37,37,37	0
57	MG	DA	3155	1/1	0.97	0.25	48,48,48,48	0
57	MG	BA	3787	1/1	0.97	0.23	45,45,45,45	0
57	MG	DA	3349	1/1	0.97	0.07	52,52,52,52	0
57	MG	BA	3565	1/1	0.97	0.17	40,40,40,40	0
57	MG	DA	3278	1/1	0.97	0.06	43,43,43,43	0
57	MG	DA	3266	1/1	0.97	0.09	57,57,57,57	0
57	MG	AA	3148	1/1	0.97	0.22	57,57,57,57	0
57	MG	AX	3006	1/1	0.97	0.10	65,65,65,65	0
57	MG	BA	3067	1/1	0.97	0.15	41,41,41,41	0
57	MG	BA	3425	1/1	0.97	0.15	40,40,40,40	0
57	MG	DA	3601	1/1	0.97	0.10	44,44,44,44	0
57	MG	DA	3105	1/1	0.97	0.19	48,48,48,48	0
57	MG	DA	3265	1/1	0.97	0.12	30,30,30,30	0
57	MG	DA	3305	1/1	0.97	0.20	50,50,50,50	0
57	MG	BA	3677	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3103	1/1	0.97	0.17	38,38,38,38	0
57	MG	BA	3483	1/1	0.97	0.15	28,28,28,28	0
57	MG	BA	3260	1/1	0.97	0.30	39,39,39,39	0
57	MG	BA	3193	1/1	0.97	0.20	48,48,48,48	0
57	MG	BA	3082	1/1	0.97	0.22	39,39,39,39	0
57	MG	AA	3125	1/1	0.97	0.24	37,37,37,37	0
57	MG	BA	3245	1/1	0.97	0.23	34,34,34,34	0
57	MG	DA	3228	1/1	0.97	0.30	38,38,38,38	0
57	MG	BA	3093	1/1	0.97	0.26	56,56,56,56	0
57	MG	BA	3116	1/1	0.97	0.28	50,50,50,50	0
57	MG	DA	3345	1/1	0.97	0.09	44,44,44,44	0
59	ZN	D9	501	1/1	0.97	0.12	68,68,68,68	0
57	MG	BA	3036	1/1	0.97	0.17	40,40,40,40	0
57	MG	BA	3326	1/1	0.97	0.19	20,20,20,20	0
57	MG	DA	3028	1/1	0.97	0.36	52,52,52,52	0
57	MG	DA	3449	1/1	0.97	0.10	54,54,54,54	0
57	MG	BA	3774	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3766	1/1	0.97	0.15	28,28,28,28	0
57	MG	DA	3261	1/1	0.97	0.12	49,49,49,49	0
57	MG	BA	3270	1/1	0.97	0.17	48,48,48,48	0
57	MG	DA	3307	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3137	1/1	0.97	0.24	39,39,39,39	0
57	MG	CA	3134	1/1	0.97	0.16	69,69,69,69	0
57	MG	BN	3003	1/1	0.97	0.19	48,48,48,48	0
57	MG	BA	3158	1/1	0.97	0.20	41,41,41,41	0
57	MG	DA	3613	1/1	0.97	0.15	54,54,54,54	0
57	MG	DA	3192	1/1	0.97	0.10	60,60,60,60	0
57	MG	BA	3042	1/1	0.97	0.20	43,43,43,43	0
57	MG	DA	3390	1/1	0.97	0.11	43,43,43,43	0
57	MG	CA	3072	1/1	0.97	0.17	54,54,54,54	0
57	MG	BA	3139	1/1	0.97	0.33	40,40,40,40	0
57	MG	DA	3370	1/1	0.97	0.14	51,51,51,51	0
57	MG	DA	3089	1/1	0.97	0.39	52,52,52,52	0
57	MG	BA	3393	1/1	0.97	0.18	51,51,51,51	0
57	MG	BA	3280	1/1	0.97	0.14	37,37,37,37	0
57	MG	DA	3143	1/1	0.97	0.18	38,38,38,38	0
57	MG	BA	3254	1/1	0.97	0.22	25,25,25,25	0
57	MG	BA	3358	1/1	0.97	0.21	49,49,49,49	0
57	MG	CA	3137	1/1	0.97	0.16	56,56,56,56	0
57	MG	BB	212	1/1	0.97	0.13	55,55,55,55	0
57	MG	CA	3167	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3371	1/1	0.97	0.14	35,35,35,35	0
57	MG	BA	3046	1/1	0.97	0.28	41,41,41,41	0
57	MG	DA	3099	1/1	0.97	0.17	32,32,32,32	0
57	MG	BB	203	1/1	0.97	0.24	43,43,43,43	0
57	MG	DA	3664	1/1	0.97	0.39	48,48,48,48	0
57	MG	DA	3086	1/1	0.97	0.09	43,43,43,43	0
57	MG	BA	3115	1/1	0.97	0.24	59,59,59,59	0
57	MG	BA	3489	1/1	0.97	0.07	59,59,59,59	0
57	MG	BA	3698	1/1	0.97	0.22	31,31,31,31	0
57	MG	BA	3725	1/1	0.97	0.14	44,44,44,44	0
57	MG	BA	3338	1/1	0.97	0.13	40,40,40,40	0
57	MG	BB	204	1/1	0.97	0.18	41,41,41,41	0
57	MG	DA	3020	1/1	0.97	0.16	55,55,55,55	0
57	MG	DA	3231	1/1	0.97	0.09	62,62,62,62	0
57	MG	CA	3034	1/1	0.97	0.14	59,59,59,59	0
57	MG	DA	3579	1/1	0.97	0.10	48,48,48,48	0
57	MG	DA	3310	1/1	0.97	0.13	38,38,38,38	0
57	MG	DA	3175	1/1	0.97	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3506	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3518	1/1	0.97	0.20	44,44,44,44	0
57	MG	DA	3384	1/1	0.97	0.10	49,49,49,49	0
57	MG	AA	3154	1/1	0.97	0.11	69,69,69,69	0
57	MG	DW	3001	1/1	0.97	0.40	54,54,54,54	0
57	MG	BA	3111	1/1	0.97	0.13	54,54,54,54	0
57	MG	BA	3232	1/1	0.97	0.20	52,52,52,52	0
57	MG	BA	3479	1/1	0.97	0.07	50,50,50,50	0
57	MG	BA	3188	1/1	0.97	0.30	49,49,49,49	0
57	MG	BA	3611	1/1	0.97	0.17	46,46,46,46	0
57	MG	DA	3460	1/1	0.97	0.13	41,41,41,41	0
57	MG	BA	3345	1/1	0.97	0.14	38,38,38,38	0
57	MG	BA	3475	1/1	0.97	0.13	42,42,42,42	0
57	MG	BA	3786	1/1	0.97	0.13	35,35,35,35	0
57	MG	AA	3186	1/1	0.97	0.12	42,42,42,42	0
57	MG	DV	3002	1/1	0.97	0.30	49,49,49,49	0
57	MG	BA	3048	1/1	0.97	0.13	47,47,47,47	0
57	MG	BA	3144	1/1	0.97	0.19	41,41,41,41	0
57	MG	BA	3789	1/1	0.97	0.18	12,12,12,12	0
57	MG	BA	3553	1/1	0.97	0.10	59,59,59,59	0
57	MG	DA	3322	1/1	0.97	0.19	51,51,51,51	0
57	MG	DA	3184	1/1	0.97	0.16	47,47,47,47	0
57	MG	BA	3756	1/1	0.97	0.20	48,48,48,48	0
57	MG	BA	3343	1/1	0.97	0.15	53,53,53,53	0
57	MG	DA	3529	1/1	0.97	0.08	38,38,38,38	0
57	MG	BA	3152	1/1	0.97	0.30	43,43,43,43	0
57	MG	DA	3016	1/1	0.97	0.34	50,50,50,50	0
57	MG	DA	3644	1/1	0.97	0.08	55,55,55,55	0
57	MG	BA	3181	1/1	0.97	0.25	43,43,43,43	0
57	MG	CA	3131	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3368	1/1	0.97	0.20	40,40,40,40	0
57	MG	AA	3092	1/1	0.97	0.14	63,63,63,63	0
57	MG	BN	3005	1/1	0.97	0.17	36,36,36,36	0
57	MG	DA	3142	1/1	0.97	0.13	47,47,47,47	0
57	MG	BA	3363	1/1	0.97	0.15	22,22,22,22	0
57	MG	BB	208	1/1	0.97	0.14	45,45,45,45	0
57	MG	CA	3071	1/1	0.97	0.15	68,68,68,68	0
57	MG	DA	3561	1/1	0.97	0.04	57,57,57,57	0
57	MG	DA	3338	1/1	0.97	0.15	61,61,61,61	0
57	MG	BA	3331	1/1	0.97	0.17	49,49,49,49	0
57	MG	DA	3352	1/1	0.97	0.19	63,63,63,63	0
57	MG	DA	3436	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3046	1/1	0.97	0.16	47,47,47,47	0
57	MG	BA	3476	1/1	0.97	0.15	55,55,55,55	0
57	MG	DA	3647	1/1	0.97	0.11	54,54,54,54	0
57	MG	BA	3221	1/1	0.97	0.17	37,37,37,37	0
57	MG	DF	3003	1/1	0.97	0.40	43,43,43,43	0
57	MG	DA	3096	1/1	0.97	0.23	42,42,42,42	0
57	MG	BA	3643	1/1	0.97	0.13	46,46,46,46	0
57	MG	DA	3058	1/1	0.97	0.14	29,29,29,29	0
57	MG	BA	3086	1/1	0.97	0.21	22,22,22,22	0
57	MG	BA	3028	1/1	0.97	0.22	51,51,51,51	0
57	MG	AK	3001	1/1	0.97	0.18	44,44,44,44	0
57	MG	BA	3004	1/1	0.97	0.19	33,33,33,33	0
57	MG	DA	3435	1/1	0.97	0.15	50,50,50,50	0
57	MG	BF	309	1/1	0.97	0.15	53,53,53,53	0
57	MG	CA	3155	1/1	0.97	0.12	53,53,53,53	0
57	MG	DA	3326	1/1	0.97	0.16	43,43,43,43	0
57	MG	BA	3097	1/1	0.97	0.14	44,44,44,44	0
57	MG	AA	3018	1/1	0.97	0.24	56,56,56,56	0
57	MG	BA	3490	1/1	0.97	0.10	54,54,54,54	0
57	MG	B7	103	1/1	0.97	0.16	42,42,42,42	0
57	MG	AA	3207	1/1	0.97	0.09	65,65,65,65	0
57	MG	BD	306	1/1	0.97	0.25	38,38,38,38	0
57	MG	DA	3373	1/1	0.97	0.15	44,44,44,44	0
57	MG	AA	3164	1/1	0.97	0.10	61,61,61,61	0
57	MG	BA	3309	1/1	0.97	0.18	41,41,41,41	0
57	MG	BA	3159	1/1	0.97	0.25	50,50,50,50	0
57	MG	BA	3360	1/1	0.97	0.16	41,41,41,41	0
57	MG	AA	3024	1/1	0.97	0.12	54,54,54,54	0
57	MG	BA	3286	1/1	0.97	0.21	34,34,34,34	0
57	MG	BA	3168	1/1	0.97	0.17	47,47,47,47	0
57	MG	BA	3380	1/1	0.97	0.10	48,48,48,48	0
57	MG	BA	3334	1/1	0.97	0.14	37,37,37,37	0
57	MG	AA	3182	1/1	0.97	0.14	49,49,49,49	0
57	MG	BA	3202	1/1	0.97	0.19	60,60,60,60	0
57	MG	BA	3435	1/1	0.97	0.27	45,45,45,45	0
57	MG	BA	3105	1/1	0.97	0.18	37,37,37,37	0
57	MG	DA	3182	1/1	0.97	0.24	51,51,51,51	0
57	MG	B8	101	1/1	0.97	0.21	44,44,44,44	0
57	MG	DA	3455	1/1	0.97	0.10	47,47,47,47	0
57	MG	CA	3147	1/1	0.97	0.12	64,64,64,64	0
57	MG	CA	3084	1/1	0.97	0.13	60,60,60,60	0
57	MG	DB	3010	1/1	0.97	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3102	1/1	0.97	0.19	44,44,44,44	0
57	MG	DA	3189	1/1	0.97	0.20	41,41,41,41	0
57	MG	AA	3120	1/1	0.97	0.19	45,45,45,45	0
57	MG	B7	101	1/1	0.97	0.24	39,39,39,39	0
57	MG	BA	3784	1/1	0.97	0.21	33,33,33,33	0
57	MG	BA	3449	1/1	0.98	0.21	35,35,35,35	0
57	MG	BA	3544	1/1	0.98	0.22	44,44,44,44	0
57	MG	DA	3508	1/1	0.98	0.10	44,44,44,44	0
57	MG	DA	3281	1/1	0.98	0.16	53,53,53,53	0
57	MG	BA	3060	1/1	0.98	0.20	30,30,30,30	0
57	MG	BA	3187	1/1	0.98	0.25	29,29,29,29	0
57	MG	BA	3705	1/1	0.98	0.11	62,62,62,62	0
57	MG	BA	3085	1/1	0.98	0.27	35,35,35,35	0
57	MG	BA	3339	1/1	0.98	0.21	23,23,23,23	0
57	MG	BA	3050	1/1	0.98	0.20	38,38,38,38	0
57	MG	BA	3281	1/1	0.98	0.28	60,60,60,60	0
57	MG	DA	3010	1/1	0.98	0.17	47,47,47,47	0
57	MG	DA	3161	1/1	0.98	0.19	38,38,38,38	0
57	MG	DQ	3001	1/1	0.98	0.13	47,47,47,47	0
57	MG	BA	3625	1/1	0.98	0.18	39,39,39,39	0
57	MG	BA	3135	1/1	0.98	0.20	43,43,43,43	0
57	MG	AA	3090	1/1	0.98	0.21	66,66,66,66	0
57	MG	DA	3363	1/1	0.98	0.16	29,29,29,29	0
57	MG	BA	3080	1/1	0.98	0.17	60,60,60,60	0
58	SF4	CD	302	8/8	0.98	0.16	60,68,83,86	0
57	MG	BA	3467	1/1	0.98	0.23	50,50,50,50	0
57	MG	DF	3002	1/1	0.98	0.18	48,48,48,48	0
57	MG	BA	3772	1/1	0.98	0.19	33,33,33,33	0
57	MG	DA	3412	1/1	0.98	0.20	50,50,50,50	0
57	MG	BA	3416	1/1	0.98	0.21	21,21,21,21	0
57	MG	BA	3521	1/1	0.98	0.20	39,39,39,39	0
57	MG	BA	3472	1/1	0.98	0.16	20,20,20,20	0
57	MG	BA	3039	1/1	0.98	0.20	32,32,32,32	0
57	MG	BA	3588	1/1	0.98	0.23	31,31,31,31	0
57	MG	DA	3115	1/1	0.98	0.24	40,40,40,40	0
57	MG	DA	3471	1/1	0.98	0.23	50,50,50,50	0
59	ZN	AN	501	1/1	0.98	0.19	69,69,69,69	0
57	MG	CA	3099	1/1	0.98	0.15	44,44,44,44	0
57	MG	BA	3313	1/1	0.98	0.07	53,53,53,53	0
57	MG	DA	3491	1/1	0.98	0.16	51,51,51,51	0
57	MG	BA	3025	1/1	0.98	0.16	27,27,27,27	0
57	MG	BA	3792	1/1	0.98	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3040	1/1	0.98	0.11	60,60,60,60	0
57	MG	AA	3053	1/1	0.98	0.20	61,61,61,61	0
57	MG	BA	3124	1/1	0.98	0.21	19,19,19,19	0
57	MG	CA	3133	1/1	0.98	0.21	59,59,59,59	0
57	MG	DA	3330	1/1	0.98	0.11	45,45,45,45	0
57	MG	AA	3062	1/1	0.98	0.28	51,51,51,51	0
57	MG	AA	3082	1/1	0.98	0.13	46,46,46,46	0
57	MG	DA	3442	1/1	0.98	0.12	39,39,39,39	0
57	MG	BA	3556	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3357	1/1	0.98	0.07	50,50,50,50	0
57	MG	DA	3258	1/1	0.98	0.14	48,48,48,48	0
57	MG	BA	3148	1/1	0.98	0.33	44,44,44,44	0
57	MG	BA	3247	1/1	0.98	0.16	25,25,25,25	0
57	MG	BA	3609	1/1	0.98	0.11	39,39,39,39	0
57	MG	DA	3555	1/1	0.98	0.29	53,53,53,53	0
57	MG	DA	3399	1/1	0.98	0.13	59,59,59,59	0
57	MG	BA	3038	1/1	0.98	0.25	35,35,35,35	0
57	MG	BA	3287	1/1	0.98	0.14	42,42,42,42	0
57	MG	BA	3450	1/1	0.98	0.13	48,48,48,48	0
57	MG	BA	3234	1/1	0.98	0.15	38,38,38,38	0
57	MG	BA	3558	1/1	0.98	0.14	32,32,32,32	0
57	MG	BA	3719	1/1	0.98	0.18	53,53,53,53	0
57	MG	DA	3453	1/1	0.98	0.22	60,60,60,60	0
57	MG	DA	3198	1/1	0.98	0.13	40,40,40,40	0
57	MG	BA	3230	1/1	0.98	0.20	53,53,53,53	0
57	MG	BA	3737	1/1	0.98	0.29	43,43,43,43	0
57	MG	AA	3168	1/1	0.98	0.11	59,59,59,59	0
57	MG	AA	3086	1/1	0.98	0.07	57,57,57,57	0
57	MG	BA	3010	1/1	0.98	0.16	39,39,39,39	0
57	MG	BA	3605	1/1	0.98	0.17	43,43,43,43	0
59	ZN	B6	103	1/1	0.98	0.24	49,49,49,49	0
57	MG	BA	3791	1/1	0.98	0.18	28,28,28,28	0
57	MG	BA	3367	1/1	0.98	0.25	29,29,29,29	0
57	MG	AA	3077	1/1	0.98	0.25	56,56,56,56	0
57	MG	BA	3762	1/1	0.98	0.20	46,46,46,46	0
57	MG	DA	3003	1/1	0.98	0.15	27,27,27,27	0
57	MG	BA	3534	1/1	0.98	0.21	44,44,44,44	0
57	MG	CA	3148	1/1	0.98	0.11	70,70,70,70	0
57	MG	DA	3500	1/1	0.98	0.10	49,49,49,49	0
57	MG	BA	3327	1/1	0.98	0.18	38,38,38,38	0
57	MG	BA	3040	1/1	0.98	0.36	35,35,35,35	0
59	ZN	CN	501	1/1	0.98	0.08	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3665	1/1	0.98	0.14	42,42,42,42	0
57	MG	DA	3190	1/1	0.98	0.20	54,54,54,54	0
57	MG	BU	203	1/1	0.98	0.21	47,47,47,47	0
57	MG	CA	3103	1/1	0.98	0.13	46,46,46,46	0
57	MG	BR	202	1/1	0.98	0.14	31,31,31,31	0
57	MG	DA	3144	1/1	0.98	0.11	38,38,38,38	0
57	MG	DA	3459	1/1	0.98	0.19	47,47,47,47	0
57	MG	DA	3525	1/1	0.98	0.13	59,59,59,59	0
57	MG	CA	3105	1/1	0.98	0.18	52,52,52,52	0
57	MG	BA	3235	1/1	0.98	0.16	42,42,42,42	0
57	MG	DD	305	1/1	0.98	0.12	36,36,36,36	0
57	MG	CA	3085	1/1	0.98	0.13	54,54,54,54	0
57	MG	BA	3167	1/1	0.98	0.12	41,41,41,41	0
57	MG	BP	203	1/1	0.98	0.15	33,33,33,33	0
57	MG	BA	3487	1/1	0.98	0.14	50,50,50,50	0
58	SF4	AD	501	8/8	0.98	0.16	62,68,73,86	0
57	MG	BA	3241	1/1	0.98	0.19	36,36,36,36	0
57	MG	BA	3278	1/1	0.98	0.18	34,34,34,34	0
57	MG	DA	3534	1/1	0.98	0.15	55,55,55,55	0
57	MG	BA	3332	1/1	0.98	0.18	38,38,38,38	0
57	MG	DA	3034	1/1	0.98	0.18	38,38,38,38	0
57	MG	BB	217	1/1	0.98	0.18	29,29,29,29	0
57	MG	DA	3177	1/1	0.98	0.15	42,42,42,42	0
57	MG	BA	3044	1/1	0.98	0.22	20,20,20,20	0
57	MG	DA	3008	1/1	0.98	0.09	36,36,36,36	0
57	MG	BA	3498	1/1	0.98	0.18	36,36,36,36	0
57	MG	DA	3294	1/1	0.98	0.16	43,43,43,43	0
57	MG	DA	3289	1/1	0.98	0.10	53,53,53,53	0
57	MG	BF	305	1/1	0.98	0.09	49,49,49,49	0
57	MG	DA	3157	1/1	0.98	0.11	47,47,47,47	0
57	MG	DU	3001	1/1	0.98	0.32	55,55,55,55	0
57	MG	DA	3292	1/1	0.98	0.17	30,30,30,30	0
59	ZN	BY	501	1/1	0.98	0.15	58,58,58,58	0
57	MG	BA	3174	1/1	0.98	0.18	37,37,37,37	0
57	MG	BA	3454	1/1	0.98	0.23	27,27,27,27	0
57	MG	BA	3364	1/1	0.98	0.27	60,60,60,60	0
57	MG	DA	3021	1/1	0.98	0.09	31,31,31,31	0
57	MG	DA	3393	1/1	0.98	0.10	50,50,50,50	0
57	MG	BA	3049	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3197	1/1	0.98	0.14	55,55,55,55	0
57	MG	DD	308	1/1	0.98	0.29	48,48,48,48	0
57	MG	BA	3735	1/1	0.98	0.43	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3043	1/1	0.98	0.11	47,47,47,47	0
57	MG	BA	3736	1/1	0.98	0.16	42,42,42,42	0
57	MG	CA	3089	1/1	0.98	0.12	47,47,47,47	0
57	MG	CA	3065	1/1	0.98	0.17	49,49,49,49	0
57	MG	DA	3512	1/1	0.98	0.09	47,47,47,47	0
57	MG	B0	101	1/1	0.98	0.17	36,36,36,36	0
57	MG	CA	3047	1/1	0.98	0.14	53,53,53,53	0
57	MG	DE	301	1/1	0.98	0.40	46,46,46,46	0
57	MG	BA	3744	1/1	0.98	0.14	39,39,39,39	0
57	MG	BV	201	1/1	0.98	0.31	33,33,33,33	0
57	MG	DN	5001	1/1	0.98	0.11	66,66,66,66	0
57	MG	B6	101	1/1	0.98	0.17	48,48,48,48	0
57	MG	DA	3404	1/1	0.98	0.12	48,48,48,48	0
57	MG	BA	3142	1/1	0.98	0.17	49,49,49,49	0
57	MG	BA	3563	1/1	0.98	0.17	36,36,36,36	0
57	MG	AA	3126	1/1	0.98	0.09	49,49,49,49	0
57	MG	DA	3094	1/1	0.98	0.22	50,50,50,50	0
57	MG	BA	3141	1/1	0.98	0.28	42,42,42,42	0
57	MG	BA	3497	1/1	0.98	0.14	28,28,28,28	0
57	MG	BA	3607	1/1	0.98	0.24	38,38,38,38	0
57	MG	BA	3259	1/1	0.98	0.21	25,25,25,25	0
57	MG	BA	3569	1/1	0.99	0.19	49,49,49,49	0
57	MG	DA	3347	1/1	0.99	0.20	27,27,27,27	0
57	MG	DA	3480	1/1	0.99	0.10	40,40,40,40	0
57	MG	BA	3458	1/1	0.99	0.18	18,18,18,18	0
57	MG	BA	3392	1/1	0.99	0.17	53,53,53,53	0
57	MG	DA	3027	1/1	0.99	0.57	51,51,51,51	0
57	MG	BA	3726	1/1	0.99	0.19	63,63,63,63	0
59	ZN	B5	102	1/1	0.99	0.22	48,48,48,48	0
57	MG	DA	3026	1/1	0.99	0.56	59,59,59,59	0
57	MG	BA	3374	1/1	0.99	0.17	40,40,40,40	0
57	MG	BA	3216	1/1	0.99	0.23	37,37,37,37	0
57	MG	DA	3535	1/1	0.99	0.18	56,56,56,56	0
57	MG	BA	3069	1/1	0.99	0.27	22,22,22,22	0
57	MG	BA	3045	1/1	0.99	0.21	36,36,36,36	0
57	MG	BD	307	1/1	0.99	0.21	40,40,40,40	0
57	MG	DA	3315	1/1	0.99	0.08	42,42,42,42	0
57	MG	DA	3671	1/1	0.99	0.13	74,74,74,74	0
59	ZN	B9	501	1/1	0.99	0.18	38,38,38,38	0
57	MG	BA	3422	1/1	0.99	0.24	33,33,33,33	0
57	MG	BA	3233	1/1	0.99	0.30	56,56,56,56	0
59	ZN	D5	501	1/1	0.99	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	ZN	D6	501	1/1	0.99	0.17	71,71,71,71	0
57	MG	DF	3004	1/1	0.99	0.38	44,44,44,44	0
57	MG	BA	3198	1/1	0.99	0.24	37,37,37,37	0
57	MG	BA	3597	1/1	0.99	0.21	25,25,25,25	0
57	MG	BA	3384	1/1	0.99	0.19	41,41,41,41	0
57	MG	DA	3560	1/1	0.99	0.07	40,40,40,40	0
57	MG	DA	3285	1/1	0.99	0.13	32,32,32,32	0
57	MG	BA	3378	1/1	0.99	0.12	28,28,28,28	0
57	MG	BA	3013	1/1	0.99	0.14	32,32,32,32	0
57	MG	DA	3344	1/1	0.99	0.16	31,31,31,31	0
57	MG	DA	3031	1/1	0.99	0.43	43,43,43,43	0
57	MG	DA	3297	1/1	0.99	0.11	39,39,39,39	0
57	MG	DA	3005	1/1	0.99	0.22	57,57,57,57	0
57	MG	BU	206	1/1	0.99	0.40	35,35,35,35	0
57	MG	BA	3037	1/1	1.00	0.24	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.