



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 02:06 AM UTC

PDB ID : 4V8I / pdb_00004v8i
Title : Crystal structure of YfiA bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-12
Resolution : 2.70 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

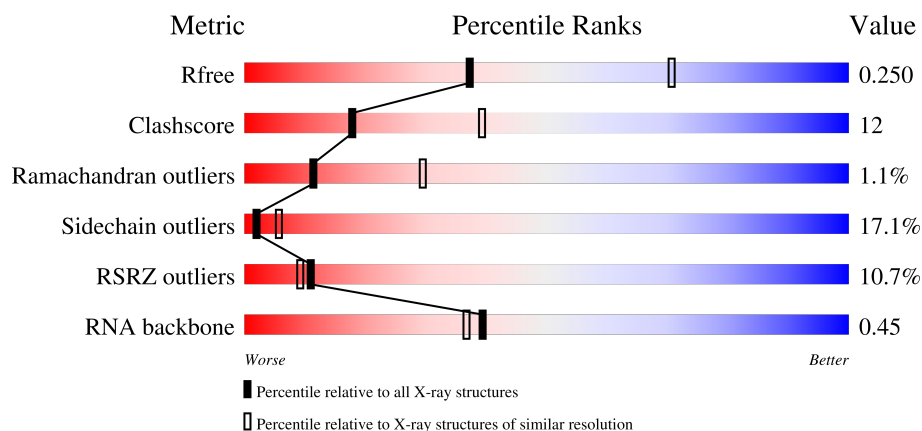
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	4% 46% 39% 13% •
1	CA	1522	8% 41% 42% 15% •
2	AB	256	29% 45% 36% 8% 11%
2	CB	256	39% 46% 37% 8% 8%

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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	AY	119	
22	CY	119	
23	BA	2915	
23	DA	2915	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	

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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	

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Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	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
54	MG	AA	1621	-	-	-	X
54	MG	CA	1630	-	-	-	X
54	MG	DB	206	-	-	-	X

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 287173 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	1493	Total	C	N	O	P	0	0	0
			32102	14287	5955	10367	1493			
1	CA	1491	Total	C	N	O	P	0	0	0
			32056	14267	5945	10353	1491			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1817	1160	325	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
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1453	908	280	264	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
			1520	960	283	272	5			
4	CD	208	Total	C	N	O	S	0	0	0
			1537	968	287	276	6			

- 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
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1106	700	204	198	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
			781	495	137	146	3			
6	CF	99	Total	C	N	O	S	0	0	0
			776	492	135	146	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
			1167	727	224	210	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1049	667	188	192	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O		0	0	0
			852	533	163	156				
9	CI	125	Total	C	N	O		0	0	0
			849	531	161	157				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O		0	0	0
			659	408	131	120				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			657	407	129	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	114	Total 828	C 516	N 155	O 154	S 3	0	0	0
11	CK	114	Total 828	C 516	N 155	O 154	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
13	CM	112	Total	C	N	O	S	0	0	0
			784	486	159	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total 478	C 303	N 99	O 72	S 4	0	0	0
14	CN	60	Total 474	C 300	N 98	O 72	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- 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
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			661	421	126	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
			819	525	150	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
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	78	Total	C	N	O	S	0	0	0
			549	345	106	96	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
			699	430	150	117	2			
20	CT	104	Total	C	N	O	S	0	0	0
			773	476	162	133	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
			180	112	41	27			

- Molecule 22 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	95	Total	C	N	O	S	0	0	0
			754	472	142	137	3			
22	CY	94	Total	C	N	O	S	0	0	0
			739	461	138	137	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	114	HIS	-	expression tag	UNP P0AD49
AY	115	HIS	-	expression tag	UNP P0AD49
AY	116	HIS	-	expression tag	UNP P0AD49
AY	117	HIS	-	expression tag	UNP P0AD49
AY	118	HIS	-	expression tag	UNP P0AD49
AY	119	HIS	-	expression tag	UNP P0AD49
CY	114	HIS	-	expression tag	UNP P0AD49
CY	115	HIS	-	expression tag	UNP P0AD49
CY	116	HIS	-	expression tag	UNP P0AD49
CY	117	HIS	-	expression tag	UNP P0AD49
CY	118	HIS	-	expression tag	UNP P0AD49
CY	119	HIS	-	expression tag	UNP P0AD49

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2827	Total	C	N	O	P	0	0	0
			60898	27101	11400	19571	2826			
23	DA	2798	Total	C	N	O	P	0	0	0
			60264	26820	11274	19374	2796			

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

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

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

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
26	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1577	1004	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1572	1003	298	269	2			

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
28	DG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
29	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1043	672	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			1043	672	180	190	1			

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
31	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
32	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
33	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				
36	DS	110	Total	C	N	O	S	0	0	0
			873	550	174	149				

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	130	Total	C	N	O	S	0	0	0
			1058	663	212	182	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
39	DV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DW	111	Total	C	N	O	S	0	0	0
			877	552	171	152	2			

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			732	477	130	124	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			781	502	145	128	6			

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
43	DZ	203	Total	C	N	O	S	0	0	0
			1528	973	268	284	3			

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	1			

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
45	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
46	D2	71	Total	C	N	O	S	0	0	0
			584	361	118	103	2			

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			463	295	87	81			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			437	272	84	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
51	D7	48	Total	C	N	O	S	0	0	0
			402	248	97	55	2			

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	217	Total	Mg	0	0
			217	217		
54	AD	2	Total	Mg	0	0
			2	2		
54	AE	1	Total	Mg	0	0
			1	1		
54	AF	1	Total	Mg	0	0
			1	1		
54	AI	1	Total	Mg	0	0
			1	1		
54	AL	1	Total	Mg	0	0
			1	1		
54	AM	2	Total	Mg	0	0
			2	2		
54	AP	1	Total	Mg	0	0
			1	1		
54	BA	729	Total	Mg	0	0
			729	729		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	19	Total 19	Mg 19	0	0
54	BD	7	Total 7	Mg 7	0	0
54	BE	6	Total 6	Mg 6	0	0
54	BF	6	Total 6	Mg 6	0	0
54	BG	1	Total 1	Mg 1	0	0
54	BH	1	Total 1	Mg 1	0	0
54	BN	2	Total 2	Mg 2	0	0
54	BO	1	Total 1	Mg 1	0	0
54	BP	2	Total 2	Mg 2	0	0
54	BQ	5	Total 5	Mg 5	0	0
54	BR	5	Total 5	Mg 5	0	0
54	BS	1	Total 1	Mg 1	0	0
54	BT	3	Total 3	Mg 3	0	0
54	BU	3	Total 3	Mg 3	0	0
54	BV	4	Total 4	Mg 4	0	0
54	BW	1	Total 1	Mg 1	0	0
54	BY	1	Total 1	Mg 1	0	0
54	BZ	2	Total 2	Mg 2	0	0
54	B0	4	Total 4	Mg 4	0	0
54	B1	1	Total 1	Mg 1	0	0
54	B2	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	B3	3	Total 3	Mg 3	0	0
54	B5	1	Total 1	Mg 1	0	0
54	B6	1	Total 1	Mg 1	0	0
54	B7	1	Total 1	Mg 1	0	0
54	B8	1	Total 1	Mg 1	0	0
54	B9	3	Total 3	Mg 3	0	0
54	CA	203	Total 203	Mg 203	0	0
54	CE	1	Total 1	Mg 1	0	0
54	CQ	1	Total 1	Mg 1	0	0
54	DA	637	Total 637	Mg 637	0	0
54	DB	10	Total 10	Mg 10	0	0
54	DD	5	Total 5	Mg 5	0	0
54	DE	3	Total 3	Mg 3	0	0
54	DF	5	Total 5	Mg 5	0	0
54	DO	3	Total 3	Mg 3	0	0
54	DP	3	Total 3	Mg 3	0	0
54	DQ	4	Total 4	Mg 4	0	0
54	DR	2	Total 2	Mg 2	0	0
54	DT	2	Total 2	Mg 2	0	0
54	DW	1	Total 1	Mg 1	0	0
54	D0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	D1	1	Total 1	Mg 1	0	0
54	D5	2	Total 2	Mg 2	0	0
54	D7	2	Total 2	Mg 2	0	0
54	D8	2	Total 2	Mg 2	0	0
54	D9	1	Total 1	Mg 1	0	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	443	Total 443	O 443	0	0
56	AD	3	Total 3	O 3	0	0
56	AE	2	Total 2	O 2	0	0
56	AF	2	Total 2	O 2	0	0
56	AG	2	Total 2	O 2	0	0
56	AJ	1	Total 1	O 1	0	0
56	AK	1	Total 1	O 1	0	0
56	AL	3	Total 3	O 3	0	0
56	AM	1	Total 1	O 1	0	0
56	AO	1	Total 1	O 1	0	0
56	AP	1	Total 1	O 1	0	0
56	AQ	3	Total 3	O 3	0	0
56	AY	1	Total 1	O 1	0	0
56	BA	1988	Total 1988	O 1988	0	0
56	BB	43	Total 43	O 43	0	0
56	BD	21	Total 21	O 21	0	0
56	BE	18	Total 18	O 18	0	0
56	BF	18	Total 18	O 18	0	0
56	BG	2	Total 2	O 2	0	0
56	BH	2	Total 2	O 2	0	0
56	BN	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BO	3	Total 3	O 3	0	0
56	BP	20	Total 20	O 20	0	0
56	BQ	9	Total 9	O 9	0	0
56	BR	8	Total 8	O 8	0	0
56	BS	2	Total 2	O 2	0	0
56	BT	5	Total 5	O 5	0	0
56	BU	9	Total 9	O 9	0	0
56	BV	13	Total 13	O 13	0	0
56	BW	6	Total 6	O 6	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	2	Total 2	O 2	0	0
56	BZ	2	Total 2	O 2	0	0
56	B0	4	Total 4	O 4	0	0
56	B1	5	Total 5	O 5	0	0
56	B3	4	Total 4	O 4	0	0
56	B5	5	Total 5	O 5	0	0
56	B6	2	Total 2	O 2	0	0
56	B7	5	Total 5	O 5	0	0
56	B8	11	Total 11	O 11	0	0
56	B9	1	Total 1	O 1	0	0
56	CA	400	Total 400	O 400	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CD	2	Total	O	0	0
			2	2		
56	CE	4	Total	O	0	0
			4	4		
56	CF	1	Total	O	0	0
			1	1		
56	CK	1	Total	O	0	0
			1	1		
56	CL	2	Total	O	0	0
			2	2		
56	CP	3	Total	O	0	0
			3	3		
56	CQ	3	Total	O	0	0
			3	3		
56	CR	1	Total	O	0	0
			1	1		
56	CT	2	Total	O	0	0
			2	2		
56	CU	1	Total	O	0	0
			1	1		
56	DA	1496	Total	O	0	0
			1496	1496		
56	DB	33	Total	O	0	0
			33	33		
56	DD	17	Total	O	0	0
			17	17		
56	DE	12	Total	O	0	0
			12	12		
56	DF	10	Total	O	0	0
			10	10		
56	DN	2	Total	O	0	0
			2	2		
56	DO	7	Total	O	0	0
			7	7		
56	DP	11	Total	O	0	0
			11	11		
56	DQ	2	Total	O	0	0
			2	2		
56	DR	5	Total	O	0	0
			5	5		
56	DT	3	Total	O	0	0
			3	3		

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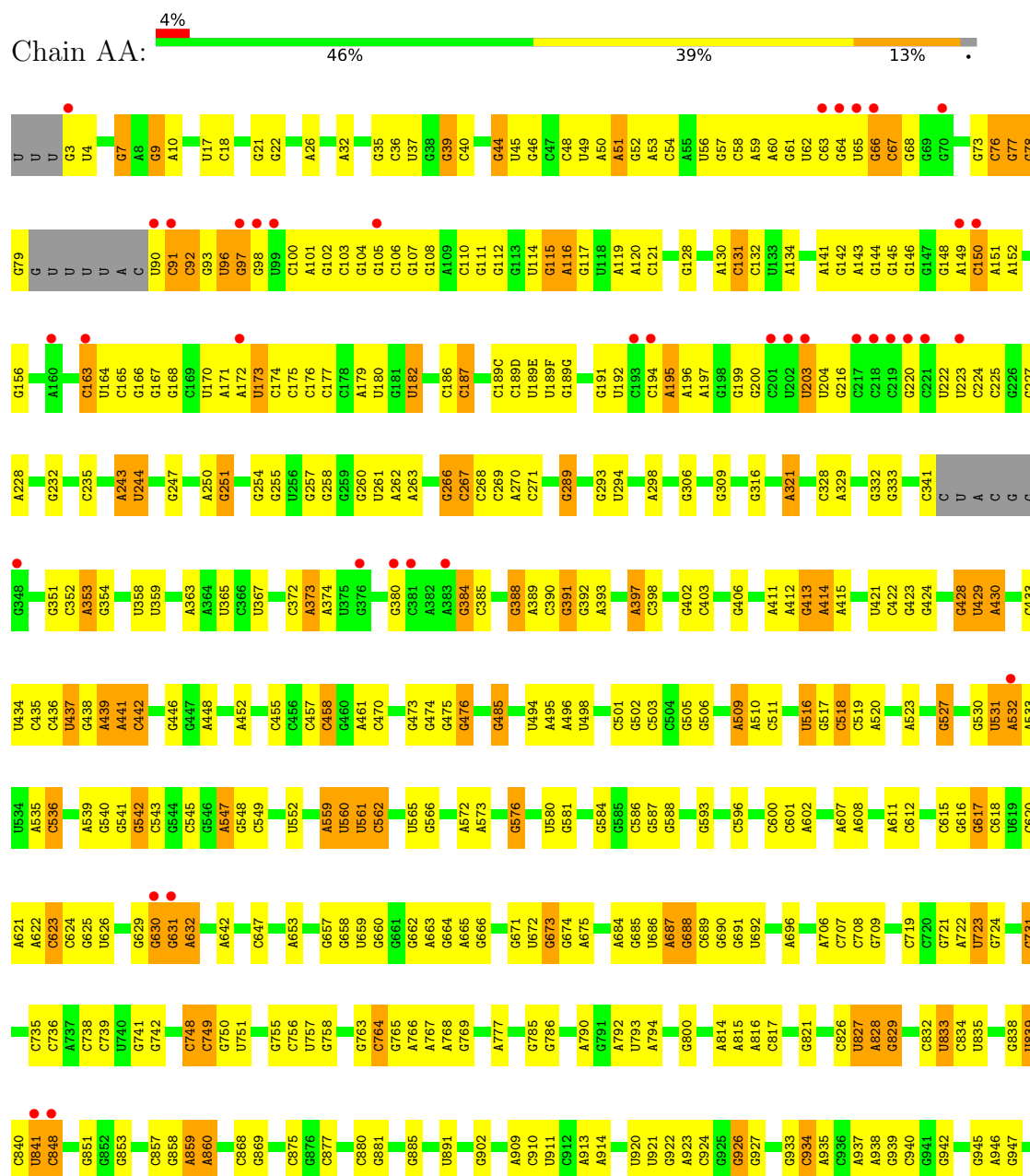
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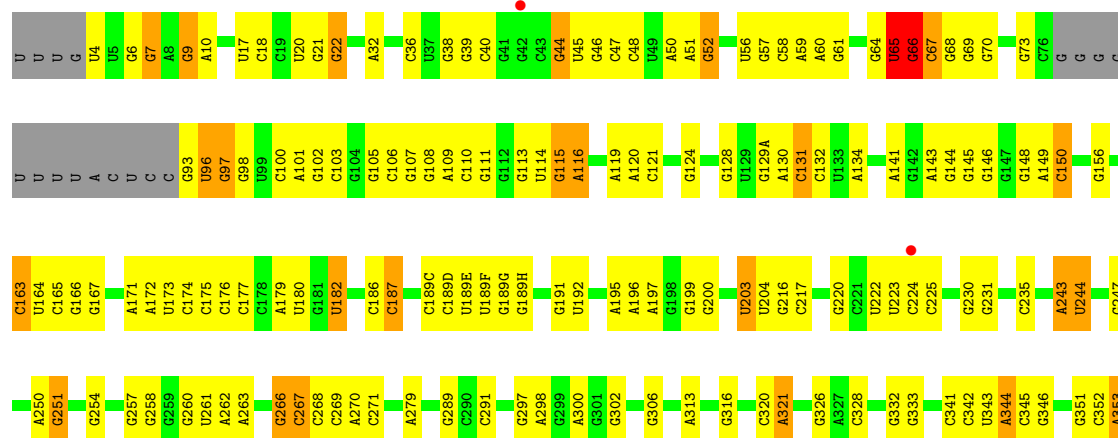
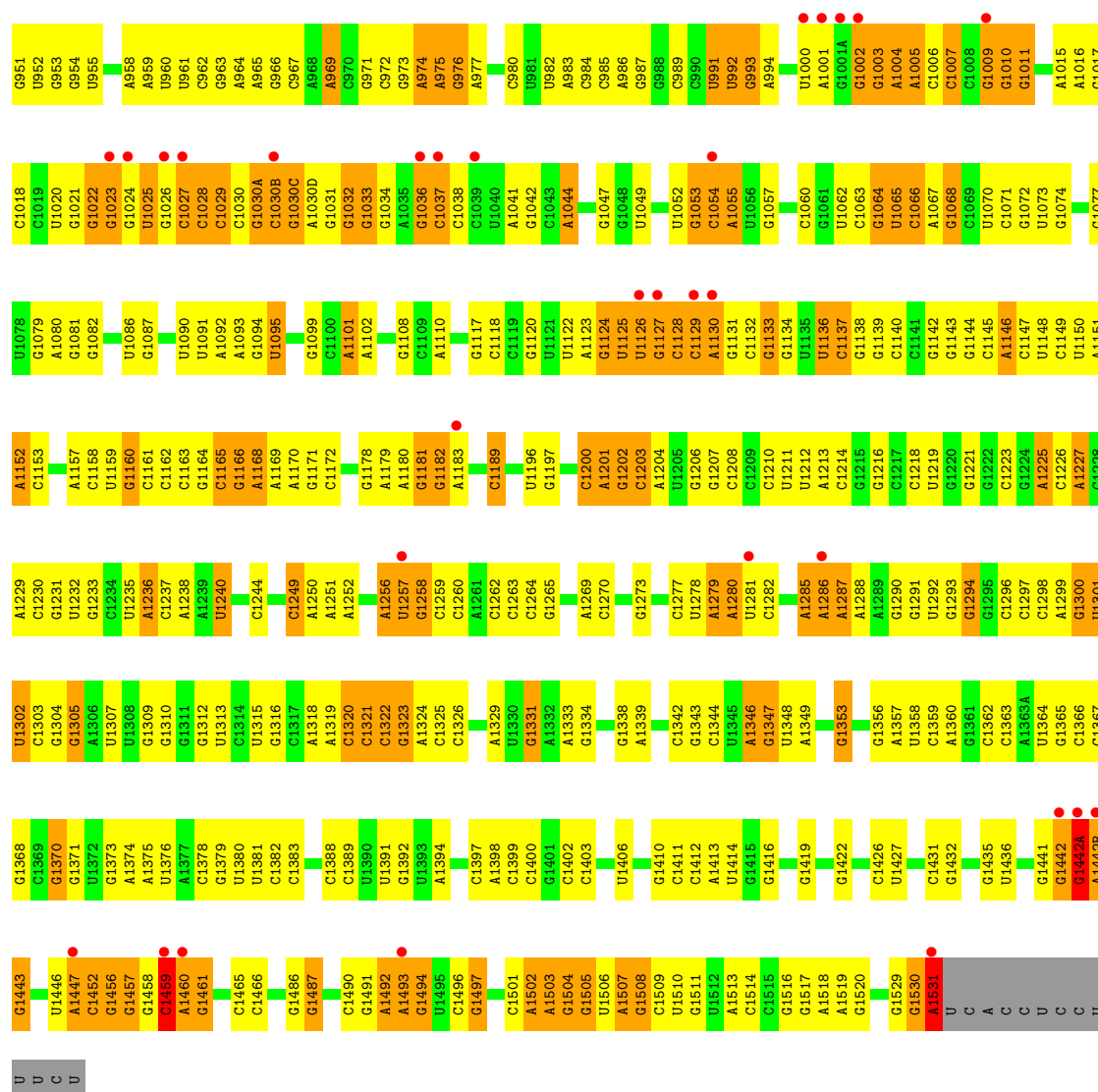
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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56	DV	1	Total	O	0	0
			1	1		
56	DW	4	Total	O	0	0
			4	4		
56	DX	2	Total	O	0	0
			2	2		
56	DY	2	Total	O	0	0
			2	2		
56	D0	2	Total	O	0	0
			2	2		
56	D1	3	Total	O	0	0
			3	3		
56	D2	1	Total	O	0	0
			1	1		
56	D3	1	Total	O	0	0
			1	1		
56	D5	3	Total	O	0	0
			3	3		
56	D6	3	Total	O	0	0
			3	3		
56	D7	3	Total	O	0	0
			3	3		
56	D8	6	Total	O	0	0
			6	6		
56	D9	1	Total	O	0	0
			1	1		

3 Residue-property plots

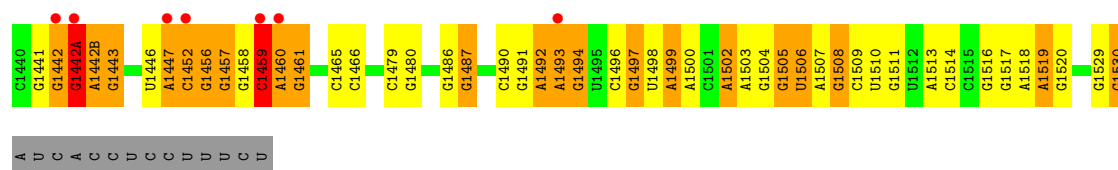
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S Ribosomal RNA

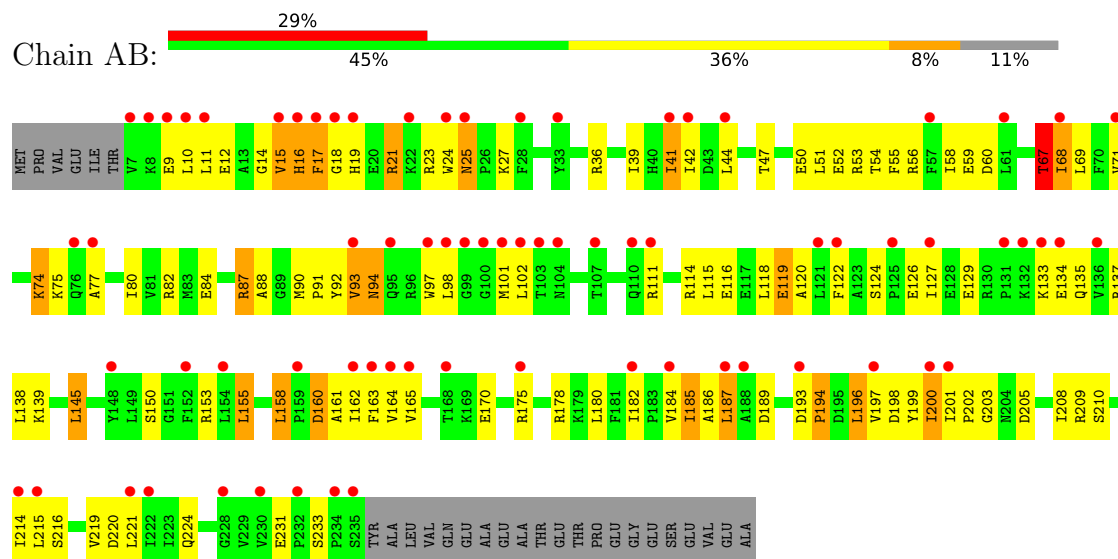




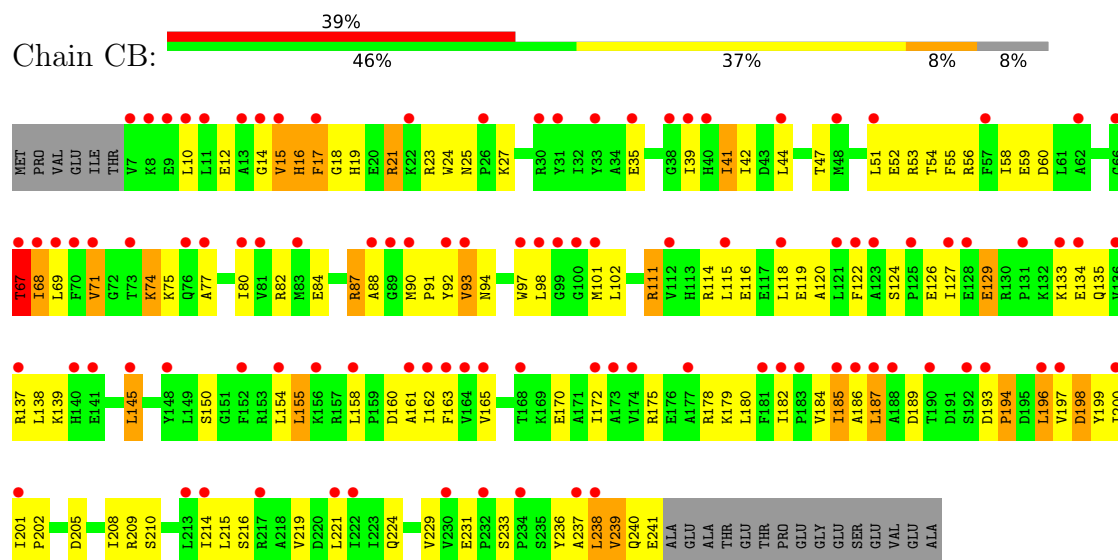




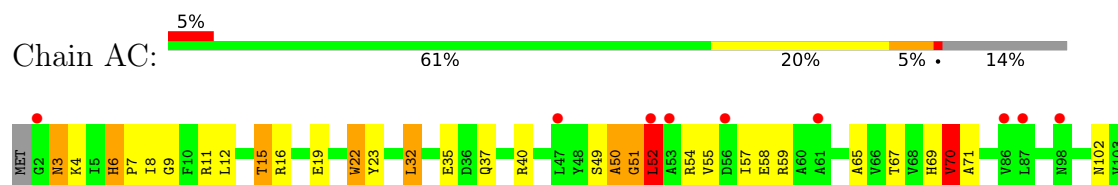
• Molecule 2: 30S Ribosomal Protein S2

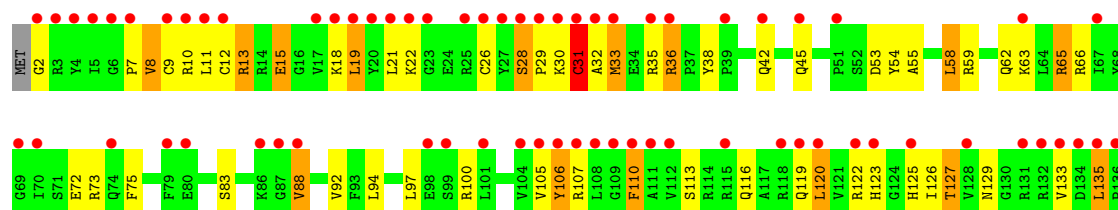


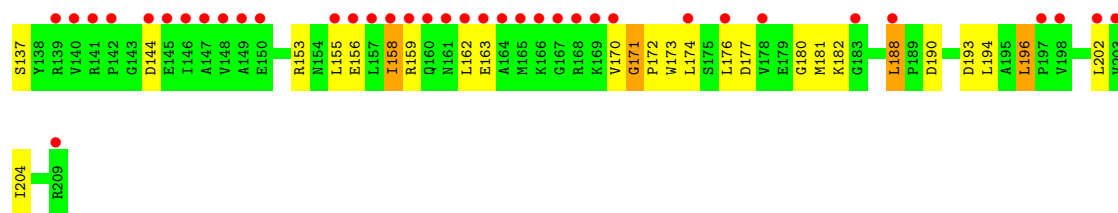
• Molecule 2: 30S Ribosomal Protein S2



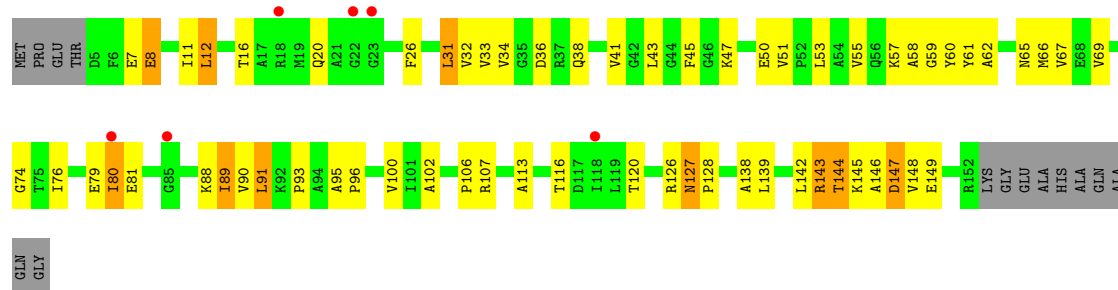
• Molecule 3: 30S Ribosomal Protein S3



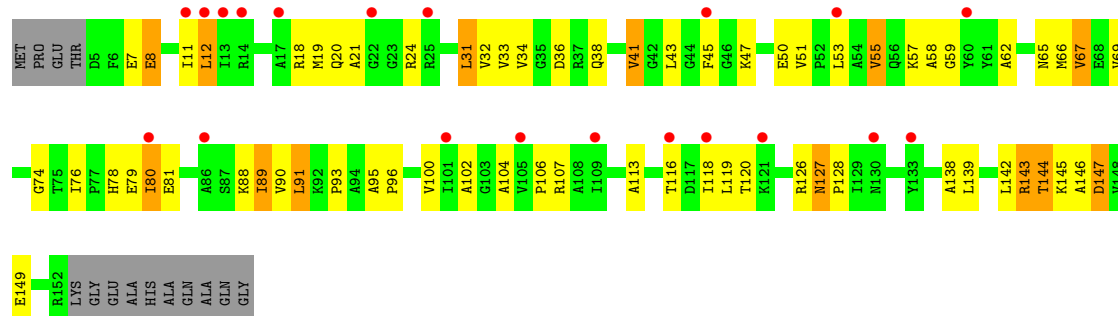




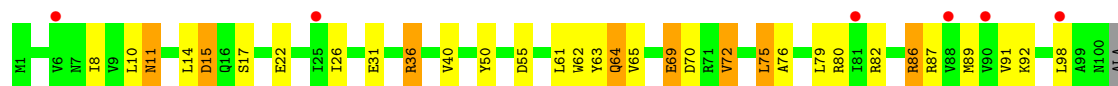
• Molecule 5: 30S Ribosomal Protein S5



• Molecule 5: 30S Ribosomal Protein S5



• Molecule 6: 30S Ribosomal Protein S6

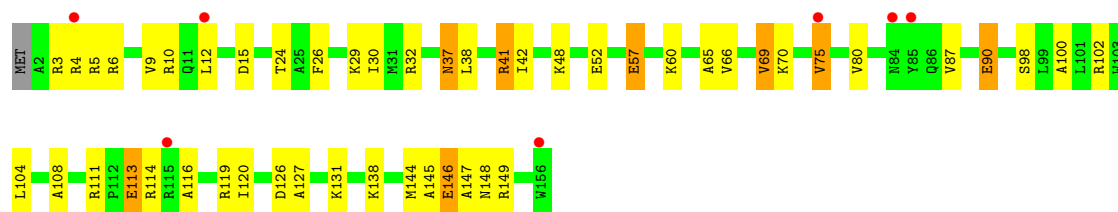


• Molecule 6: 30S Ribosomal Protein S6



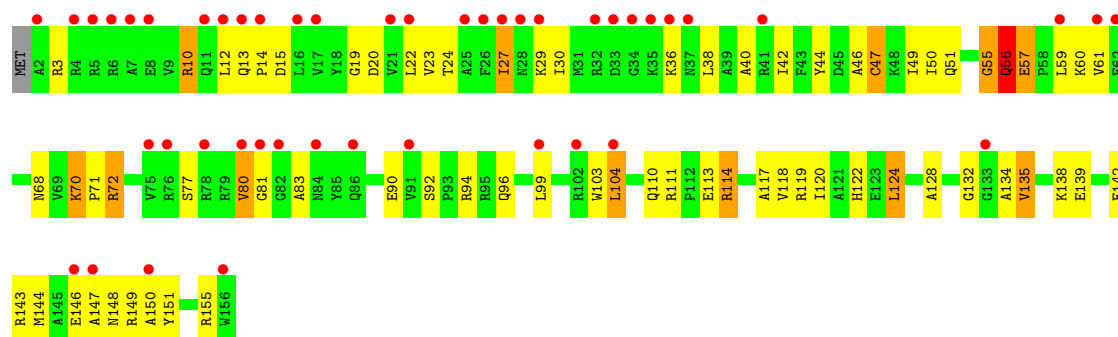
• Molecule 7: 30S Ribosomal Protein S7

Chain AG: 



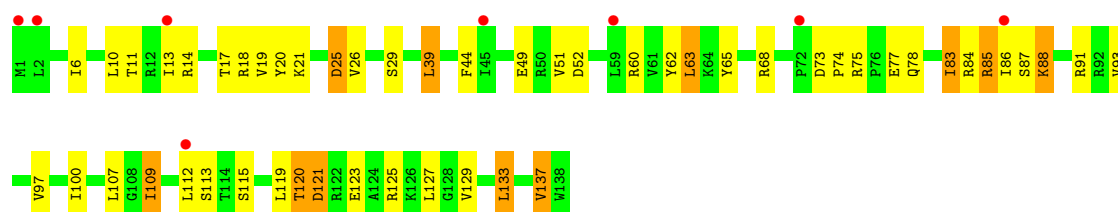
• Molecule 7: 30S Ribosomal Protein S7

Chain CG: 



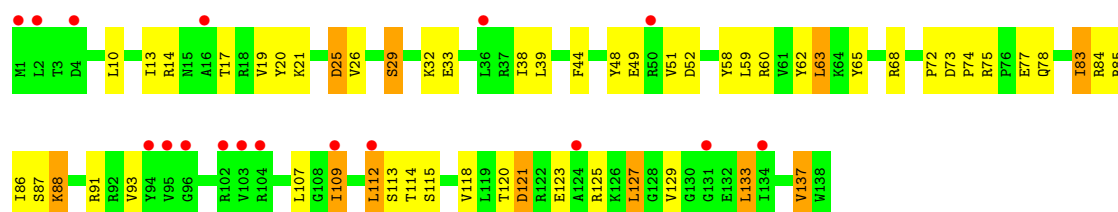
• Molecule 8: 30S Ribosomal Protein S8

Chain AH: 



• Molecule 8: 30S Ribosomal Protein S8

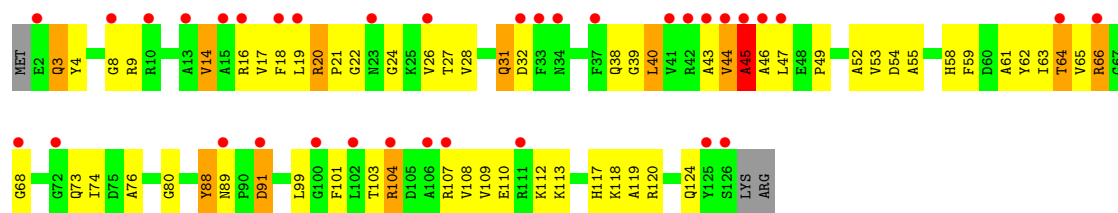
Chain CH: 



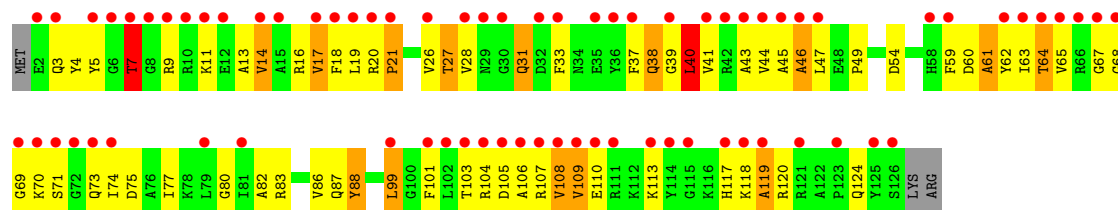
• Molecule 9: 30S Ribosomal Protein S9

Chain AI: 

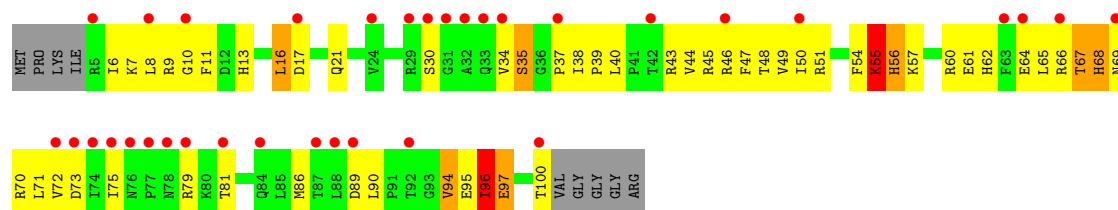




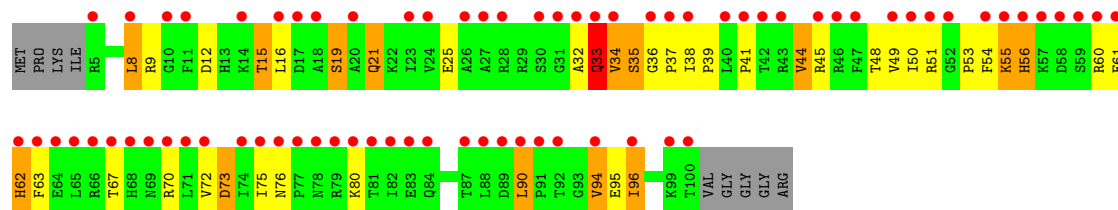
• Molecule 9: 30S Ribosomal Protein S9



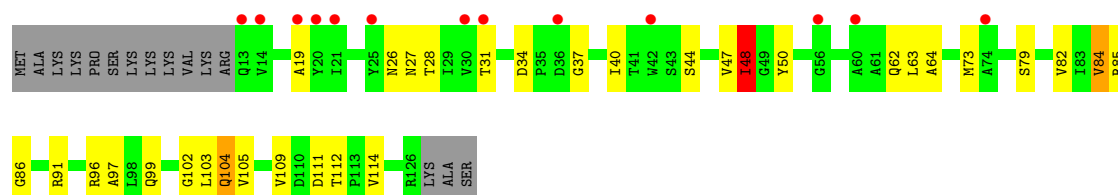
• Molecule 10: 30S Ribosomal Protein S10



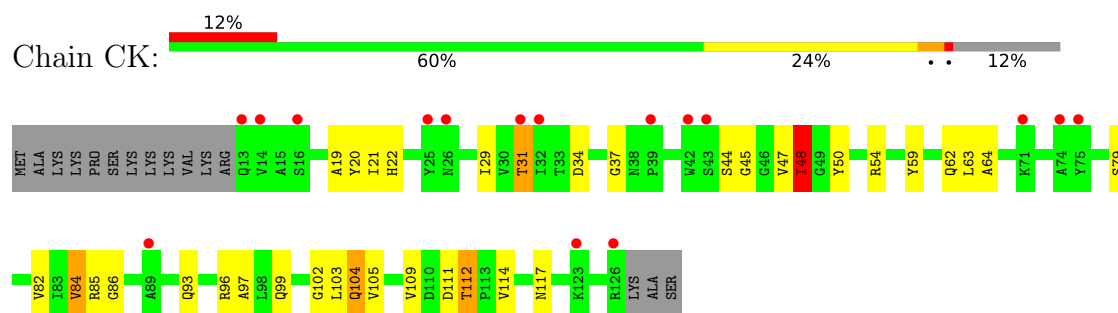
• Molecule 10: 30S Ribosomal Protein S10



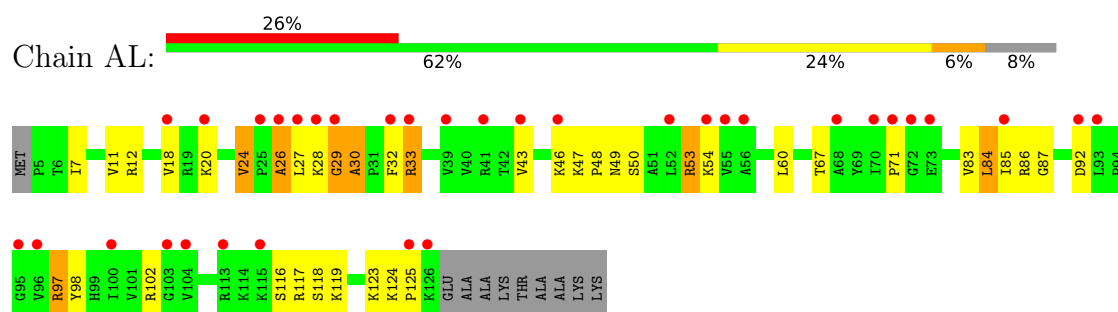
• Molecule 11: 30S Ribosomal Protein S11



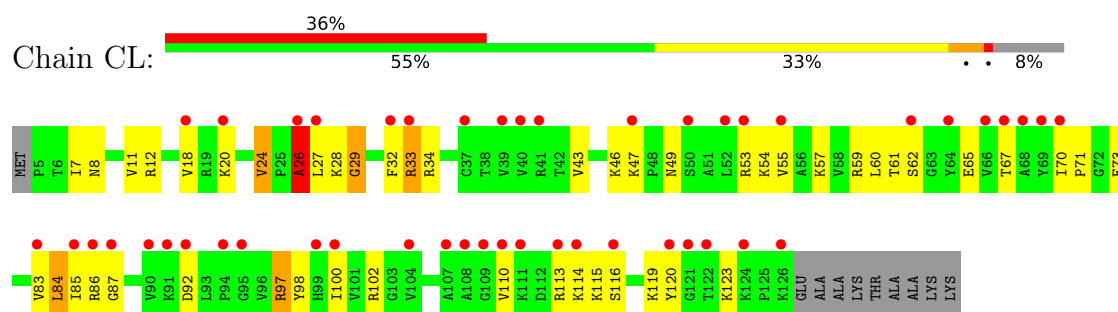
- Molecule 11: 30S Ribosomal Protein S11



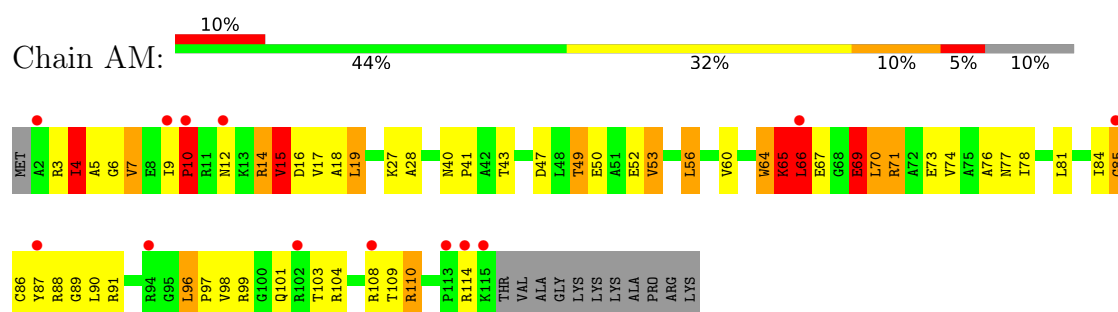
- Molecule 12: 30S Ribosomal Protein S12



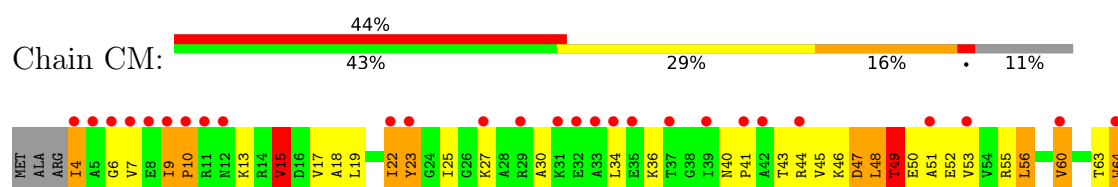
- Molecule 12: 30S Ribosomal Protein S12

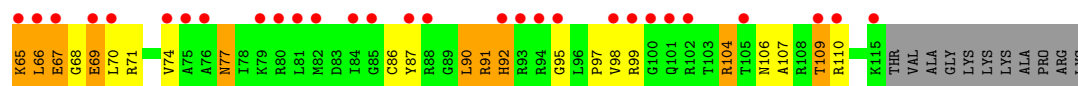


- Molecule 13: 30S Ribosomal Protein S13

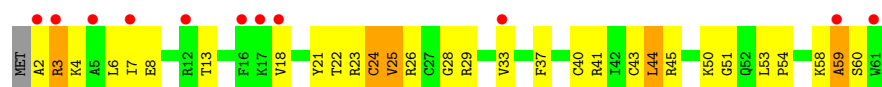


- Molecule 13: 30S Ribosomal Protein S13

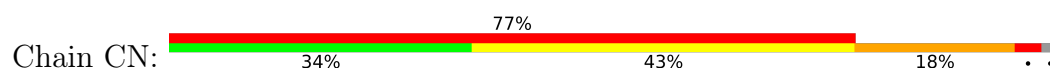




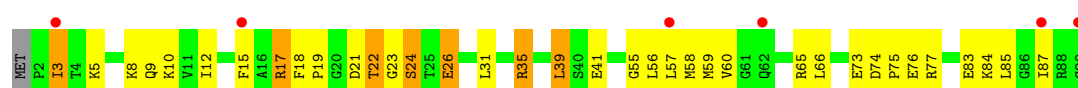
• Molecule 14: 30S Ribosomal Protein S14



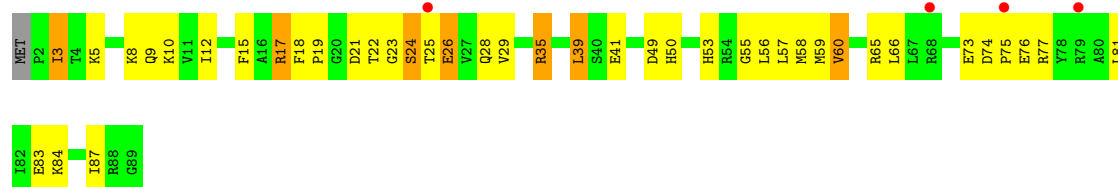
• Molecule 14: 30S Ribosomal Protein S14



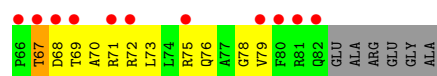
• Molecule 15: 30S Ribosomal Protein S15



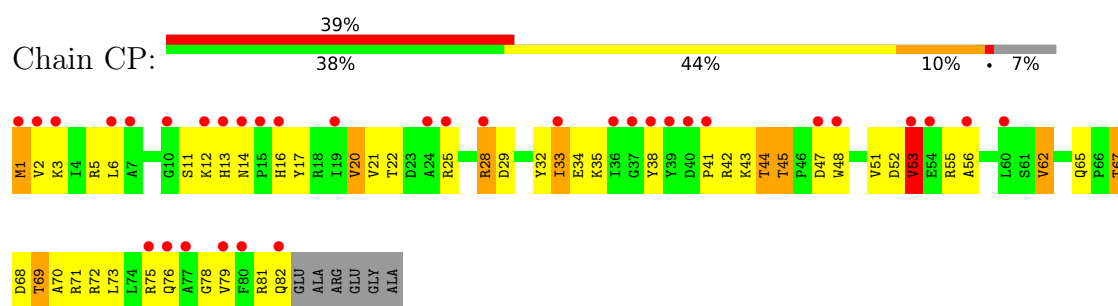
• Molecule 15: 30S Ribosomal Protein S15



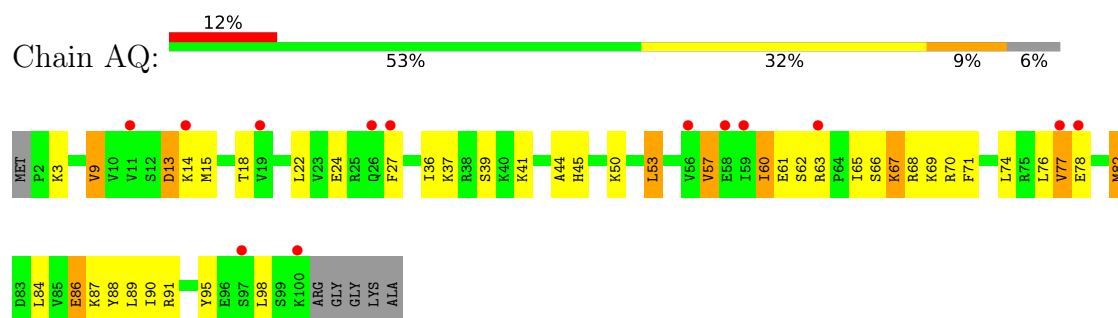
• Molecule 16: 30S Ribosomal Protein S16



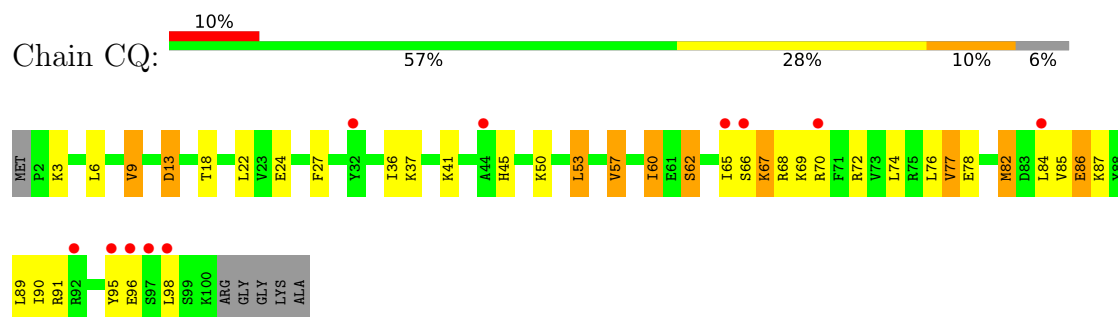
• Molecule 16: 30S Ribosomal Protein S16



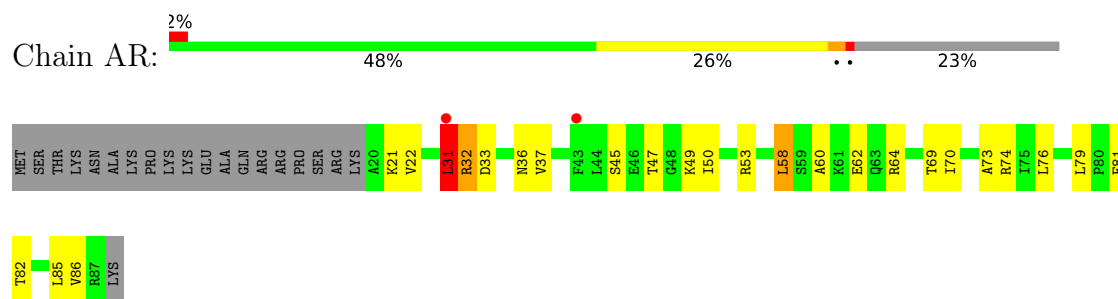
• Molecule 17: 30S Ribosomal Protein S17



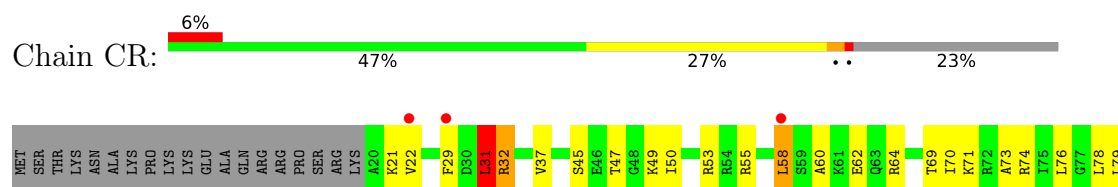
• Molecule 17: 30S Ribosomal Protein S17

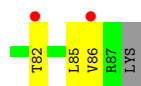


• Molecule 18: 30S Ribosomal Protein S18

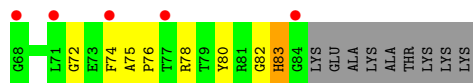
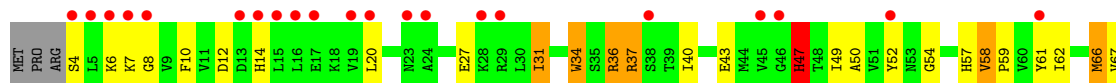


• Molecule 18: 30S Ribosomal Protein S18

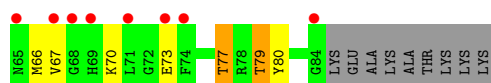
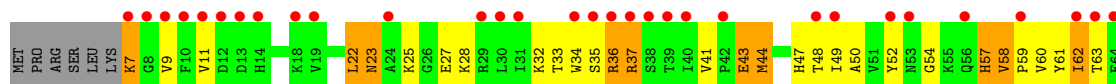
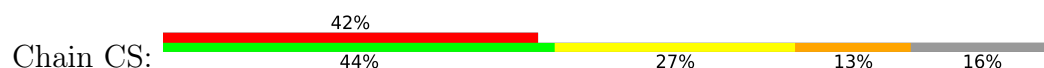




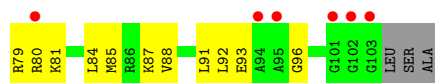
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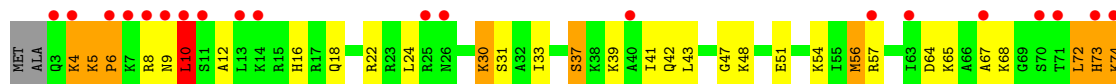
● Molecule 19: 30S Ribosomal Protein S19



● Molecule 20: 30S Ribosomal Protein S20

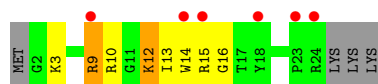


● Molecule 20: 30S Ribosomal Protein S20

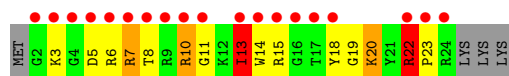
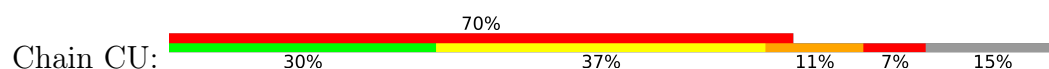


● Molecule 21: 30S Ribosomal Protein THX

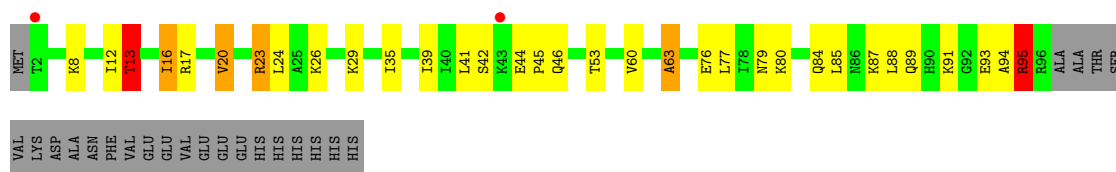




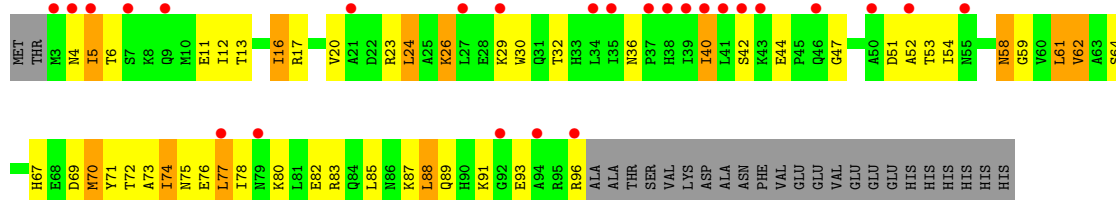
• Molecule 21: 30S Ribosomal Protein THX



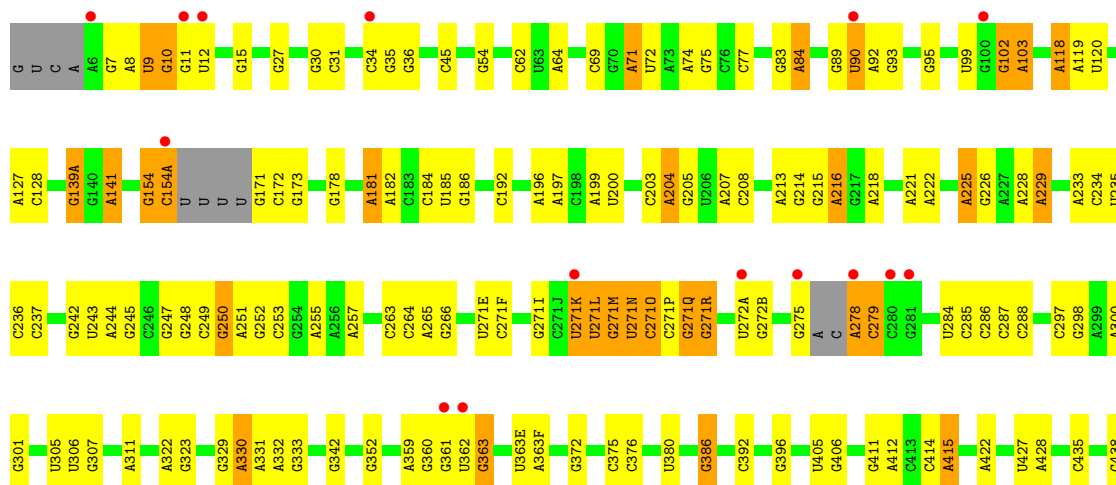
• Molecule 22: Ribosome-associated inhibitor A



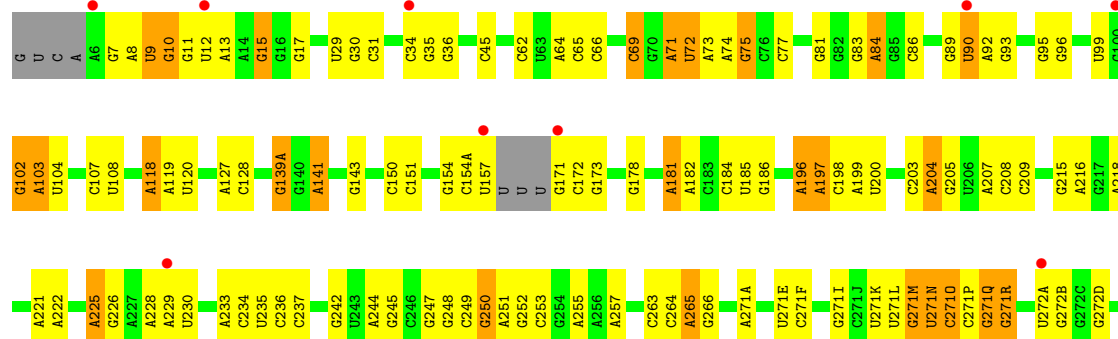
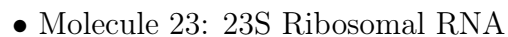
• Molecule 22: Ribosome-associated inhibitor A

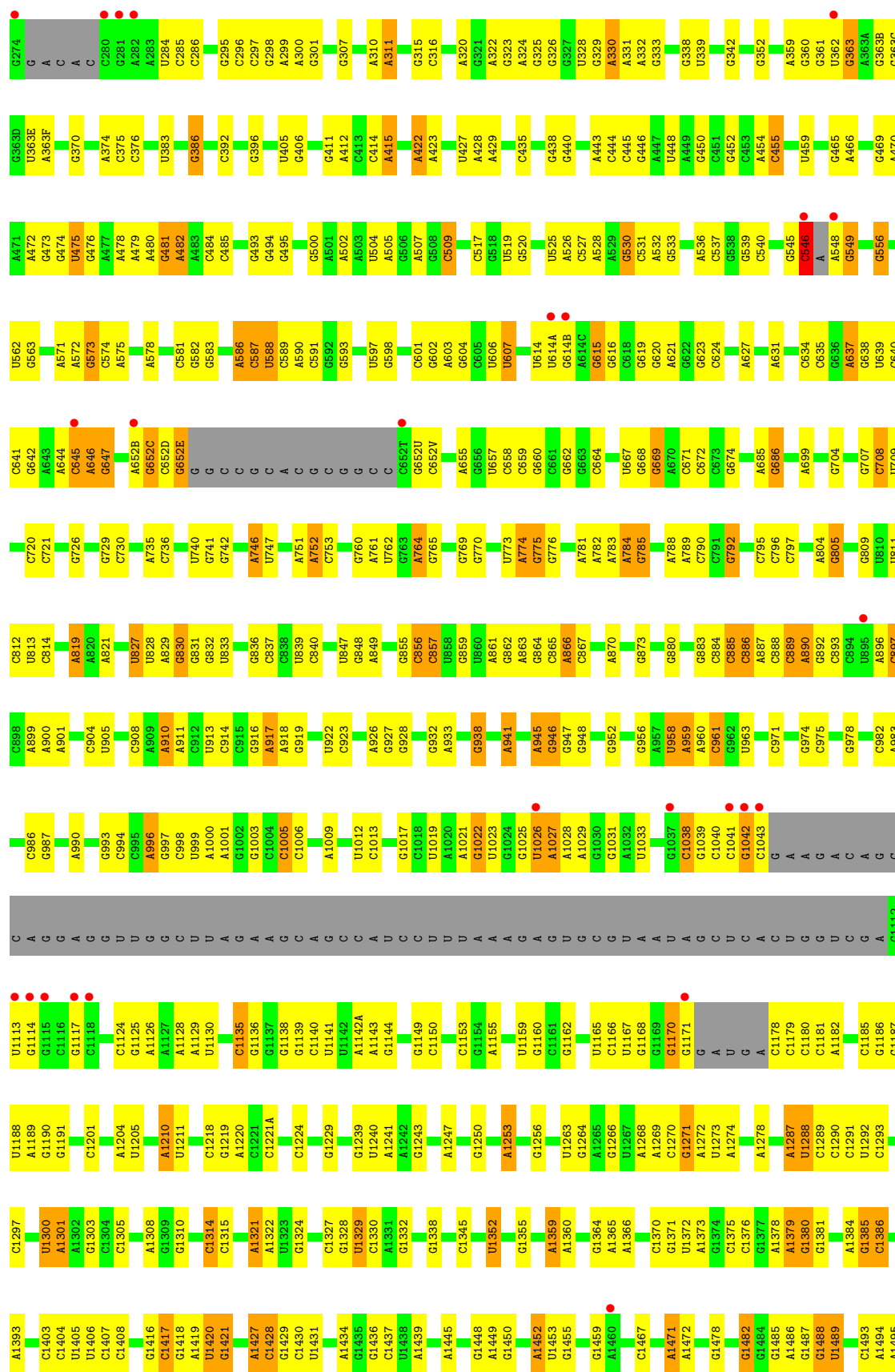


• Molecule 23: 23S Ribosomal RNA

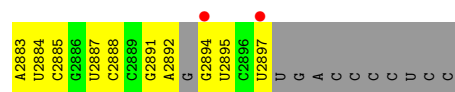


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C1793	G1541	U1540	G1435	G1310	U1188	C	G1044	A941	G832	C730	G652C	C444
U1794	G1542	A1543	G1436	C1314	C1201	G1106	A1045	A945	U833	U740	C652D	U448
C1795	G1543	A1544	C1437	C1315	A1204	U1108	A1046	G947	G839	G741	G652E	G570
U1796	A1545	U1546	A1445	A1321	A1204	C1109	A1048	G948	C840	A746	G652F	A454
U1798	C1546	C1547	G1448	A1322	A1210	G1110	C1049	G949	U847	U747	G652G	C455
G1799	C1551	C1552	A1449	U1329	A1211	A1111	G1051	G948	U848	U748	G652H	C456
C1800	C1557	C1558	C1330	A1331	G1212	U1113	G1052	G952	A849	G748	G652J	U459
G1801	C1558	A1558	G1450	G1332	G1218	G1114	C	G956	C856	A751	C	U459
A1802	G1559	G1560	A1452	G1332	G1219	G1117	A	A957	C857	A752	A	G459
A1803	U1560	G1561	G1459	C1345	A1220	G1125	G	U958	U858	C753	G	A470
G1810	G1566	A1566	C1467	U1352	C1224	A1126	C	A960	U860	A764	C652D	G473
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G1816	C1575	C1576	A1472	G1355	U1240	A1128	U	G962	G862	A766	G652Q	U475
U1817	U1576	U1577	G1482	G1358	A1241	U1130	G	G974	G864	G775	C652R	G476
U1818	G1577	C1577	G1485	A1359	G1243	U1135	G	C975	C865	G776	C652S	A477
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U1820	A1579	U1579	G1487	G1364	A1250	G1137	U	U989	C867	A782	A655	A480
G1823	C1580	C1580	A1488	A1365	G1251	G1138	A	G993	G880	A783	G656	G481
A1825	G1581	G1581	U1489	C1251	C1252	G1139	G	C994	G883	A784	G657	A482
A1829	C1582	C1582	C1493	C1370	A1253	C1140	A	A995	U885	G786	G658	A483
C1830	A1583	A1583	A1494	G1371	G1256	U1142	G	G997	C886	U787	G662	C484
U1833	A1586	A1586	A1495	U1372	A1268	A1142A	A	C999	C888	A788	G663	C485
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G1835	U1588	U1588	U1497	G1378	A1269	G1149	C	G1003	C890	C791	A667	A501
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G1843	G1593	G1594	U1503	A1384	C1270	C1153	C	G1005	C893	C796	C671	A503
C1847	C1594	C1594	C1504	G1385	G1271	G1154	U	U1012	A896	C797	C672	U504
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G1858	C1604	C1604	A1507	C1403	U1273	A1156	U	U1019	C898	G805	C674	G506
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A1876	C1617	C1617	G1525	C1408	C1291	C1166	U	A1027	C912	U811	G690	A529
A1877	A1618	A1618	G1529	G1416	C1293	G1170	G	A1028	U913	U813	C691	C530
G1878	G1619	G1619	G1530	C1417	C1297	G1171	C	U1032	G916	C814	G695	A532
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G1882	C1631	C1631	G1532	U1420	A1302	U1175	A	A1032	U922	C820	C708	G539
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A1889	U1639	U1639	A	C1428	C1305	C1179	G	U1039	U826	U827	A718	C546
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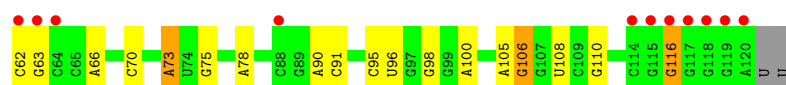
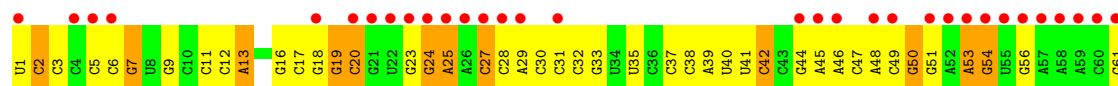




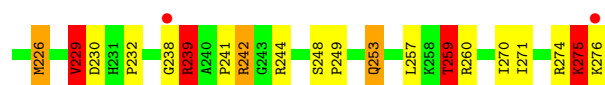
• Molecule 24: 5S Ribosomal RNA



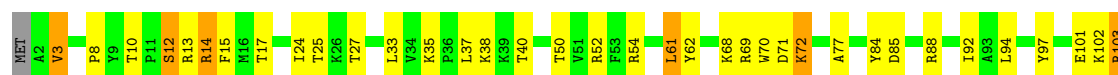
• Molecule 24: 5S Ribosomal RNA



• Molecule 25: 50S Ribosomal Protein L2

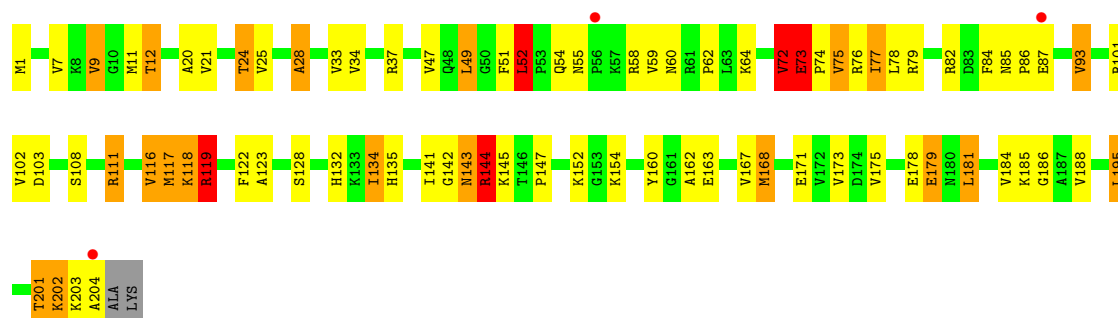


• Molecule 25: 50S Ribosomal Protein L2





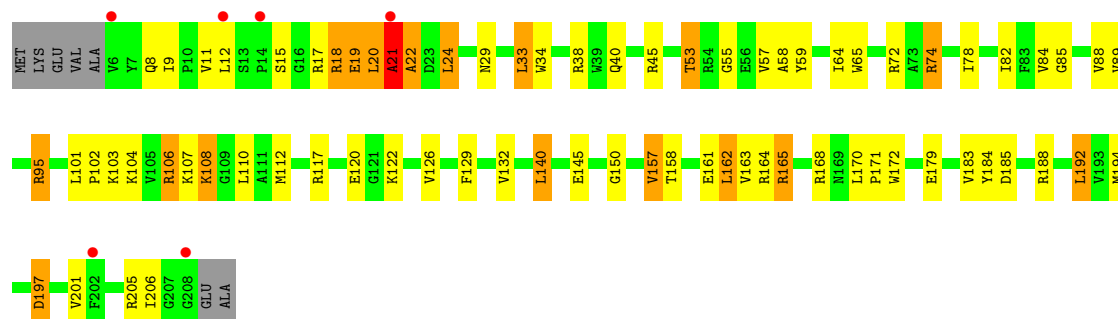
• Molecule 26: 50S Ribosomal Protein L3



• Molecule 26: 50S Ribosomal Protein L3

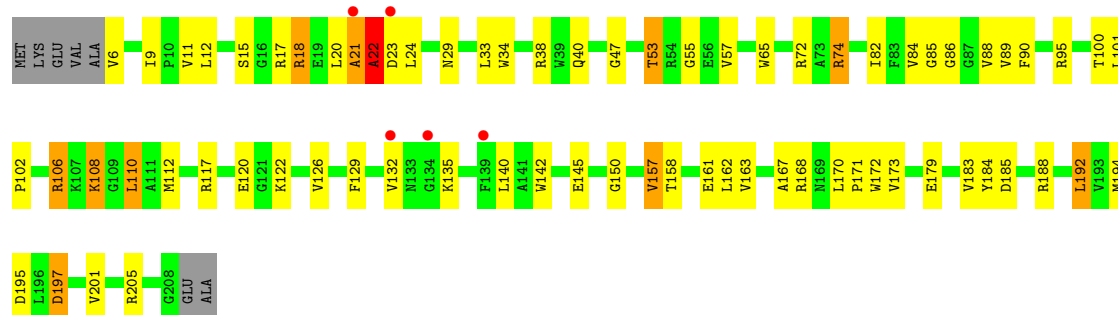


• Molecule 27: 50S Ribosomal Protein L4

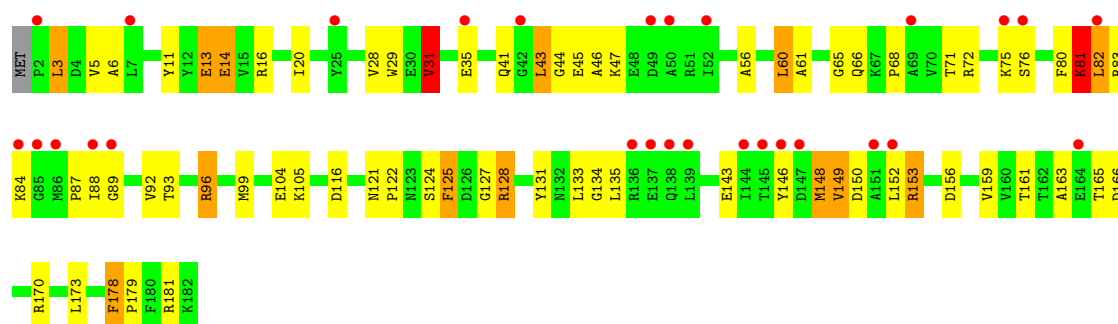


• Molecule 27: 50S Ribosomal Protein L4

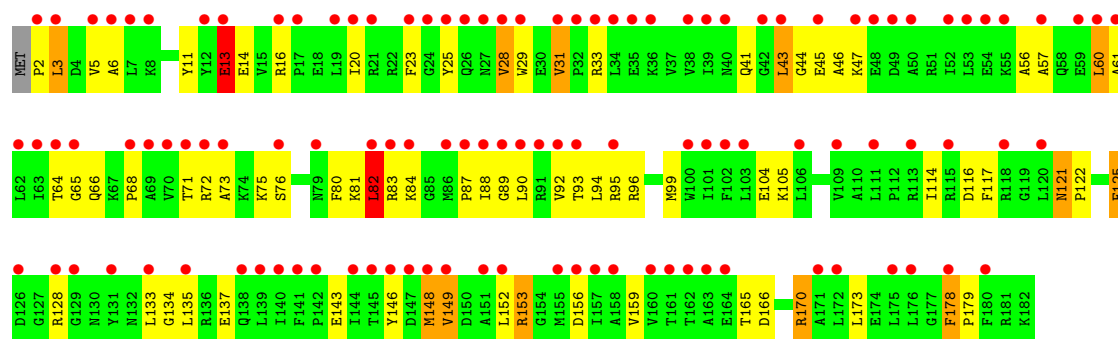




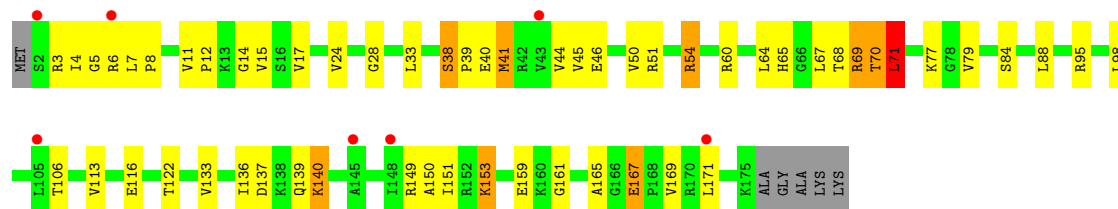
• Molecule 28: 50S Ribosomal Protein L5



• Molecule 28: 50S Ribosomal Protein L5

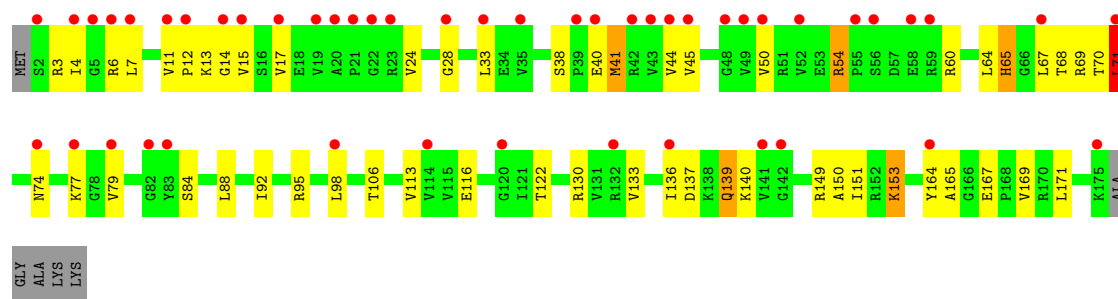


• Molecule 29: 50S Ribosomal Protein L6



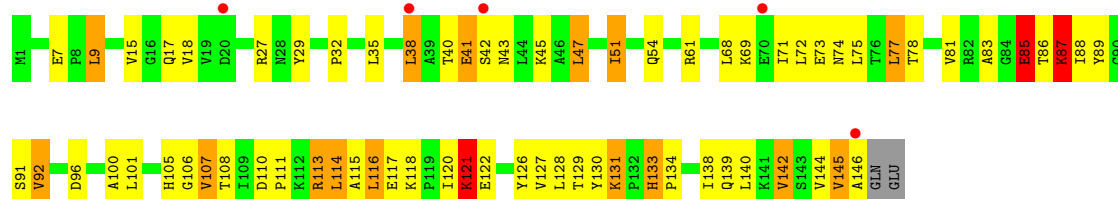
• Molecule 29: 50S Ribosomal Protein L6

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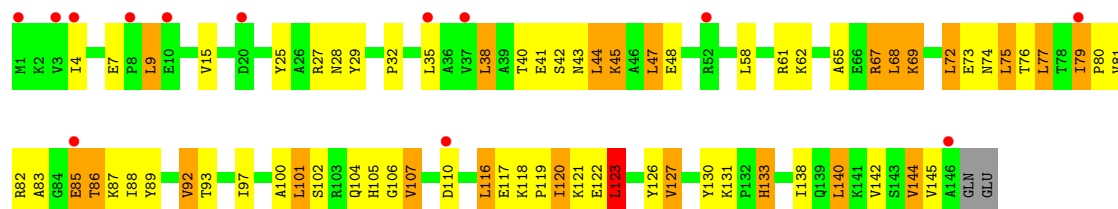
• Molecule 30: 50S Ribosomal Protein L9

Chain BI: 



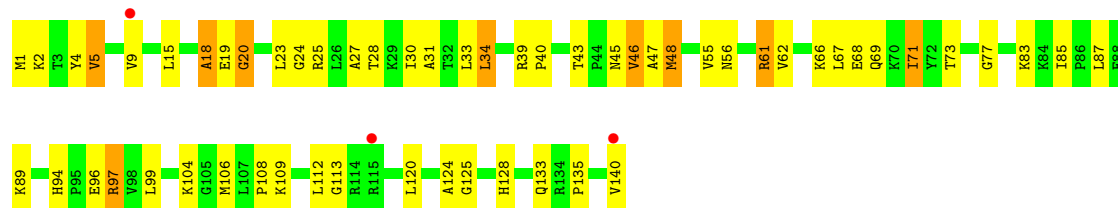
• Molecule 30: 50S Ribosomal Protein L9

Chain DI: 



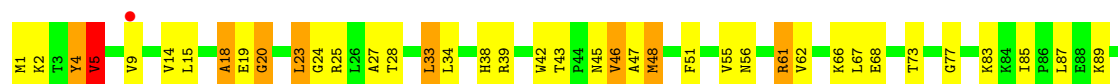
• Molecule 31: 50S Ribosomal Protein L13

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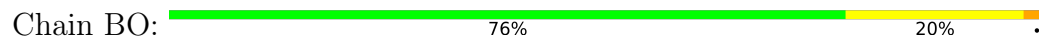
• Molecule 31: 50S Ribosomal Protein L13

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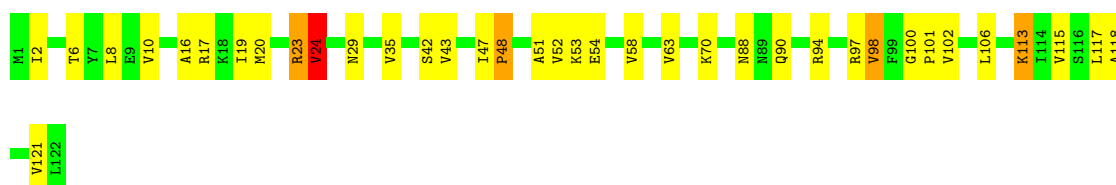




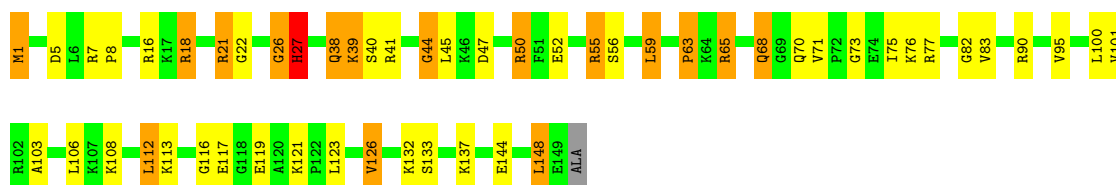
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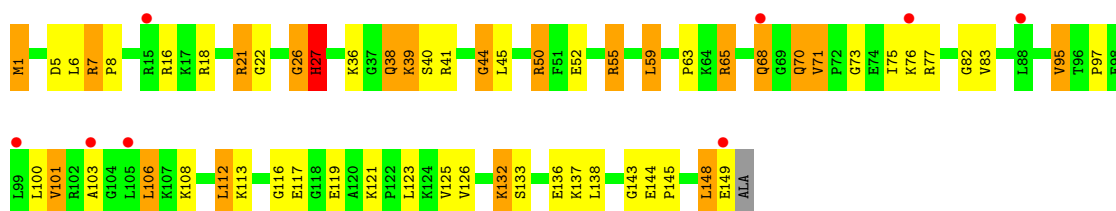
• Molecule 32: 50S Ribosomal Protein L14



• Molecule 33: 50S Ribosomal Protein L15



• Molecule 33: 50S Ribosomal Protein L15



• Molecule 34: 50S Ribosomal Protein L16

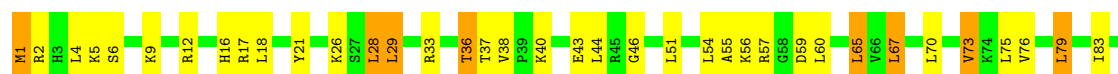




• Molecule 34: 50S Ribosomal Protein L16



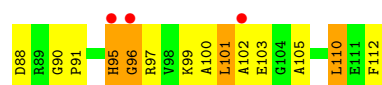
• Molecule 35: 50S Ribosomal Protein L17



• Molecule 35: 50S Ribosomal Protein L17

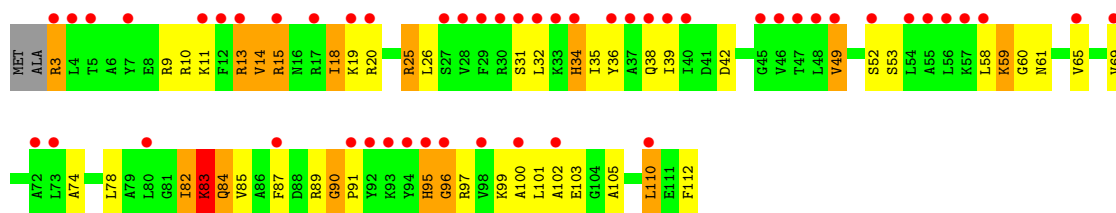


• Molecule 36: 50S Ribosomal Protein L18

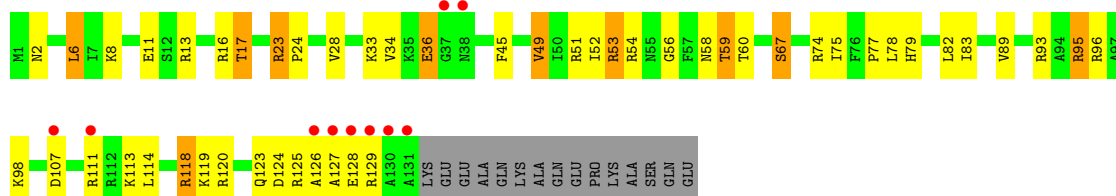


• Molecule 36: 50S Ribosomal Protein L18

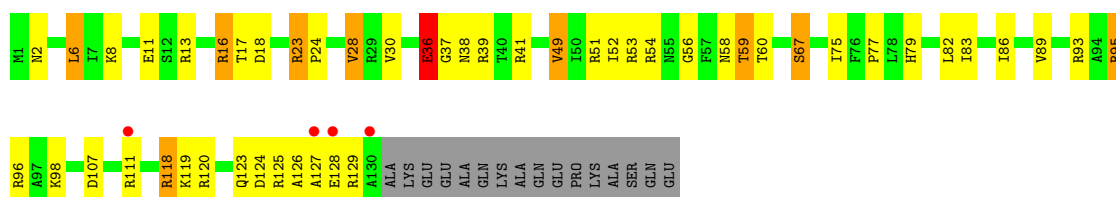




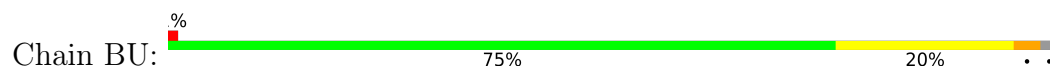
• Molecule 37: 50S Ribosomal Protein L19



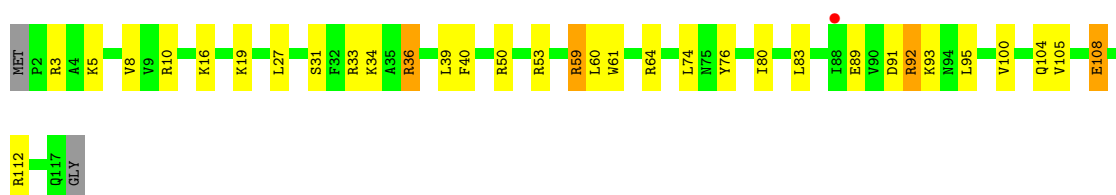
• Molecule 37: 50S Ribosomal Protein L19



• Molecule 38: 50S Ribosomal Protein L20

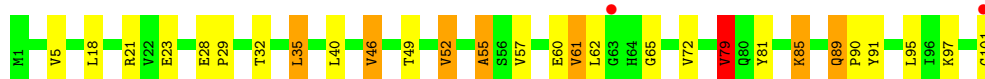


• Molecule 38: 50S Ribosomal Protein L20

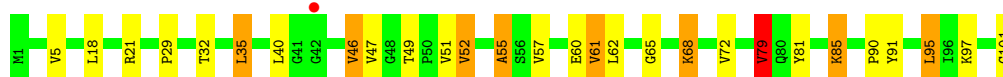
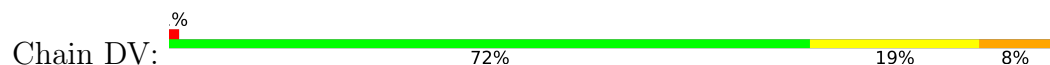


• Molecule 39: 50S Ribosomal Protein L21

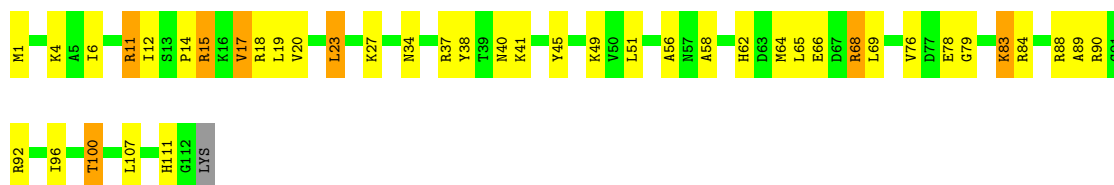




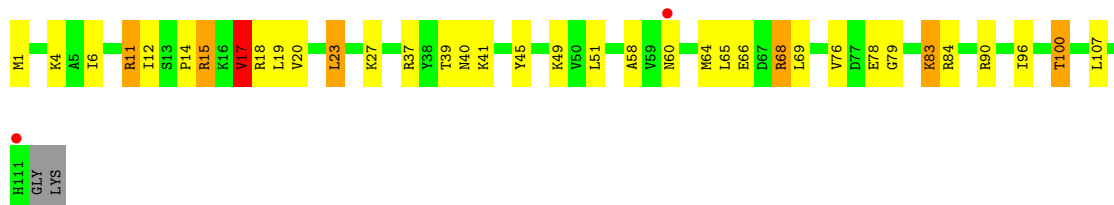
- Molecule 39: 50S Ribosomal Protein L21



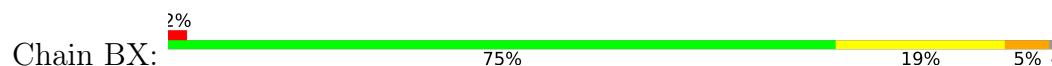
- Molecule 40: 50S Ribosomal Protein L22



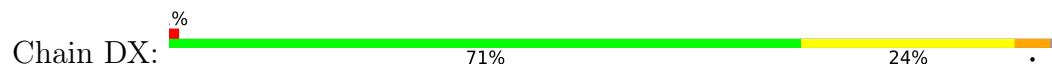
- Molecule 40: 50S Ribosomal Protein L22



- Molecule 41: 50S Ribosomal Protein L23

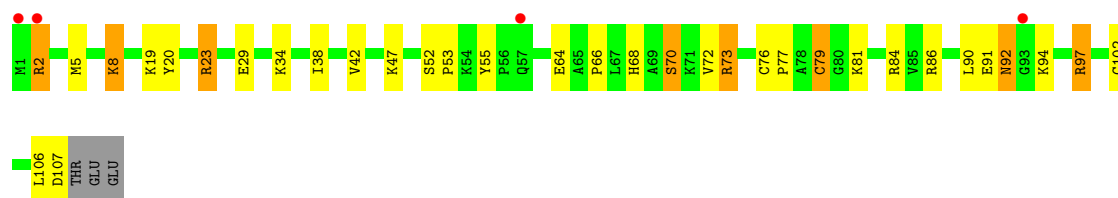


- Molecule 41: 50S Ribosomal Protein L23

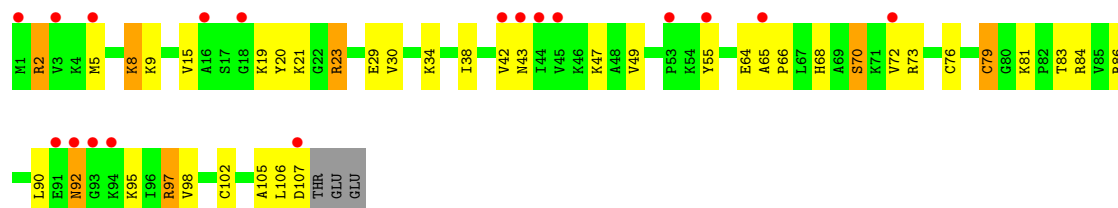


- Molecule 42: 50S Ribosomal Protein L24

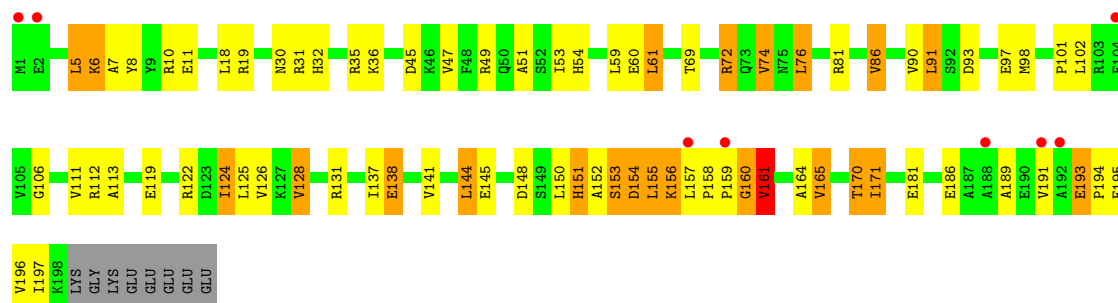




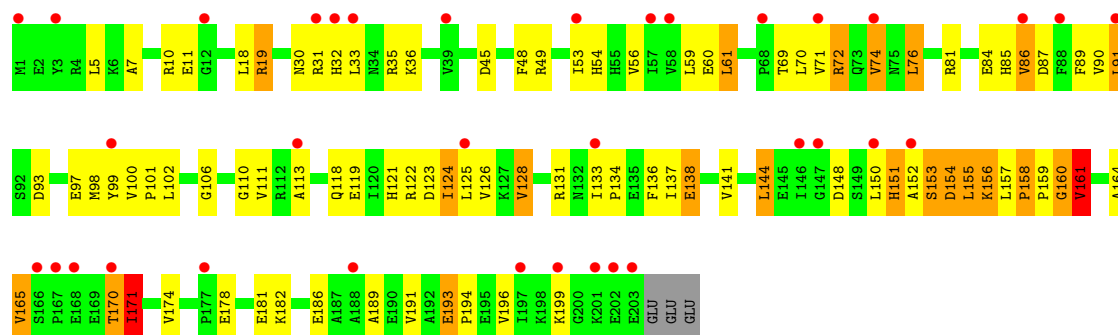
• Molecule 42: 50S Ribosomal Protein L24



• Molecule 43: 50S Ribosomal Protein L25



• Molecule 43: 50S Ribosomal Protein L25



• Molecule 44: 50S Ribosomal Protein L27





• Molecule 44: 50S Ribosomal Protein L27



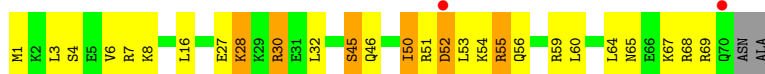
• Molecule 45: 50S Ribosomal Protein L28



• Molecule 45: 50S Ribosomal Protein L28



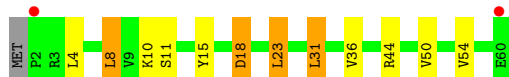
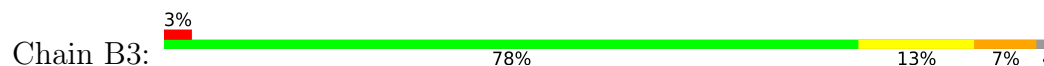
• Molecule 46: 50S Ribosomal Protein L29



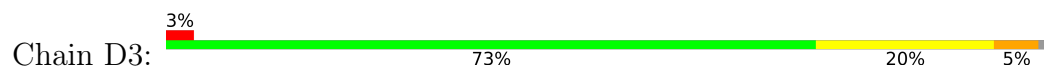
• Molecule 46: 50S Ribosomal Protein L29



• Molecule 47: 50S Ribosomal Protein L30

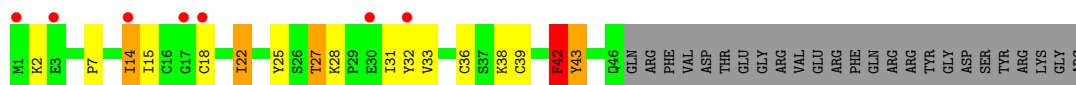


• Molecule 47: 50S Ribosomal Protein L30

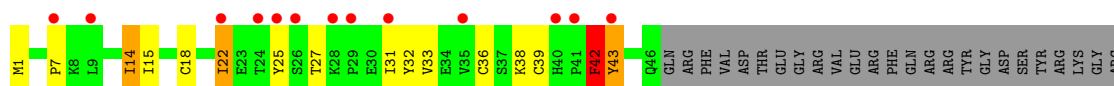




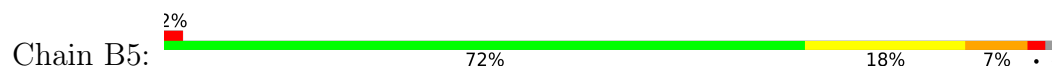
• Molecule 48: 50S Ribosomal Protein L31



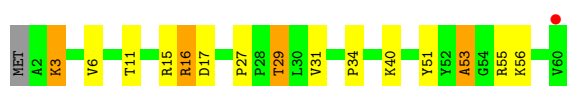
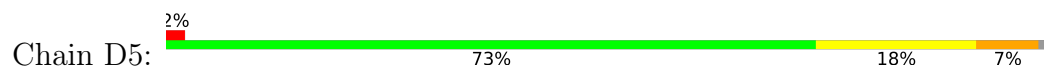
• Molecule 48: 50S Ribosomal Protein L31



• Molecule 49: 50S Ribosomal Protein L32



• Molecule 49: 50S Ribosomal Protein L32



• Molecule 50: 50S Ribosomal Protein L33

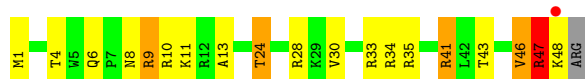


• Molecule 50: 50S Ribosomal Protein L33

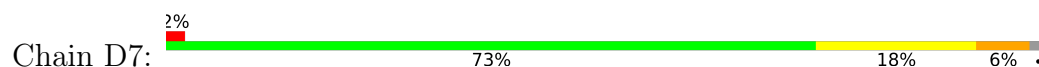


• Molecule 51: 50S Ribosomal Protein L34





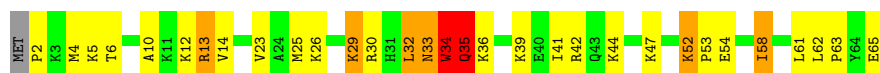
- Molecule 51: 50S Ribosomal Protein L34



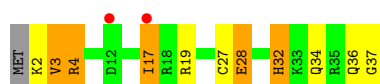
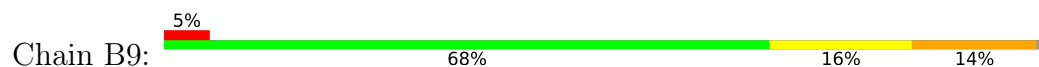
- Molecule 52: 50S Ribosomal Protein L35



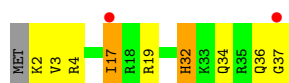
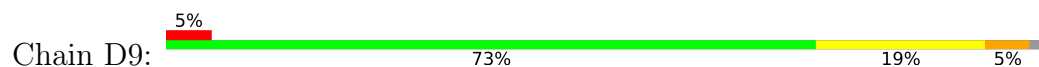
- Molecule 52: 50S Ribosomal Protein L35



- Molecule 53: 50S ribosomal protein L36



- Molecule 53: 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	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.217 , 0.254 0.213 , 0.250	Depositor DCC
R_{free} test set	78243 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	287173	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: MG, ZN

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	0.58	22/35935 (0.1%)	0.54	3/56084 (0.0%)
1	CA	0.56	21/35884 (0.1%)	0.54	4/56006 (0.0%)
2	AB	0.71	0/1811	1.14	12/2452 (0.5%)
2	CB	0.80	1/1852 (0.1%)	1.15	11/2510 (0.4%)
3	AC	0.82	0/1474	1.25	10/2003 (0.5%)
3	CC	0.88	0/1477	1.38	20/2006 (1.0%)
4	AD	0.84	2/1550 (0.1%)	1.29	13/2106 (0.6%)
4	CD	0.80	0/1567	1.27	12/2125 (0.6%)
5	AE	0.80	1/1121 (0.1%)	1.20	10/1517 (0.7%)
5	CE	0.81	0/1122	1.22	10/1518 (0.7%)
6	AF	0.76	0/794	1.11	3/1082 (0.3%)
6	CF	0.70	0/789	1.09	0/1074
7	AG	0.73	0/1186	1.17	9/1603 (0.6%)
7	CG	0.78	1/1183 (0.1%)	1.18	6/1599 (0.4%)
8	AH	0.70	0/1065	1.07	3/1445 (0.2%)
8	CH	0.68	0/1069	1.05	3/1450 (0.2%)
9	AI	0.81	0/867	1.31	8/1180 (0.7%)
9	CI	0.98	0/864	1.37	13/1177 (1.1%)
10	AJ	0.91	0/672	1.20	4/919 (0.4%)
10	CJ	1.05	0/670	1.36	7/917 (0.8%)
11	AK	0.78	0/843	1.21	4/1144 (0.3%)
11	CK	0.78	0/843	1.18	5/1144 (0.4%)
12	AL	0.88	0/925	1.23	8/1251 (0.6%)
12	CL	0.86	0/921	1.24	8/1247 (0.6%)
13	AM	0.89	0/811	1.37	13/1103 (1.2%)
13	CM	0.98	1/794 (0.1%)	1.45	13/1081 (1.2%)
14	AN	0.75	0/487	1.30	4/649 (0.6%)
14	CN	0.82	0/483	1.59	10/645 (1.6%)
15	AO	0.72	0/735	1.11	1/981 (0.1%)
15	CO	0.66	0/735	1.07	1/981 (0.1%)
16	AP	0.76	0/667	1.23	6/905 (0.7%)
16	CP	0.76	0/677	1.18	6/917 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.75	0/836	1.04	2/1117 (0.2%)
17	CQ	0.75	0/832	1.08	3/1113 (0.3%)
18	AR	0.70	0/519	1.18	3/699 (0.4%)
18	CR	0.67	0/519	1.12	2/699 (0.3%)
19	AS	0.81	0/574	1.42	7/781 (0.9%)
19	CS	0.86	0/563	1.40	9/766 (1.2%)
20	AT	0.78	1/701 (0.1%)	1.22	4/930 (0.4%)
20	CT	0.82	0/776	1.23	5/1026 (0.5%)
21	AU	0.63	0/203	1.00	0/266
21	CU	0.94	0/184	1.44	6/244 (2.5%)
22	AY	0.82	0/766	1.21	4/1034 (0.4%)
22	CY	0.87	0/751	1.14	4/1017 (0.4%)
23	BA	0.83	48/68200 (0.1%)	0.62	10/106454 (0.0%)
23	DA	0.66	11/67486 (0.0%)	0.59	6/105338 (0.0%)
24	BB	0.64	2/2878 (0.1%)	0.55	0/4490
24	DB	0.68	2/2878 (0.1%)	0.55	0/4490
25	BD	1.13	3/2186 (0.1%)	1.35	23/2944 (0.8%)
25	DD	0.95	0/2186	1.31	12/2944 (0.4%)
26	BE	1.10	4/1588 (0.3%)	1.35	20/2145 (0.9%)
26	DE	0.95	1/1588 (0.1%)	1.35	16/2145 (0.7%)
27	BF	1.05	0/1612	1.24	9/2184 (0.4%)
27	DF	0.88	0/1607	1.26	12/2178 (0.6%)
28	BG	0.70	0/1393	1.24	15/1892 (0.8%)
28	DG	0.79	0/1393	1.24	14/1892 (0.7%)
29	BH	0.89	0/1343	1.18	9/1820 (0.5%)
29	DH	0.74	0/1343	1.14	6/1820 (0.3%)
30	BI	0.83	0/1058	1.25	12/1449 (0.8%)
30	DI	0.84	0/1058	1.36	16/1449 (1.1%)
31	BN	1.07	2/1139 (0.2%)	1.39	14/1538 (0.9%)
31	DN	0.86	1/1139 (0.1%)	1.37	14/1538 (0.9%)
32	BO	1.07	0/933	1.25	7/1257 (0.6%)
32	DO	0.93	1/933 (0.1%)	1.24	10/1257 (0.8%)
33	BP	1.05	0/1148	1.31	14/1529 (0.9%)
33	DP	0.87	0/1148	1.29	14/1529 (0.9%)
34	BQ	1.07	0/1143	1.28	7/1527 (0.5%)
34	DQ	0.91	0/1143	1.26	4/1527 (0.3%)
35	BR	1.10	0/982	1.24	9/1312 (0.7%)
35	DR	0.88	0/982	1.19	5/1312 (0.4%)
36	BS	0.91	0/875	1.28	7/1168 (0.6%)
36	DS	0.88	0/883	1.27	6/1176 (0.5%)
37	BT	0.98	0/1077	1.31	7/1444 (0.5%)
37	DT	0.87	0/1072	1.29	6/1437 (0.4%)
38	BU	1.13	1/977 (0.1%)	1.18	3/1301 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	0.88	0/977	1.12	1/1301 (0.1%)
39	BV	1.05	0/782	1.24	4/1049 (0.4%)
39	DV	0.89	0/786	1.22	2/1053 (0.2%)
40	BW	1.25	1/891 (0.1%)	1.22	3/1197 (0.3%)
40	DW	1.03	0/887	1.18	4/1192 (0.3%)
41	BX	1.11	2/756 (0.3%)	1.20	1/1016 (0.1%)
41	DX	0.91	0/746	1.18	2/1005 (0.2%)
42	BY	0.94	0/798	1.35	11/1073 (1.0%)
42	DY	0.85	0/794	1.36	9/1067 (0.8%)
43	BZ	0.87	0/1555	1.29	16/2118 (0.8%)
43	DZ	0.86	0/1561	1.30	17/2131 (0.8%)
44	B0	0.98	0/602	1.17	3/804 (0.4%)
44	D0	0.91	0/615	1.19	4/820 (0.5%)
45	B1	1.06	2/752 (0.3%)	1.12	1/1003 (0.1%)
45	D1	0.90	1/752 (0.1%)	1.14	1/1003 (0.1%)
46	B2	0.98	0/590	1.17	5/781 (0.6%)
46	D2	0.81	0/586	1.18	4/779 (0.5%)
47	B3	0.99	0/463	1.14	2/623 (0.3%)
47	D3	0.88	0/468	1.16	2/628 (0.3%)
48	B4	0.70	0/358	1.18	2/487 (0.4%)
48	D4	0.84	0/358	1.12	2/487 (0.4%)
49	B5	1.22	3/469 (0.6%)	1.36	2/634 (0.3%)
49	D5	1.07	2/465 (0.4%)	1.28	1/630 (0.2%)
50	B6	1.04	0/456	1.30	4/609 (0.7%)
50	D6	0.90	0/444	1.25	4/595 (0.7%)
51	B7	1.27	2/426 (0.5%)	1.31	4/561 (0.7%)
51	D7	1.04	1/410 (0.2%)	1.22	4/543 (0.7%)
52	B8	1.17	0/516	1.29	5/679 (0.7%)
52	D8	0.96	0/516	1.34	6/679 (0.9%)
53	B9	1.44	5/300 (1.7%)	1.43	5/395 (1.3%)
53	D9	0.96	1/300 (0.3%)	1.33	2/395 (0.5%)
All	All	0.76	146/304847 (0.0%)	0.82	729/456336 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
2	CB	0	2
3	AC	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	3
4	AD	0	1
4	CD	0	1
9	AI	0	3
9	CI	0	1
10	AJ	0	3
10	CJ	0	2
12	CL	0	2
13	AM	0	2
13	CM	0	1
14	CN	0	2
18	AR	0	1
18	CR	0	1
23	BA	0	4
23	DA	0	1
25	BD	0	1
25	DD	0	1
26	BE	0	1
26	DE	0	1
27	BF	0	3
27	DF	0	2
28	BG	0	1
28	DG	0	1
29	BH	0	1
29	DH	0	1
30	BI	0	1
31	BN	0	1
31	DN	0	1
33	BP	0	2
33	DP	0	2
36	BS	0	1
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
43	BZ	0	1
43	DZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	1
48	D4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	B5	0	1
49	D5	0	1
52	D8	0	1
All	All	0	68

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1459	C	C1'-N1	12.10	1.66	1.48
1	CA	1459	C	C1'-N1	11.66	1.66	1.48
23	DA	2123	G	P-OP2	-10.34	1.28	1.49
1	CA	66	G	P-OP2	-10.34	1.28	1.49
23	BA	2123	G	P-OP1	-10.21	1.28	1.49

The worst 5 of 729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	CN	13	THR	CA-C-N	15.03	138.63	119.84
14	CN	13	THR	C-N-CA	15.03	138.63	119.84
31	DN	46	VAL	N-CA-C	14.89	129.66	113.43
31	BN	46	VAL	N-CA-C	14.71	129.46	113.43
4	AD	31	CYS	N-CA-C	-12.15	97.98	112.92

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	14	GLY	Peptide
3	AC	180	ALA	Peptide
3	AC	50	ALA	Peptide
4	AD	29	PRO	Peptide
9	AI	39	GLY	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	32102	0	16201	702	0
1	CA	32056	0	16179	905	0
2	AB	1777	0	1747	82	0
2	CB	1817	0	1785	82	0
3	AC	1450	0	1314	43	0
3	CC	1453	0	1320	80	0
4	AD	1520	0	1406	45	0
4	CD	1537	0	1430	89	0
5	AE	1105	0	1130	39	0
5	CE	1106	0	1132	41	0
6	AF	781	0	741	18	0
6	CF	776	0	733	20	0
7	AG	1167	0	1108	34	0
7	CG	1164	0	1106	49	0
8	AH	1045	0	1033	32	0
8	CH	1049	0	1037	34	0
9	AI	852	0	742	49	0
9	CI	849	0	735	56	0
10	AJ	659	0	552	40	0
10	CJ	657	0	547	38	0
11	AK	828	0	822	16	0
11	CK	828	0	822	24	0
12	AL	909	0	927	29	0
12	CL	905	0	916	30	0
13	AM	801	0	743	44	0
13	CM	784	0	730	41	0
14	AN	478	0	496	25	0
14	CN	474	0	485	36	0
15	AO	724	0	749	25	0
15	CO	724	0	749	31	0
16	AP	651	0	638	39	0
16	CP	661	0	653	51	0
17	AQ	823	0	891	28	0
17	CQ	819	0	880	26	0
18	AR	514	0	530	14	0
18	CR	514	0	530	20	0
19	AS	560	0	466	32	0
19	CS	549	0	468	28	0
20	AT	699	0	746	27	0
20	CT	773	0	836	34	0
21	AU	199	0	208	6	0
21	CU	180	0	173	10	0
22	AY	754	0	776	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CY	739	0	740	38	0
23	BA	60898	0	30697	764	0
23	DA	60264	0	30391	919	0
24	BB	2573	0	1306	28	0
24	DB	2573	0	1306	51	0
25	BD	2136	0	2218	56	0
25	DD	2136	0	2218	63	0
26	BE	1555	0	1607	44	0
26	DE	1555	0	1607	48	0
27	BF	1577	0	1612	46	0
27	DF	1572	0	1613	44	0
28	BG	1368	0	1324	39	0
28	DG	1368	0	1324	54	0
29	BH	1317	0	1376	27	0
29	DH	1317	0	1376	24	0
30	BI	1043	0	1054	44	0
30	DI	1043	0	1054	52	0
31	BN	1112	0	1180	26	0
31	DN	1112	0	1180	29	0
32	BO	923	0	981	11	0
32	DO	923	0	981	16	0
33	BP	1131	0	1201	38	0
33	DP	1131	0	1201	45	0
34	BQ	1122	0	1179	27	0
34	DQ	1122	0	1179	32	0
35	BR	968	0	1033	26	0
35	DR	968	0	1033	31	0
36	BS	865	0	905	39	0
36	DS	873	0	927	49	0
37	BT	1063	0	1103	29	0
37	DT	1058	0	1098	33	0
38	BU	959	0	1019	11	0
38	DU	959	0	1019	23	0
39	BV	771	0	830	14	1
39	DV	775	0	841	16	0
40	BW	881	0	935	23	0
40	DW	877	0	932	18	0
41	BX	742	0	799	14	0
41	DX	732	0	777	17	0
42	BY	785	0	828	17	0
42	DY	781	0	829	24	0
43	BZ	1522	0	1511	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DZ	1528	0	1476	62	0
44	B0	594	0	604	7	0
44	D0	607	0	622	17	0
45	B1	745	0	804	20	0
45	D1	745	0	804	22	0
46	B2	588	0	643	14	0
46	D2	584	0	623	18	0
47	B3	458	0	503	6	0
47	D3	463	0	507	8	0
48	B4	349	0	336	11	0
48	D4	349	0	336	13	0
49	B5	455	0	472	10	0
49	D5	451	0	461	11	0
50	B6	449	0	462	15	0
50	D6	437	0	440	15	0
51	B7	418	0	467	10	0
51	D7	402	0	434	4	0
52	B8	509	0	565	24	0
52	D8	509	0	565	29	0
53	B9	297	0	316	7	0
53	D9	297	0	316	6	0
54	AA	217	0	0	0	0
54	AD	2	0	0	0	0
54	AE	1	0	0	0	0
54	AF	1	0	0	0	0
54	AI	1	0	0	0	0
54	AL	1	0	0	0	0
54	AM	2	0	0	0	0
54	AP	1	0	0	0	0
54	B0	4	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	3	0	0	0	0
54	B5	1	0	0	0	0
54	B6	1	0	0	0	0
54	B7	1	0	0	0	0
54	B8	1	0	0	0	0
54	B9	3	0	0	0	0
54	BA	729	0	0	0	0
54	BB	19	0	0	0	0
54	BD	7	0	0	0	0
54	BE	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BF	6	0	0	0	0
54	BG	1	0	0	0	0
54	BH	1	0	0	0	0
54	BN	2	0	0	0	0
54	BO	1	0	0	0	0
54	BP	2	0	0	0	0
54	BQ	5	0	0	0	0
54	BR	5	0	0	0	0
54	BS	1	0	0	0	0
54	BT	3	0	0	0	0
54	BU	3	0	0	0	0
54	BV	4	0	0	0	0
54	BW	1	0	0	0	0
54	BY	1	0	0	0	0
54	BZ	2	0	0	0	0
54	CA	203	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	1	0	0	0	0
54	D1	1	0	0	0	0
54	D5	2	0	0	0	0
54	D7	2	0	0	0	0
54	D8	2	0	0	0	0
54	D9	1	0	0	0	0
54	DA	637	0	0	0	0
54	DB	10	0	0	0	0
54	DD	5	0	0	0	0
54	DE	3	0	0	0	0
54	DF	5	0	0	0	0
54	DO	3	0	0	0	0
54	DP	3	0	0	0	0
54	DQ	4	0	0	0	0
54	DR	2	0	0	0	0
54	DT	2	0	0	0	0
54	DW	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	443	0	0	25	0
56	AD	3	0	0	2	0
56	AE	2	0	0	0	0
56	AF	2	0	0	0	0
56	AG	2	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	3	0	0	0	0
56	AM	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AQ	3	0	0	0	0
56	AY	1	0	0	0	0
56	B0	4	0	0	0	0
56	B1	5	0	0	0	0
56	B3	4	0	0	0	0
56	B5	5	0	0	0	0
56	B6	2	0	0	0	0
56	B7	5	0	0	2	0
56	B8	11	0	0	1	0
56	B9	1	0	0	0	0
56	BA	1988	0	0	66	1
56	BB	43	0	0	1	0
56	BD	21	0	0	2	0
56	BE	18	0	0	1	0
56	BF	18	0	0	0	0
56	BG	2	0	0	0	0
56	BH	2	0	0	0	0
56	BN	7	0	0	0	0
56	BO	3	0	0	0	0
56	BP	20	0	0	0	0
56	BQ	9	0	0	0	0
56	BR	8	0	0	0	1
56	BS	2	0	0	0	0
56	BT	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BU	9	0	0	0	0
56	BV	13	0	0	1	1
56	BW	6	0	0	0	0
56	BX	2	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	2	0	0	0	0
56	CA	400	0	0	32	0
56	CD	2	0	0	1	0
56	CE	4	0	0	0	0
56	CF	1	0	0	0	0
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CP	3	0	0	0	0
56	CQ	3	0	0	0	0
56	CR	1	0	0	1	0
56	CT	2	0	0	0	0
56	CU	1	0	0	1	0
56	D0	2	0	0	0	0
56	D1	3	0	0	0	0
56	D2	1	0	0	0	0
56	D3	1	0	0	1	0
56	D5	3	0	0	0	0
56	D6	3	0	0	0	0
56	D7	3	0	0	0	0
56	D8	6	0	0	0	0
56	D9	1	0	0	0	0
56	DA	1496	0	0	107	0
56	DB	33	0	0	6	0
56	DD	17	0	0	2	0
56	DE	12	0	0	0	0
56	DF	10	0	0	0	0
56	DN	2	0	0	0	0
56	DO	7	0	0	0	0
56	DP	11	0	0	0	0
56	DQ	2	0	0	1	0
56	DR	5	0	0	0	0
56	DT	3	0	0	0	0
56	DU	1	0	0	0	0
56	DV	1	0	0	0	0
56	DW	4	0	0	0	0
56	DX	2	0	0	0	0
56	DY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	287173	0	187292	5699	2

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

The worst 5 of 5699 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)
23:BA:2296:U:O4	23:BA:2335:A:N6	1.59	1.34
23:DA:2296:U:O4	23:DA:2335:A:N6	1.59	1.33
1:CA:1164:G:H1	1:CA:1172:C:N4	1.45	1.15
23:BA:885:C:N4	23:BA:890:A:N6	1.97	1.13
1:AA:40:C:N4	1:AA:402:G:H1	1.47	1.12

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BR:308:HOH:O	56:BV:310:HOH:O[4_445]	2.03	0.17
39:BV:101:GLY:O	56:BA:5729:HOH:O[4_545]	2.17	0.03

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	227/256 (89%)	185 (82%)	40 (18%)	2 (1%)	14	35
2	CB	233/256 (91%)	187 (80%)	43 (18%)	3 (1%)	9	25
3	AC	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
3	CC	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	6	16
4	AD	206/209 (99%)	186 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	206/209 (99%)	182 (88%)	23 (11%)	1 (0%)	24	48
5	AE	146/162 (90%)	128 (88%)	17 (12%)	1 (1%)	18	41
5	CE	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	18	41
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	97/101 (96%)	95 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	18	41
7	CG	153/156 (98%)	130 (85%)	22 (14%)	1 (1%)	18	41
8	AH	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
8	CH	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
9	AI	123/128 (96%)	108 (88%)	13 (11%)	2 (2%)	7	20
9	CI	123/128 (96%)	104 (85%)	14 (11%)	5 (4%)	2	5
10	AJ	94/105 (90%)	72 (77%)	15 (16%)	7 (7%)	1	1
10	CJ	94/105 (90%)	72 (77%)	18 (19%)	4 (4%)	2	4
11	AK	112/129 (87%)	103 (92%)	9 (8%)	0	100	100
11	CK	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	16	37
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	16	37
13	AM	112/126 (89%)	86 (77%)	22 (20%)	4 (4%)	2	6
13	CM	110/126 (87%)	86 (78%)	18 (16%)	6 (6%)	1	2
14	AN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	19
14	CN	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1	1
15	AO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	CO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	25
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	25
17	AQ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	32
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	AR	66/88 (75%)	55 (83%)	11 (17%)	0	100	100
18	CR	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	9	25
19	CS	76/93 (82%)	57 (75%)	18 (24%)	1 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	94/106 (89%)	77 (82%)	17 (18%)	0	100	100
20	CT	102/106 (96%)	79 (78%)	20 (20%)	3 (3%)	3	9
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
22	AY	93/119 (78%)	85 (91%)	7 (8%)	1 (1%)	11	29
22	CY	92/119 (77%)	87 (95%)	5 (5%)	0	100	100
25	BD	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	11	29
25	DD	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	11	29
26	BE	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	8	22
26	DE	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	8	22
27	BF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	12	32
27	DF	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	12	32
28	BG	179/182 (98%)	149 (83%)	26 (14%)	4 (2%)	5	14
28	DG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	11	29
29	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	44
29	DH	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	7	19
30	BI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	4	9
30	DI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	5	15
31	BN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	23
31	DN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	23
32	BO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	BP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	9	23
33	DP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	23
34	BQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	18	41
34	DQ	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	9	23
35	BR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
35	DR	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
36	BS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	35
36	DS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	35
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	DT	128/146 (88%)	124 (97%)	3 (2%)	1 (1%)	16	37
38	BU	114/118 (97%)	114 (100%)	0	0	100	100
38	DU	114/118 (97%)	114 (100%)	0	0	100	100
39	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
39	DV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
40	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
40	DW	109/113 (96%)	108 (99%)	1 (1%)	0	100	100
41	BX	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	29
42	BY	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
42	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
43	BZ	196/206 (95%)	178 (91%)	14 (7%)	4 (2%)	6	16
43	DZ	201/206 (98%)	181 (90%)	15 (8%)	5 (2%)	4	11
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
44	D0	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
45	B1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	5	15
45	D1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	5	15
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
46	D2	69/72 (96%)	65 (94%)	4 (6%)	0	100	100
47	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	B4	44/71 (62%)	35 (80%)	8 (18%)	1 (2%)	5	13
48	D4	44/71 (62%)	34 (77%)	10 (23%)	0	100	100
49	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
49	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	14
51	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	14
52	B8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	20
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	3	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	11568/12366 (94%)	10478 (91%)	965 (8%)	125 (1%)	11	29

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AJ	56	HIS
13	AM	84	ILE
27	BF	21	ALA
28	BG	82	LEU
30	BI	107	VAL

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	177/220 (80%)	147 (83%)	30 (17%)	2	6
2	CB	181/220 (82%)	147 (81%)	34 (19%)	1	4
3	AC	114/188 (61%)	93 (82%)	21 (18%)	1	4
3	CC	114/188 (61%)	84 (74%)	30 (26%)	0	2
4	AD	139/181 (77%)	119 (86%)	20 (14%)	3	8
4	CD	142/181 (78%)	119 (84%)	23 (16%)	2	6
5	AE	108/123 (88%)	95 (88%)	13 (12%)	5	12
5	CE	108/123 (88%)	94 (87%)	14 (13%)	4	10
6	AF	77/90 (86%)	64 (83%)	13 (17%)	2	6
6	CF	75/90 (83%)	64 (85%)	11 (15%)	3	8
7	AG	104/127 (82%)	90 (86%)	14 (14%)	4	9
7	CG	103/127 (81%)	82 (80%)	21 (20%)	1	3
8	AH	103/119 (87%)	83 (81%)	20 (19%)	1	4
8	CH	104/119 (87%)	84 (81%)	20 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	62/99 (63%)	52 (84%)	10 (16%)	2	6
9	CI	62/99 (63%)	52 (84%)	10 (16%)	2	6
10	AJ	52/92 (56%)	42 (81%)	10 (19%)	1	4
10	CJ	52/92 (56%)	40 (77%)	12 (23%)	1	2
11	AK	81/99 (82%)	73 (90%)	8 (10%)	7	19
11	CK	81/99 (82%)	73 (90%)	8 (10%)	7	19
12	AL	92/109 (84%)	83 (90%)	9 (10%)	7	19
12	CL	91/109 (84%)	78 (86%)	13 (14%)	3	8
13	AM	63/101 (62%)	46 (73%)	17 (27%)	0	1
13	CM	62/101 (61%)	42 (68%)	20 (32%)	0	1
14	AN	46/50 (92%)	38 (83%)	8 (17%)	2	5
14	CN	45/50 (90%)	33 (73%)	12 (27%)	0	1
15	AO	77/80 (96%)	62 (80%)	15 (20%)	1	4
15	CO	77/80 (96%)	62 (80%)	15 (20%)	1	4
16	AP	63/74 (85%)	49 (78%)	14 (22%)	1	3
16	CP	65/74 (88%)	50 (77%)	15 (23%)	1	2
17	AQ	94/97 (97%)	83 (88%)	11 (12%)	5	13
17	CQ	93/97 (96%)	80 (86%)	13 (14%)	3	9
18	AR	49/77 (64%)	40 (82%)	9 (18%)	1	4
18	CR	49/77 (64%)	40 (82%)	9 (18%)	1	4
19	AS	43/80 (54%)	35 (81%)	8 (19%)	1	4
19	CS	44/80 (55%)	30 (68%)	14 (32%)	0	1
20	AT	62/82 (76%)	54 (87%)	8 (13%)	4	10
20	CT	72/82 (88%)	62 (86%)	10 (14%)	3	9
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	6
21	CU	14/22 (64%)	9 (64%)	5 (36%)	0	0
22	AY	82/104 (79%)	66 (80%)	16 (20%)	1	4
22	CY	79/104 (76%)	60 (76%)	19 (24%)	1	2
25	BD	215/218 (99%)	188 (87%)	27 (13%)	4	11
25	DD	215/218 (99%)	187 (87%)	28 (13%)	4	10
26	BE	163/166 (98%)	132 (81%)	31 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DE	163/166 (98%)	131 (80%)	32 (20%)	1	4
27	BF	158/166 (95%)	130 (82%)	28 (18%)	2	5
27	DF	157/166 (95%)	130 (83%)	27 (17%)	2	6
28	BG	128/156 (82%)	106 (83%)	22 (17%)	2	6
28	DG	128/156 (82%)	107 (84%)	21 (16%)	2	6
29	BH	141/148 (95%)	122 (86%)	19 (14%)	4	9
29	DH	141/148 (95%)	122 (86%)	19 (14%)	4	9
30	BI	100/124 (81%)	76 (76%)	24 (24%)	1	2
30	DI	100/124 (81%)	76 (76%)	24 (24%)	1	2
31	BN	117/119 (98%)	96 (82%)	21 (18%)	2	5
31	DN	117/119 (98%)	94 (80%)	23 (20%)	1	4
32	BO	98/100 (98%)	87 (89%)	11 (11%)	6	15
32	DO	98/100 (98%)	85 (87%)	13 (13%)	4	10
33	BP	114/116 (98%)	93 (82%)	21 (18%)	1	4
33	DP	114/116 (98%)	93 (82%)	21 (18%)	1	4
34	BQ	111/111 (100%)	91 (82%)	20 (18%)	2	5
34	DQ	111/111 (100%)	91 (82%)	20 (18%)	2	5
35	BR	101/101 (100%)	81 (80%)	20 (20%)	1	4
35	DR	101/101 (100%)	80 (79%)	21 (21%)	1	3
36	BS	84/88 (96%)	67 (80%)	17 (20%)	1	4
36	DS	86/88 (98%)	67 (78%)	19 (22%)	1	3
37	BT	110/127 (87%)	88 (80%)	22 (20%)	1	4
37	DT	110/127 (87%)	89 (81%)	21 (19%)	1	4
38	BU	93/94 (99%)	78 (84%)	15 (16%)	2	6
38	DU	93/94 (99%)	80 (86%)	13 (14%)	3	9
39	BV	80/82 (98%)	66 (82%)	14 (18%)	2	5
39	DV	81/82 (99%)	67 (83%)	14 (17%)	2	5
40	BW	89/92 (97%)	77 (86%)	12 (14%)	4	9
40	DW	89/92 (97%)	77 (86%)	12 (14%)	4	9
41	BX	75/78 (96%)	65 (87%)	10 (13%)	4	10
41	DX	73/78 (94%)	64 (88%)	9 (12%)	4	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BY	80/91 (88%)	65 (81%)	15 (19%)	1	4
42	DY	79/91 (87%)	64 (81%)	15 (19%)	1	4
43	BZ	159/179 (89%)	131 (82%)	28 (18%)	2	5
43	DZ	155/179 (87%)	129 (83%)	26 (17%)	2	6
44	B0	59/67 (88%)	50 (85%)	9 (15%)	3	7
44	D0	61/67 (91%)	51 (84%)	10 (16%)	2	6
45	B1	78/83 (94%)	63 (81%)	15 (19%)	1	4
45	D1	78/83 (94%)	63 (81%)	15 (19%)	1	4
46	B2	65/67 (97%)	57 (88%)	8 (12%)	4	12
46	D2	63/67 (94%)	54 (86%)	9 (14%)	3	8
47	B3	49/52 (94%)	43 (88%)	6 (12%)	5	12
47	D3	50/52 (96%)	43 (86%)	7 (14%)	3	9
48	B4	39/63 (62%)	32 (82%)	7 (18%)	2	5
48	D4	39/63 (62%)	33 (85%)	6 (15%)	2	7
49	B5	50/52 (96%)	43 (86%)	7 (14%)	3	9
49	D5	49/52 (94%)	44 (90%)	5 (10%)	7	18
50	B6	50/52 (96%)	41 (82%)	9 (18%)	2	5
50	D6	48/52 (92%)	38 (79%)	10 (21%)	1	3
51	B7	41/42 (98%)	34 (83%)	7 (17%)	2	6
51	D7	38/42 (90%)	33 (87%)	5 (13%)	4	10
52	B8	52/55 (94%)	45 (86%)	7 (14%)	4	9
52	D8	52/55 (94%)	45 (86%)	7 (14%)	4	9
53	B9	32/34 (94%)	30 (94%)	2 (6%)	16	39
53	D9	32/34 (94%)	30 (94%)	2 (6%)	16	39
All	All	8871/10274 (86%)	7358 (83%)	1513 (17%)	2	6

5 of 1513 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	CL	119	LYS
28	DG	3	LEU
14	CN	31	ARG
12	CL	100	ILE
22	CY	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
9	CI	87	GLN
22	CY	89	GLN
10	CJ	56	HIS
16	CP	16	HIS
27	DF	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1490/1522 (97%)	308 (20%)	32 (2%)
1	CA	1490/1522 (97%)	330 (22%)	34 (2%)
23	BA	2819/2915 (96%)	524 (18%)	72 (2%)
23	DA	2788/2915 (95%)	496 (17%)	64 (2%)
24	BB	119/122 (97%)	19 (15%)	0
24	DB	119/122 (97%)	21 (17%)	0
All	All	8825/9118 (96%)	1698 (19%)	202 (2%)

5 of 1698 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G

5 of 202 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	495	A
23	DA	215	G
23	DA	2778	A
1	CA	687	A
1	CA	1136	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1945 ligands modelled in this entry, 1945 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1493/1522 (98%)	0.43	68 (4%) 37 34	37, 73, 129, 165	0
1	CA	1491/1522 (97%)	0.73	118 (7%) 18 16	40, 84, 135, 175	0
2	AB	229/256 (89%)	1.66	73 (31%) 1 1	76, 103, 123, 135	0
2	CB	235/256 (91%)	2.00	101 (42%) 0 0	80, 108, 127, 135	0
3	AC	206/239 (86%)	0.80	13 (6%) 26 23	62, 81, 98, 105	0
3	CC	206/239 (86%)	1.62	57 (27%) 1 1	85, 109, 122, 130	0
4	AD	208/209 (99%)	2.22	108 (51%) 0 0	64, 85, 105, 113	0
4	CD	208/209 (99%)	2.20	105 (50%) 0 0	68, 85, 103, 111	0
5	AE	148/162 (91%)	0.67	6 (4%) 41 37	59, 73, 86, 101	0
5	CE	148/162 (91%)	1.19	20 (13%) 7 6	62, 77, 91, 105	0
6	AF	100/101 (99%)	0.91	6 (6%) 27 24	61, 72, 85, 100	0
6	CF	99/101 (98%)	1.02	4 (4%) 42 38	62, 74, 86, 95	0
7	AG	155/156 (99%)	0.55	7 (4%) 38 34	64, 76, 91, 100	0
7	CG	155/156 (99%)	1.59	46 (29%) 1 1	86, 102, 111, 118	0
8	AH	138/138 (100%)	0.96	8 (5%) 29 25	61, 75, 83, 94	0
8	CH	138/138 (100%)	1.25	17 (12%) 8 7	64, 79, 87, 95	0
9	AI	125/128 (97%)	1.55	35 (28%) 1 1	64, 93, 106, 114	0
9	CI	125/128 (97%)	2.49	73 (58%) 0 0	89, 118, 126, 133	0
10	AJ	96/105 (91%)	1.70	34 (35%) 1 1	63, 96, 120, 124	0
10	CJ	96/105 (91%)	2.81	73 (76%) 0 0	95, 118, 135, 144	0
11	AK	114/129 (88%)	0.87	13 (11%) 10 8	50, 72, 91, 107	0
11	CK	114/129 (88%)	1.19	16 (14%) 6 5	54, 77, 95, 109	0
12	AL	122/132 (92%)	1.62	34 (27%) 1 1	54, 68, 82, 95	0
12	CL	122/132 (92%)	1.86	47 (38%) 1 0	55, 72, 85, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	1.00	13 (11%) 10 8	68, 82, 97, 102	0
13	CM	112/126 (88%)	2.12	56 (50%) 0 0	94, 117, 126, 134	0
14	AN	60/61 (98%)	1.29	11 (18%) 3 3	68, 79, 92, 102	0
14	CN	60/61 (98%)	2.81	47 (78%) 0 0	99, 110, 121, 128	0
15	AO	88/89 (98%)	0.83	6 (6%) 23 20	52, 73, 90, 94	0
15	CO	88/89 (98%)	0.81	4 (4%) 38 34	58, 77, 91, 96	0
16	AP	82/88 (93%)	2.11	47 (57%) 0 0	68, 82, 100, 110	0
16	CP	82/88 (93%)	1.80	34 (41%) 0 0	66, 79, 94, 103	0
17	AQ	99/105 (94%)	1.23	13 (13%) 7 6	57, 74, 87, 92	0
17	CQ	99/105 (94%)	1.12	11 (11%) 10 8	60, 75, 85, 94	0
18	AR	68/88 (77%)	0.79	2 (2%) 53 50	62, 73, 92, 96	0
18	CR	68/88 (77%)	0.94	5 (7%) 20 18	65, 76, 92, 96	0
19	AS	81/93 (87%)	1.50	26 (32%) 1 1	74, 89, 105, 128	0
19	CS	78/93 (83%)	2.16	39 (50%) 0 0	100, 118, 130, 133	0
20	AT	96/106 (90%)	1.77	29 (30%) 1 1	66, 82, 100, 106	0
20	CT	104/106 (98%)	1.67	26 (25%) 2 1	64, 83, 103, 119	0
21	AU	23/27 (85%)	1.54	6 (26%) 1 1	71, 80, 83, 90	0
21	CU	23/27 (85%)	3.09	19 (82%) 0 0	97, 106, 115, 119	0
22	AY	95/119 (79%)	0.42	2 (2%) 63 61	51, 64, 81, 92	0
22	CY	94/119 (78%)	1.56	26 (27%) 1 1	76, 95, 113, 120	0
23	BA	2827/2915 (96%)	-0.38	99 (3%) 47 43	24, 40, 120, 169	0
23	DA	2798/2915 (95%)	-0.18	98 (3%) 47 43	27, 46, 118, 170	0
24	BB	120/122 (98%)	0.28	4 (3%) 49 45	39, 65, 76, 119	0
24	DB	120/122 (98%)	1.63	43 (35%) 1 0	50, 81, 97, 130	0
25	BD	275/276 (99%)	-0.18	2 (0%) 84 83	24, 39, 51, 79	0
25	DD	275/276 (99%)	-0.18	1 (0%) 88 87	26, 43, 55, 84	0
26	BE	204/206 (99%)	-0.08	3 (1%) 72 70	24, 44, 64, 81	0
26	DE	204/206 (99%)	0.04	2 (0%) 79 78	27, 48, 69, 84	0
27	BF	203/210 (96%)	0.26	6 (2%) 52 49	25, 49, 82, 113	0
27	DF	203/210 (96%)	0.42	5 (2%) 58 55	28, 58, 84, 115	0
28	BG	181/182 (99%)	1.23	28 (15%) 5 4	64, 83, 108, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	2.41	113 (62%) 0 0	78, 96, 116, 140	0
29	BH	174/180 (96%)	0.77	7 (4%) 42 38	49, 64, 80, 92	0
29	DH	174/180 (96%)	1.58	48 (27%) 1 1	61, 78, 92, 101	0
30	BI	146/148 (98%)	0.71	5 (3%) 48 44	46, 75, 91, 98	0
30	DI	146/148 (98%)	0.93	13 (8%) 15 13	49, 81, 99, 107	0
31	BN	140/140 (100%)	0.18	3 (2%) 63 61	30, 44, 66, 83	0
31	DN	140/140 (100%)	0.31	2 (1%) 73 72	35, 52, 73, 86	0
32	BO	122/122 (100%)	-0.11	0 100 100	34, 43, 62, 65	0
32	DO	122/122 (100%)	-0.02	0 100 100	37, 47, 65, 68	0
33	BP	149/150 (99%)	0.27	0 100 100	25, 51, 77, 96	0
33	DP	149/150 (99%)	0.59	8 (5%) 31 27	30, 60, 87, 99	0
34	BQ	141/141 (100%)	0.21	0 100 100	31, 47, 59, 74	0
34	DQ	141/141 (100%)	0.67	10 (7%) 22 19	39, 55, 69, 79	0
35	BR	118/118 (100%)	-0.10	0 100 100	30, 38, 51, 62	0
35	DR	118/118 (100%)	0.11	1 (0%) 82 81	33, 42, 55, 67	0
36	BS	110/112 (98%)	0.77	10 (9%) 15 12	48, 62, 77, 85	0
36	DS	110/112 (98%)	2.01	51 (46%) 0 0	59, 74, 87, 93	0
37	BT	131/146 (89%)	0.16	10 (7%) 20 17	38, 46, 76, 103	0
37	DT	130/146 (89%)	0.26	4 (3%) 51 48	41, 50, 73, 105	0
38	BU	116/118 (98%)	-0.04	1 (0%) 81 80	28, 38, 53, 70	0
38	DU	116/118 (98%)	0.25	1 (0%) 81 80	33, 45, 61, 70	0
39	BV	101/101 (100%)	0.08	2 (1%) 65 62	27, 48, 67, 83	0
39	DV	101/101 (100%)	0.45	1 (0%) 79 78	32, 59, 76, 85	0
40	BW	112/113 (99%)	-0.20	0 100 100	28, 35, 52, 92	0
40	DW	111/113 (98%)	-0.11	2 (1%) 67 65	32, 40, 58, 85	0
41	BX	95/96 (98%)	0.14	2 (2%) 63 61	33, 43, 65, 84	0
41	DX	95/96 (98%)	0.49	1 (1%) 78 76	39, 50, 68, 89	0
42	BY	107/110 (97%)	0.56	4 (3%) 45 41	44, 55, 77, 88	0
42	DY	107/110 (97%)	1.20	18 (16%) 4 3	53, 63, 82, 91	0
43	BZ	198/206 (96%)	0.65	8 (4%) 42 38	48, 68, 91, 103	0
43	DZ	203/206 (98%)	1.39	35 (17%) 4 3	57, 78, 100, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	0.09	0 100 100	37, 44, 57, 75	0
44	D0	77/85 (90%)	0.77	5 (6%) 25 22	44, 52, 67, 101	0
45	B1	97/98 (98%)	0.00	2 (2%) 63 61	31, 44, 74, 82	0
45	D1	97/98 (98%)	0.18	3 (3%) 51 48	33, 48, 78, 85	0
46	B2	70/72 (97%)	0.54	2 (2%) 53 50	42, 56, 67, 93	0
46	D2	71/72 (98%)	0.90	4 (5%) 30 26	51, 65, 76, 94	0
47	B3	59/60 (98%)	0.16	2 (3%) 48 44	33, 42, 66, 84	0
47	D3	59/60 (98%)	0.69	2 (3%) 48 44	39, 50, 76, 96	0
48	B4	46/71 (64%)	0.97	7 (15%) 5 4	73, 96, 111, 116	0
48	D4	46/71 (64%)	1.71	13 (28%) 1 1	89, 107, 118, 124	0
49	B5	59/60 (98%)	-0.17	1 (1%) 69 67	23, 38, 56, 68	0
49	D5	59/60 (98%)	-0.08	1 (1%) 69 67	27, 43, 61, 73	0
50	B6	53/54 (98%)	-0.10	0 100 100	40, 46, 59, 66	0
50	D6	53/54 (98%)	0.17	0 100 100	47, 52, 60, 70	0
51	B7	48/49 (97%)	-0.17	1 (2%) 63 61	26, 30, 50, 71	0
51	D7	48/49 (97%)	-0.11	1 (2%) 63 61	28, 33, 54, 82	0
52	B8	64/65 (98%)	0.02	1 (1%) 70 68	34, 38, 45, 57	0
52	D8	64/65 (98%)	0.22	0 100 100	38, 44, 50, 60	0
53	B9	36/37 (97%)	0.35	2 (5%) 30 26	38, 46, 57, 69	0
53	D9	36/37 (97%)	0.66	2 (5%) 30 26	45, 55, 66, 76	0
All	All	20617/21484 (95%)	0.52	2204 (10%) 11 9	23, 63, 117, 175	0

The worst 5 of 2204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	AI	126	SER	8.4
8	CH	1	MET	7.9
2	CB	163	PHE	7.8
23	BA	2793	G	7.4
14	AN	2	ALA	7.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
54	MG	AA	1675	1/1	0.17	0.27	106,106,106,106	0
54	MG	CA	1607	1/1	0.39	0.38	96,96,96,96	0
54	MG	BA	3605	1/1	0.41	0.24	89,89,89,89	0
54	MG	AA	1757	1/1	0.50	0.30	91,91,91,91	0
54	MG	CA	1653	1/1	0.54	0.22	85,85,85,85	0
54	MG	BA	3600	1/1	0.55	0.17	58,58,58,58	0
54	MG	CA	1777	1/1	0.56	0.18	130,130,130,130	0
54	MG	CA	1797	1/1	0.56	0.16	68,68,68,68	0
54	MG	BA	3530	1/1	0.57	0.27	95,95,95,95	0
54	MG	CA	1742	1/1	0.57	0.15	99,99,99,99	0
54	MG	DA	3547	1/1	0.57	0.17	89,89,89,89	0
54	MG	AA	1646	1/1	0.58	0.23	87,87,87,87	0
54	MG	DA	3410	1/1	0.60	0.18	80,80,80,80	0
54	MG	CA	1762	1/1	0.60	0.25	86,86,86,86	0
54	MG	CA	1664	1/1	0.62	0.16	62,62,62,62	0
54	MG	DA	3399	1/1	0.62	0.20	80,80,80,80	0
54	MG	DA	3558	1/1	0.62	0.20	70,70,70,70	0
54	MG	DA	3614	1/1	0.62	0.40	92,92,92,92	0
54	MG	DA	3395	1/1	0.63	0.20	75,75,75,75	0
54	MG	BA	3560	1/1	0.63	0.22	93,93,93,93	0
54	MG	BA	3128	1/1	0.64	0.15	63,63,63,63	0
54	MG	DA	3565	1/1	0.66	0.14	62,62,62,62	0
54	MG	BA	3726	1/1	0.66	0.15	73,73,73,73	0
54	MG	DB	206	1/1	0.67	0.42	115,115,115,115	0
54	MG	CA	1629	1/1	0.68	0.37	81,81,81,81	0
54	MG	BA	3491	1/1	0.68	0.14	72,72,72,72	0
54	MG	BA	3683	1/1	0.68	0.14	95,95,95,95	0
54	MG	CA	1713	1/1	0.68	0.25	95,95,95,95	0
54	MG	CA	1781	1/1	0.69	0.20	100,100,100,100	0
54	MG	DA	3479	1/1	0.69	0.12	66,66,66,66	0
54	MG	DA	3486	1/1	0.69	0.19	44,44,44,44	0
54	MG	DA	3175	1/1	0.69	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3537	1/1	0.70	0.28	66,66,66,66	0
54	MG	DA	3393	1/1	0.70	0.22	52,52,52,52	0
54	MG	DA	3347	1/1	0.71	0.17	87,87,87,87	0
54	MG	BA	3111	1/1	0.71	0.33	67,67,67,67	0
54	MG	DA	3573	1/1	0.71	0.22	68,68,68,68	0
54	MG	AA	1686	1/1	0.71	0.21	68,68,68,68	0
54	MG	DA	3632	1/1	0.71	0.12	72,72,72,72	0
54	MG	CA	1631	1/1	0.71	0.17	87,87,87,87	0
54	MG	AA	1698	1/1	0.72	0.29	78,78,78,78	0
54	MG	DA	3389	1/1	0.72	0.15	82,82,82,82	0
54	MG	CA	1715	1/1	0.72	0.26	85,85,85,85	0
54	MG	BA	3169	1/1	0.72	0.14	60,60,60,60	0
54	MG	AA	1756	1/1	0.72	0.16	107,107,107,107	0
54	MG	CA	1707	1/1	0.73	0.34	73,73,73,73	0
54	MG	DA	3554	1/1	0.73	0.16	70,70,70,70	0
54	MG	BA	3500	1/1	0.73	0.17	68,68,68,68	0
54	MG	CA	1624	1/1	0.73	0.24	65,65,65,65	0
54	MG	CA	1791	1/1	0.73	0.18	72,72,72,72	0
54	MG	CA	1719	1/1	0.73	0.33	90,90,90,90	0
54	MG	BA	3206	1/1	0.73	0.21	67,67,67,67	0
54	MG	CA	1746	1/1	0.73	0.13	113,113,113,113	0
54	MG	DA	3141	1/1	0.74	0.10	70,70,70,70	0
54	MG	DA	3159	1/1	0.74	0.12	66,66,66,66	0
54	MG	BA	3517	1/1	0.74	0.14	91,91,91,91	0
54	MG	BA	3590	1/1	0.74	0.12	77,77,77,77	0
54	MG	CA	1604	1/1	0.74	0.26	70,70,70,70	0
54	MG	CA	1787	1/1	0.74	0.27	84,84,84,84	0
54	MG	AA	1714	1/1	0.74	0.13	58,58,58,58	0
54	MG	AA	1817	1/1	0.74	0.17	78,78,78,78	0
54	MG	DA	3404	1/1	0.74	0.19	62,62,62,62	0
54	MG	DA	3124	1/1	0.74	0.19	69,69,69,69	0
54	MG	AA	1794	1/1	0.75	0.15	111,111,111,111	0
54	MG	BA	3192	1/1	0.75	0.24	62,62,62,62	0
54	MG	BA	3510	1/1	0.75	0.17	77,77,77,77	0
54	MG	DA	3377	1/1	0.75	0.12	74,74,74,74	0
54	MG	DA	3388	1/1	0.75	0.22	73,73,73,73	0
54	MG	BA	3579	1/1	0.75	0.21	57,57,57,57	0
54	MG	BA	3003	1/1	0.75	0.26	68,68,68,68	0
54	MG	CA	1654	1/1	0.76	0.14	63,63,63,63	0
54	MG	DA	3316	1/1	0.76	0.10	87,87,87,87	0
54	MG	DA	3435	1/1	0.76	0.12	77,77,77,77	0
54	MG	DA	3466	1/1	0.76	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3014	1/1	0.76	0.23	61,61,61,61	0
54	MG	DA	3359	1/1	0.76	0.23	69,69,69,69	0
54	MG	CA	1758	1/1	0.76	0.14	64,64,64,64	0
54	MG	DA	3559	1/1	0.77	0.16	76,76,76,76	0
54	MG	BA	3529	1/1	0.77	0.15	52,52,52,52	0
54	MG	AA	1621	1/1	0.77	0.41	63,63,63,63	0
54	MG	CA	1660	1/1	0.77	0.20	65,65,65,65	0
54	MG	AA	1797	1/1	0.77	0.14	106,106,106,106	0
54	MG	DA	3374	1/1	0.77	0.20	73,73,73,73	0
54	MG	CA	1720	1/1	0.78	0.26	84,84,84,84	0
54	MG	CA	1729	1/1	0.78	0.18	84,84,84,84	0
54	MG	AA	1613	1/1	0.78	0.38	77,77,77,77	0
54	MG	CA	1625	1/1	0.78	0.13	69,69,69,69	0
54	MG	AA	1769	1/1	0.78	0.11	69,69,69,69	0
54	MG	AA	1611	1/1	0.78	0.22	75,75,75,75	0
54	MG	BA	3020	1/1	0.78	0.18	69,69,69,69	0
54	MG	AA	1622	1/1	0.78	0.19	60,60,60,60	0
54	MG	D0	101	1/1	0.78	0.29	78,78,78,78	0
54	MG	D5	103	1/1	0.78	0.11	61,61,61,61	0
54	MG	CA	1647	1/1	0.79	0.19	103,103,103,103	0
54	MG	DA	3253	1/1	0.79	0.14	58,58,58,58	0
54	MG	BA	3715	1/1	0.79	0.12	88,88,88,88	0
54	MG	BA	3345	1/1	0.79	0.18	54,54,54,54	0
54	MG	BA	3479	1/1	0.79	0.18	77,77,77,77	0
54	MG	DA	3371	1/1	0.79	0.21	76,76,76,76	0
54	MG	AA	1658	1/1	0.79	0.19	73,73,73,73	0
54	MG	BA	3205	1/1	0.79	0.10	67,67,67,67	0
54	MG	BA	3639	1/1	0.79	0.12	56,56,56,56	0
54	MG	CA	1626	1/1	0.79	0.37	86,86,86,86	0
54	MG	BA	3679	1/1	0.79	0.14	80,80,80,80	0
54	MG	DA	3618	1/1	0.79	0.17	93,93,93,93	0
54	MG	DA	3016	1/1	0.79	0.18	64,64,64,64	0
54	MG	CA	1630	1/1	0.79	0.46	78,78,78,78	0
54	MG	AD	302	1/1	0.79	0.27	73,73,73,73	0
54	MG	CA	1741	1/1	0.79	0.11	117,117,117,117	0
54	MG	DA	3292	1/1	0.80	0.14	59,59,59,59	0
54	MG	DA	3478	1/1	0.80	0.21	64,64,64,64	0
54	MG	CA	1616	1/1	0.80	0.26	71,71,71,71	0
54	MG	BA	3619	1/1	0.80	0.15	75,75,75,75	0
54	MG	DA	3536	1/1	0.80	0.14	76,76,76,76	0
54	MG	DA	3011	1/1	0.80	0.10	45,45,45,45	0
54	MG	DA	3014	1/1	0.80	0.41	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1643	1/1	0.80	0.35	76,76,76,76	0
54	MG	DA	3050	1/1	0.80	0.17	52,52,52,52	0
54	MG	DA	3108	1/1	0.80	0.19	70,70,70,70	0
54	MG	CA	1645	1/1	0.80	0.21	69,69,69,69	0
54	MG	DA	3592	1/1	0.80	0.11	72,72,72,72	0
54	MG	BA	3499	1/1	0.80	0.19	35,35,35,35	0
54	MG	AA	1793	1/1	0.80	0.19	78,78,78,78	0
54	MG	DA	3624	1/1	0.80	0.10	56,56,56,56	0
54	MG	AA	1813	1/1	0.80	0.17	86,86,86,86	0
54	MG	DA	3196	1/1	0.80	0.23	37,37,37,37	0
54	MG	CA	1657	1/1	0.80	0.12	85,85,85,85	0
54	MG	DA	3264	1/1	0.80	0.10	91,91,91,91	0
54	MG	DA	3282	1/1	0.81	0.12	64,64,64,64	0
54	MG	DA	3283	1/1	0.81	0.13	51,51,51,51	0
54	MG	AA	1674	1/1	0.81	0.19	75,75,75,75	0
54	MG	CA	1739	1/1	0.81	0.27	76,76,76,76	0
54	MG	DA	3507	1/1	0.81	0.12	90,90,90,90	0
54	MG	DA	3337	1/1	0.81	0.15	65,65,65,65	0
54	MG	CA	1612	1/1	0.81	0.40	84,84,84,84	0
54	MG	CA	1637	1/1	0.81	0.21	98,98,98,98	0
54	MG	DA	3032	1/1	0.81	0.18	59,59,59,59	0
54	MG	CA	1684	1/1	0.81	0.29	82,82,82,82	0
54	MG	CA	1754	1/1	0.81	0.20	77,77,77,77	0
54	MG	CA	1695	1/1	0.81	0.22	76,76,76,76	0
54	MG	DA	3136	1/1	0.81	0.55	62,62,62,62	0
54	MG	CA	1761	1/1	0.81	0.14	92,92,92,92	0
54	MG	AA	1694	1/1	0.81	0.14	76,76,76,76	0
54	MG	BA	3117	1/1	0.81	0.16	67,67,67,67	0
54	MG	BA	3719	1/1	0.81	0.13	83,83,83,83	0
54	MG	DA	3634	1/1	0.81	0.22	75,75,75,75	0
54	MG	BA	3577	1/1	0.81	0.14	59,59,59,59	0
54	MG	AA	1759	1/1	0.81	0.24	74,74,74,74	0
54	MG	DA	3463	1/1	0.81	0.19	67,67,67,67	0
54	MG	CA	1681	1/1	0.82	0.21	83,83,83,83	0
54	MG	DA	3020	1/1	0.82	0.24	66,66,66,66	0
54	MG	DA	3326	1/1	0.82	0.12	69,69,69,69	0
54	MG	BA	3197	1/1	0.82	0.14	58,58,58,58	0
54	MG	CA	1641	1/1	0.82	0.28	62,62,62,62	0
54	MG	DA	3497	1/1	0.82	0.12	40,40,40,40	0
54	MG	DA	3501	1/1	0.82	0.19	85,85,85,85	0
54	MG	CA	1697	1/1	0.82	0.15	95,95,95,95	0
54	MG	DA	3522	1/1	0.82	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3530	1/1	0.82	0.12	66,66,66,66	0
54	MG	CA	1613	1/1	0.82	0.24	68,68,68,68	0
54	MG	BA	3612	1/1	0.82	0.17	58,58,58,58	0
54	MG	DA	3140	1/1	0.82	0.12	60,60,60,60	0
54	MG	BA	3591	1/1	0.82	0.11	104,104,104,104	0
54	MG	BA	3721	1/1	0.82	0.17	53,53,53,53	0
54	MG	BA	3624	1/1	0.82	0.18	36,36,36,36	0
54	MG	BR	204	1/1	0.82	0.11	49,49,49,49	0
54	MG	DA	3574	1/1	0.82	0.10	77,77,77,77	0
54	MG	CA	1736	1/1	0.82	0.15	94,94,94,94	0
54	MG	CA	1803	1/1	0.82	0.14	55,55,55,55	0
54	MG	BA	3592	1/1	0.82	0.15	62,62,62,62	0
54	MG	DA	3416	1/1	0.82	0.15	64,64,64,64	0
54	MG	DA	3432	1/1	0.82	0.16	67,67,67,67	0
54	MG	AA	1659	1/1	0.82	0.18	75,75,75,75	0
54	MG	DA	3439	1/1	0.82	0.23	57,57,57,57	0
54	MG	DB	208	1/1	0.82	0.14	96,96,96,96	0
54	MG	DQ	204	1/1	0.82	0.09	67,67,67,67	0
54	MG	DA	3446	1/1	0.82	0.12	68,68,68,68	0
54	MG	DA	3449	1/1	0.82	0.13	57,57,57,57	0
54	MG	CA	1776	1/1	0.83	0.16	76,76,76,76	0
54	MG	DA	3272	1/1	0.83	0.07	69,69,69,69	0
54	MG	CA	1627	1/1	0.83	0.16	72,72,72,72	0
54	MG	AA	1667	1/1	0.83	0.21	84,84,84,84	0
54	MG	BA	3281	1/1	0.83	0.11	43,43,43,43	0
54	MG	BA	3314	1/1	0.83	0.11	39,39,39,39	0
54	MG	BA	3165	1/1	0.83	0.15	41,41,41,41	0
54	MG	BV	202	1/1	0.83	0.18	83,83,83,83	0
54	MG	DA	3523	1/1	0.83	0.11	73,73,73,73	0
54	MG	B6	102	1/1	0.83	0.15	69,69,69,69	0
54	MG	DA	3351	1/1	0.83	0.12	68,68,68,68	0
54	MG	DA	3013	1/1	0.83	0.23	60,60,60,60	0
54	MG	BA	3617	1/1	0.83	0.17	44,44,44,44	0
54	MG	CA	1722	1/1	0.83	0.14	58,58,58,58	0
54	MG	AA	1752	1/1	0.83	0.26	102,102,102,102	0
54	MG	CA	1650	1/1	0.83	0.28	65,65,65,65	0
54	MG	CA	1737	1/1	0.83	0.24	75,75,75,75	0
54	MG	CA	1652	1/1	0.83	0.15	88,88,88,88	0
54	MG	AA	1760	1/1	0.83	0.23	74,74,74,74	0
54	MG	DA	3134	1/1	0.83	0.31	71,71,71,71	0
54	MG	AA	1755	1/1	0.83	0.19	76,76,76,76	0
54	MG	BA	3677	1/1	0.83	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1633	1/1	0.83	0.26	69,69,69,69	0
54	MG	BA	3501	1/1	0.83	0.12	51,51,51,51	0
54	MG	CA	1759	1/1	0.83	0.22	95,95,95,95	0
54	MG	DA	3185	1/1	0.83	0.17	47,47,47,47	0
54	MG	DD	303	1/1	0.83	0.15	53,53,53,53	0
54	MG	CA	1677	1/1	0.83	0.13	86,86,86,86	0
54	MG	DA	3247	1/1	0.83	0.17	73,73,73,73	0
54	MG	BA	3507	1/1	0.83	0.13	67,67,67,67	0
54	MG	CA	1606	1/1	0.84	0.34	83,83,83,83	0
54	MG	DA	3398	1/1	0.84	0.14	53,53,53,53	0
54	MG	DA	3543	1/1	0.84	0.09	54,54,54,54	0
54	MG	DA	3276	1/1	0.84	0.10	76,76,76,76	0
54	MG	DA	3551	1/1	0.84	0.12	69,69,69,69	0
54	MG	DA	3051	1/1	0.84	0.22	73,73,73,73	0
54	MG	AA	1649	1/1	0.84	0.15	71,71,71,71	0
54	MG	DA	3285	1/1	0.84	0.21	68,68,68,68	0
54	MG	CA	1786	1/1	0.84	0.26	83,83,83,83	0
54	MG	DA	3307	1/1	0.84	0.20	79,79,79,79	0
54	MG	AA	1652	1/1	0.84	0.17	63,63,63,63	0
54	MG	DA	3323	1/1	0.84	0.15	69,69,69,69	0
54	MG	DA	3606	1/1	0.84	0.14	82,82,82,82	0
54	MG	AA	1623	1/1	0.84	0.35	85,85,85,85	0
54	MG	BA	3260	1/1	0.84	0.22	31,31,31,31	0
54	MG	BA	3152	1/1	0.84	0.13	48,48,48,48	0
54	MG	DA	3628	1/1	0.84	0.11	59,59,59,59	0
54	MG	DA	3149	1/1	0.84	0.20	46,46,46,46	0
54	MG	AA	1696	1/1	0.84	0.25	66,66,66,66	0
54	MG	DB	201	1/1	0.84	0.20	67,67,67,67	0
54	MG	BP	202	1/1	0.84	0.33	54,54,54,54	0
54	MG	BA	3626	1/1	0.84	0.13	68,68,68,68	0
54	MG	AA	1767	1/1	0.84	0.10	70,70,70,70	0
54	MG	DP	201	1/1	0.84	0.18	78,78,78,78	0
54	MG	BA	3671	1/1	0.84	0.12	50,50,50,50	0
54	MG	BA	3105	1/1	0.84	0.18	44,44,44,44	0
54	MG	DA	3038	1/1	0.84	0.13	85,85,85,85	0
54	MG	DA	3286	1/1	0.85	0.14	69,69,69,69	0
54	MG	BA	3287	1/1	0.85	0.15	44,44,44,44	0
54	MG	CA	1728	1/1	0.85	0.16	79,79,79,79	0
54	MG	BA	3716	1/1	0.85	0.11	54,54,54,54	0
54	MG	AA	1780	1/1	0.85	0.11	72,72,72,72	0
54	MG	AA	1721	1/1	0.85	0.23	77,77,77,77	0
54	MG	BA	3386	1/1	0.85	0.22	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3338	1/1	0.85	0.22	67,67,67,67	0
54	MG	DA	3340	1/1	0.85	0.16	72,72,72,72	0
54	MG	DA	3341	1/1	0.85	0.11	60,60,60,60	0
54	MG	BB	205	1/1	0.85	0.13	48,48,48,48	0
54	MG	DA	3069	1/1	0.85	0.19	67,67,67,67	0
54	MG	DA	3086	1/1	0.85	0.14	54,54,54,54	0
54	MG	DA	3365	1/1	0.85	0.12	51,51,51,51	0
54	MG	BA	3469	1/1	0.85	0.12	65,65,65,65	0
54	MG	AA	1764	1/1	0.85	0.15	70,70,70,70	0
54	MG	CA	1750	1/1	0.85	0.13	88,88,88,88	0
54	MG	BA	3487	1/1	0.85	0.13	49,49,49,49	0
54	MG	DA	3579	1/1	0.85	0.12	52,52,52,52	0
54	MG	BZ	301	1/1	0.85	0.25	61,61,61,61	0
54	MG	DA	3594	1/1	0.85	0.11	62,62,62,62	0
54	MG	DA	3596	1/1	0.85	0.20	60,60,60,60	0
54	MG	AA	1796	1/1	0.85	0.14	100,100,100,100	0
54	MG	BA	3608	1/1	0.85	0.10	21,21,21,21	0
54	MG	BA	3189	1/1	0.85	0.17	71,71,71,71	0
54	MG	BA	3072	1/1	0.85	0.12	48,48,48,48	0
54	MG	BA	3073	1/1	0.85	0.23	74,74,74,74	0
54	MG	CA	1778	1/1	0.85	0.10	83,83,83,83	0
54	MG	BA	3088	1/1	0.85	0.11	42,42,42,42	0
54	MG	AA	1609	1/1	0.85	0.20	66,66,66,66	0
54	MG	BA	3627	1/1	0.85	0.11	40,40,40,40	0
54	MG	AA	1603	1/1	0.85	0.13	62,62,62,62	0
54	MG	BA	3267	1/1	0.85	0.13	56,56,56,56	0
54	MG	DA	3281	1/1	0.85	0.14	85,85,85,85	0
54	MG	BA	3277	1/1	0.85	0.12	32,32,32,32	0
54	MG	AA	1777	1/1	0.85	0.09	100,100,100,100	0
54	MG	BA	3545	1/1	0.85	0.10	63,63,63,63	0
54	MG	BA	3309	1/1	0.86	0.10	69,69,69,69	0
54	MG	AA	1608	1/1	0.86	0.19	66,66,66,66	0
54	MG	BA	3532	1/1	0.86	0.16	31,31,31,31	0
54	MG	DA	3147	1/1	0.86	0.14	52,52,52,52	0
54	MG	DA	3436	1/1	0.86	0.23	77,77,77,77	0
54	MG	CA	1635	1/1	0.86	0.24	63,63,63,63	0
54	MG	BA	3322	1/1	0.86	0.10	54,54,54,54	0
54	MG	DA	3168	1/1	0.86	0.11	41,41,41,41	0
54	MG	DA	3459	1/1	0.86	0.14	90,90,90,90	0
54	MG	CA	1639	1/1	0.86	0.40	57,57,57,57	0
54	MG	BA	3334	1/1	0.86	0.10	39,39,39,39	0
54	MG	DA	3467	1/1	0.86	0.11	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1723	1/1	0.86	0.18	82,82,82,82	0
54	MG	BA	3717	1/1	0.86	0.10	45,45,45,45	0
54	MG	BA	3564	1/1	0.86	0.10	67,67,67,67	0
54	MG	BA	3377	1/1	0.86	0.14	44,44,44,44	0
54	MG	CA	1768	1/1	0.86	0.23	95,95,95,95	0
54	MG	AA	1639	1/1	0.86	0.20	64,64,64,64	0
54	MG	DA	3519	1/1	0.86	0.10	61,61,61,61	0
54	MG	BA	3452	1/1	0.86	0.10	54,54,54,54	0
54	MG	BD	307	1/1	0.86	0.16	65,65,65,65	0
54	MG	CA	1779	1/1	0.86	0.10	116,116,116,116	0
54	MG	CA	1655	1/1	0.86	0.13	66,66,66,66	0
54	MG	DA	3542	1/1	0.86	0.16	65,65,65,65	0
54	MG	AA	1802	1/1	0.86	0.21	64,64,64,64	0
54	MG	CA	1659	1/1	0.86	0.12	89,89,89,89	0
54	MG	DA	3294	1/1	0.86	0.14	67,67,67,67	0
54	MG	DA	3306	1/1	0.86	0.21	68,68,68,68	0
54	MG	CA	1789	1/1	0.86	0.14	66,66,66,66	0
54	MG	DA	3308	1/1	0.86	0.10	70,70,70,70	0
54	MG	BA	3477	1/1	0.86	0.10	101,101,101,101	0
54	MG	DA	3318	1/1	0.86	0.20	75,75,75,75	0
54	MG	BA	3102	1/1	0.86	0.15	33,33,33,33	0
54	MG	AA	1704	1/1	0.86	0.16	75,75,75,75	0
54	MG	B0	103	1/1	0.86	0.18	71,71,71,71	0
54	MG	BA	3106	1/1	0.86	0.13	48,48,48,48	0
54	MG	CA	1686	1/1	0.86	0.25	67,67,67,67	0
54	MG	DA	3597	1/1	0.86	0.14	73,73,73,73	0
54	MG	DA	3598	1/1	0.86	0.14	64,64,64,64	0
54	MG	CA	1602	1/1	0.86	0.28	70,70,70,70	0
54	MG	BA	3210	1/1	0.86	0.11	58,58,58,58	0
54	MG	AA	1630	1/1	0.86	0.18	76,76,76,76	0
54	MG	AA	1715	1/1	0.86	0.18	61,61,61,61	0
54	MG	DA	3626	1/1	0.86	0.18	75,75,75,75	0
54	MG	AA	1785	1/1	0.86	0.18	61,61,61,61	0
54	MG	BA	3150	1/1	0.86	0.14	70,70,70,70	0
54	MG	DA	3065	1/1	0.86	0.33	74,74,74,74	0
54	MG	BA	3511	1/1	0.86	0.12	72,72,72,72	0
54	MG	AA	1717	1/1	0.86	0.13	79,79,79,79	0
54	MG	DA	3090	1/1	0.86	0.15	45,45,45,45	0
54	MG	DA	3093	1/1	0.86	0.09	55,55,55,55	0
54	MG	BA	3640	1/1	0.86	0.14	55,55,55,55	0
54	MG	BA	3656	1/1	0.86	0.16	50,50,50,50	0
54	MG	DA	3130	1/1	0.86	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3664	1/1	0.86	0.10	56,56,56,56	0
54	MG	D7	102	1/1	0.86	0.13	65,65,65,65	0
54	MG	AA	1762	1/1	0.87	0.24	78,78,78,78	0
54	MG	AA	1678	1/1	0.87	0.25	75,75,75,75	0
54	MG	DA	3198	1/1	0.87	0.14	52,52,52,52	0
54	MG	CA	1675	1/1	0.87	0.11	75,75,75,75	0
54	MG	CA	1785	1/1	0.87	0.16	84,84,84,84	0
54	MG	BA	3512	1/1	0.87	0.11	71,71,71,71	0
54	MG	CA	1603	1/1	0.87	0.46	83,83,83,83	0
54	MG	DA	3494	1/1	0.87	0.12	64,64,64,64	0
54	MG	AA	1632	1/1	0.87	0.14	64,64,64,64	0
54	MG	BA	3526	1/1	0.87	0.12	55,55,55,55	0
54	MG	DA	3505	1/1	0.87	0.16	66,66,66,66	0
54	MG	CA	1688	1/1	0.87	0.15	110,110,110,110	0
54	MG	DA	3514	1/1	0.87	0.13	92,92,92,92	0
54	MG	CA	1800	1/1	0.87	0.12	76,76,76,76	0
54	MG	BA	3327	1/1	0.87	0.12	69,69,69,69	0
54	MG	DA	3004	1/1	0.87	0.26	64,64,64,64	0
54	MG	AA	1605	1/1	0.87	0.27	62,62,62,62	0
54	MG	BA	3343	1/1	0.87	0.10	48,48,48,48	0
54	MG	CA	1709	1/1	0.87	0.21	76,76,76,76	0
54	MG	CA	1712	1/1	0.87	0.09	55,55,55,55	0
54	MG	BA	3666	1/1	0.87	0.12	78,78,78,78	0
54	MG	DA	3028	1/1	0.87	0.20	62,62,62,62	0
54	MG	BA	3669	1/1	0.87	0.12	44,44,44,44	0
54	MG	BA	3174	1/1	0.87	0.16	73,73,73,73	0
54	MG	DA	3040	1/1	0.87	0.21	58,58,58,58	0
54	MG	AA	1695	1/1	0.87	0.12	57,57,57,57	0
54	MG	BA	3556	1/1	0.87	0.16	52,52,52,52	0
54	MG	BA	3059	1/1	0.87	0.15	54,54,54,54	0
54	MG	DA	3576	1/1	0.87	0.27	36,36,36,36	0
54	MG	BA	3709	1/1	0.87	0.09	47,47,47,47	0
54	MG	BA	3714	1/1	0.87	0.09	47,47,47,47	0
54	MG	AA	1736	1/1	0.87	0.15	67,67,67,67	0
54	MG	BA	3453	1/1	0.87	0.16	65,65,65,65	0
54	MG	DA	3100	1/1	0.87	0.23	56,56,56,56	0
54	MG	DA	3106	1/1	0.87	0.10	55,55,55,55	0
54	MG	AA	1740	1/1	0.87	0.23	70,70,70,70	0
54	MG	DA	3110	1/1	0.87	0.10	56,56,56,56	0
54	MG	AA	1606	1/1	0.87	0.14	63,63,63,63	0
54	MG	AA	1619	1/1	0.87	0.28	45,45,45,45	0
54	MG	BA	3228	1/1	0.87	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3727	1/1	0.87	0.11	94,94,94,94	0
54	MG	BA	3595	1/1	0.87	0.19	78,78,78,78	0
54	MG	AA	1699	1/1	0.87	0.14	65,65,65,65	0
54	MG	DA	3635	1/1	0.87	0.13	54,54,54,54	0
54	MG	DA	3143	1/1	0.87	0.22	62,62,62,62	0
54	MG	BE	304	1/1	0.87	0.15	53,53,53,53	0
54	MG	AA	1700	1/1	0.87	0.30	69,69,69,69	0
54	MG	DB	210	1/1	0.87	0.10	82,82,82,82	0
54	MG	DA	3152	1/1	0.87	0.16	52,52,52,52	0
54	MG	DO	201	1/1	0.87	0.11	67,67,67,67	0
54	MG	AA	1620	1/1	0.87	0.26	61,61,61,61	0
54	MG	DA	3164	1/1	0.87	0.13	64,64,64,64	0
54	MG	AA	1805	1/1	0.87	0.18	82,82,82,82	0
54	MG	AA	1651	1/1	0.87	0.14	62,62,62,62	0
54	MG	D7	101	1/1	0.87	0.27	41,41,41,41	0
54	MG	DA	3178	1/1	0.87	0.10	42,42,42,42	0
54	MG	AA	1665	1/1	0.88	0.20	66,66,66,66	0
54	MG	DA	3148	1/1	0.88	0.14	55,55,55,55	0
54	MG	BF	305	1/1	0.88	0.27	29,29,29,29	0
54	MG	BN	201	1/1	0.88	0.09	57,57,57,57	0
54	MG	BA	3336	1/1	0.88	0.11	71,71,71,71	0
54	MG	BA	3615	1/1	0.88	0.22	60,60,60,60	0
54	MG	BA	3129	1/1	0.88	0.16	69,69,69,69	0
54	MG	AA	1800	1/1	0.88	0.22	70,70,70,70	0
54	MG	BA	3621	1/1	0.88	0.13	35,35,35,35	0
54	MG	CA	1793	1/1	0.88	0.21	89,89,89,89	0
54	MG	BA	3513	1/1	0.88	0.12	46,46,46,46	0
54	MG	CA	1798	1/1	0.88	0.26	67,67,67,67	0
54	MG	DA	3222	1/1	0.88	0.17	37,37,37,37	0
54	MG	DA	3231	1/1	0.88	0.12	51,51,51,51	0
54	MG	DA	3496	1/1	0.88	0.16	38,38,38,38	0
54	MG	DA	3244	1/1	0.88	0.10	32,32,32,32	0
54	MG	DA	3500	1/1	0.88	0.16	56,56,56,56	0
54	MG	CA	1601	1/1	0.88	0.20	55,55,55,55	0
54	MG	CA	1692	1/1	0.88	0.14	64,64,64,64	0
54	MG	BA	3360	1/1	0.88	0.13	41,41,41,41	0
54	MG	BA	3235	1/1	0.88	0.14	45,45,45,45	0
54	MG	CA	1705	1/1	0.88	0.14	72,72,72,72	0
54	MG	DA	3279	1/1	0.88	0.14	66,66,66,66	0
54	MG	BA	3239	1/1	0.88	0.08	63,63,63,63	0
54	MG	BA	3432	1/1	0.88	0.16	68,68,68,68	0
54	MG	BA	3444	1/1	0.88	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3023	1/1	0.88	0.37	68,68,68,68	0
54	MG	BA	3536	1/1	0.88	0.12	54,54,54,54	0
54	MG	DA	3288	1/1	0.88	0.11	51,51,51,51	0
54	MG	BA	3449	1/1	0.88	0.08	40,40,40,40	0
54	MG	DA	3037	1/1	0.88	0.12	52,52,52,52	0
54	MG	DA	3296	1/1	0.88	0.21	61,61,61,61	0
54	MG	DA	3297	1/1	0.88	0.09	49,49,49,49	0
54	MG	DA	3302	1/1	0.88	0.10	51,51,51,51	0
54	MG	AA	1779	1/1	0.88	0.13	68,68,68,68	0
54	MG	AA	1666	1/1	0.88	0.21	71,71,71,71	0
54	MG	DA	3042	1/1	0.88	0.17	50,50,50,50	0
54	MG	DA	3577	1/1	0.88	0.13	57,57,57,57	0
54	MG	BA	3672	1/1	0.88	0.15	69,69,69,69	0
54	MG	DA	3583	1/1	0.88	0.32	35,35,35,35	0
54	MG	BA	3458	1/1	0.88	0.09	45,45,45,45	0
54	MG	BA	3462	1/1	0.88	0.34	36,36,36,36	0
54	MG	BA	3569	1/1	0.88	0.09	67,67,67,67	0
54	MG	DA	3083	1/1	0.88	0.07	50,50,50,50	0
54	MG	BA	3684	1/1	0.88	0.20	64,64,64,64	0
54	MG	DA	3605	1/1	0.88	0.11	49,49,49,49	0
54	MG	BA	3702	1/1	0.88	0.10	66,66,66,66	0
54	MG	DA	3092	1/1	0.88	0.13	54,54,54,54	0
54	MG	BA	3570	1/1	0.88	0.08	50,50,50,50	0
54	MG	DA	3348	1/1	0.88	0.09	87,87,87,87	0
54	MG	DA	3096	1/1	0.88	0.24	61,61,61,61	0
54	MG	AA	1753	1/1	0.88	0.17	71,71,71,71	0
54	MG	AA	1816	1/1	0.88	0.12	75,75,75,75	0
54	MG	AA	1635	1/1	0.88	0.18	77,77,77,77	0
54	MG	DA	3109	1/1	0.88	0.27	57,57,57,57	0
54	MG	BA	3306	1/1	0.88	0.10	61,61,61,61	0
54	MG	DA	3118	1/1	0.88	0.26	75,75,75,75	0
54	MG	AA	1654	1/1	0.88	0.12	77,77,77,77	0
54	MG	BA	3594	1/1	0.88	0.14	56,56,56,56	0
54	MG	DA	3133	1/1	0.88	0.33	50,50,50,50	0
54	MG	AA	1795	1/1	0.88	0.10	87,87,87,87	0
54	MG	BA	3201	1/1	0.88	0.17	57,57,57,57	0
54	MG	AA	1662	1/1	0.88	0.15	64,64,64,64	0
54	MG	BB	211	1/1	0.88	0.10	61,61,61,61	0
54	MG	DA	3415	1/1	0.88	0.10	53,53,53,53	0
54	MG	BA	3607	1/1	0.88	0.13	76,76,76,76	0
54	MG	DA	3428	1/1	0.88	0.10	36,36,36,36	0
54	MG	BA	3265	1/1	0.89	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3293	1/1	0.89	0.14	85,85,85,85	0
54	MG	DA	3094	1/1	0.89	0.14	54,54,54,54	0
54	MG	BA	3153	1/1	0.89	0.10	36,36,36,36	0
54	MG	DA	3502	1/1	0.89	0.12	78,78,78,78	0
54	MG	CA	1774	1/1	0.89	0.18	73,73,73,73	0
54	MG	DA	3102	1/1	0.89	0.16	48,48,48,48	0
54	MG	DA	3509	1/1	0.89	0.11	70,70,70,70	0
54	MG	AA	1660	1/1	0.89	0.21	62,62,62,62	0
54	MG	CA	1663	1/1	0.89	0.13	75,75,75,75	0
54	MG	BA	3559	1/1	0.89	0.17	56,56,56,56	0
54	MG	B2	102	1/1	0.89	0.14	60,60,60,60	0
54	MG	BA	3461	1/1	0.89	0.08	62,62,62,62	0
54	MG	CA	1783	1/1	0.89	0.23	73,73,73,73	0
54	MG	DA	3538	1/1	0.89	0.23	60,60,60,60	0
54	MG	DA	3125	1/1	0.89	0.16	59,59,59,59	0
54	MG	DA	3328	1/1	0.89	0.09	52,52,52,52	0
54	MG	BA	3100	1/1	0.89	0.11	41,41,41,41	0
54	MG	BA	3467	1/1	0.89	0.09	63,63,63,63	0
54	MG	BA	3285	1/1	0.89	0.21	96,96,96,96	0
54	MG	DA	3555	1/1	0.89	0.23	63,63,63,63	0
54	MG	BA	3674	1/1	0.89	0.07	62,62,62,62	0
54	MG	BA	3574	1/1	0.89	0.11	41,41,41,41	0
54	MG	CA	1694	1/1	0.89	0.13	69,69,69,69	0
54	MG	AA	1770	1/1	0.89	0.11	80,80,80,80	0
54	MG	CA	1610	1/1	0.89	0.23	67,67,67,67	0
54	MG	BA	3291	1/1	0.89	0.07	68,68,68,68	0
54	MG	CA	1801	1/1	0.89	0.17	88,88,88,88	0
54	MG	DA	3578	1/1	0.89	0.12	45,45,45,45	0
54	MG	AA	1725	1/1	0.89	0.18	62,62,62,62	0
54	MG	AA	1707	1/1	0.89	0.12	79,79,79,79	0
54	MG	BA	3704	1/1	0.89	0.16	70,70,70,70	0
54	MG	BA	3495	1/1	0.89	0.12	57,57,57,57	0
54	MG	BA	3015	1/1	0.89	0.21	32,32,32,32	0
54	MG	BA	3113	1/1	0.89	0.13	48,48,48,48	0
54	MG	AA	1644	1/1	0.89	0.12	58,58,58,58	0
54	MG	AA	1604	1/1	0.89	0.31	66,66,66,66	0
54	MG	BA	3606	1/1	0.89	0.12	63,63,63,63	0
54	MG	DA	3608	1/1	0.89	0.16	74,74,74,74	0
54	MG	DA	3212	1/1	0.89	0.07	32,32,32,32	0
54	MG	DA	3617	1/1	0.89	0.08	74,74,74,74	0
54	MG	DA	3413	1/1	0.89	0.19	78,78,78,78	0
54	MG	BA	3208	1/1	0.89	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3228	1/1	0.89	0.13	60,60,60,60	0
54	MG	BA	3068	1/1	0.89	0.13	40,40,40,40	0
54	MG	DA	3235	1/1	0.89	0.11	58,58,58,58	0
54	MG	BA	3148	1/1	0.89	0.15	21,21,21,21	0
54	MG	BA	3149	1/1	0.89	0.10	24,24,24,24	0
54	MG	BA	3238	1/1	0.89	0.09	39,39,39,39	0
54	MG	DA	3047	1/1	0.89	0.11	52,52,52,52	0
54	MG	AA	1617	1/1	0.89	0.22	58,58,58,58	0
54	MG	BA	3248	1/1	0.89	0.13	30,30,30,30	0
54	MG	BA	3436	1/1	0.89	0.11	41,41,41,41	0
54	MG	BA	3251	1/1	0.89	0.08	24,24,24,24	0
54	MG	DA	3079	1/1	0.89	0.19	54,54,54,54	0
54	MG	DA	3469	1/1	0.89	0.16	56,56,56,56	0
54	MG	CA	1757	1/1	0.89	0.11	75,75,75,75	0
54	MG	AA	1641	1/1	0.89	0.11	62,62,62,62	0
54	MG	BQ	201	1/1	0.89	0.15	61,61,61,61	0
54	MG	BR	203	1/1	0.89	0.14	33,33,33,33	0
55	ZN	CD	301	1/1	0.89	0.24	93,93,93,93	0
54	MG	DA	3409	1/1	0.90	0.12	53,53,53,53	0
54	MG	BA	3242	1/1	0.90	0.08	45,45,45,45	0
54	MG	BA	3030	1/1	0.90	0.08	44,44,44,44	0
54	MG	BA	3144	1/1	0.90	0.14	51,51,51,51	0
54	MG	BA	3031	1/1	0.90	0.21	66,66,66,66	0
54	MG	BA	3567	1/1	0.90	0.08	66,66,66,66	0
54	MG	BA	3033	1/1	0.90	0.19	31,31,31,31	0
54	MG	DA	3144	1/1	0.90	0.14	54,54,54,54	0
54	MG	BA	3056	1/1	0.90	0.07	32,32,32,32	0
54	MG	DA	3437	1/1	0.90	0.15	54,54,54,54	0
54	MG	AA	1693	1/1	0.90	0.20	72,72,72,72	0
54	MG	AA	1804	1/1	0.90	0.17	64,64,64,64	0
54	MG	AA	1732	1/1	0.90	0.29	68,68,68,68	0
54	MG	BA	3580	1/1	0.90	0.11	49,49,49,49	0
54	MG	DA	3462	1/1	0.90	0.14	63,63,63,63	0
54	MG	BA	3588	1/1	0.90	0.09	55,55,55,55	0
54	MG	AA	1645	1/1	0.90	0.10	54,54,54,54	0
54	MG	BA	3718	1/1	0.90	0.10	49,49,49,49	0
54	MG	BA	3288	1/1	0.90	0.13	44,44,44,44	0
54	MG	DA	3182	1/1	0.90	0.10	45,45,45,45	0
54	MG	AA	1791	1/1	0.90	0.13	68,68,68,68	0
54	MG	DA	3484	1/1	0.90	0.13	34,34,34,34	0
54	MG	DA	3193	1/1	0.90	0.09	66,66,66,66	0
54	MG	BA	3485	1/1	0.90	0.13	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3495	1/1	0.90	0.08	34,34,34,34	0
54	MG	BA	3293	1/1	0.90	0.09	36,36,36,36	0
54	MG	DA	3200	1/1	0.90	0.07	34,34,34,34	0
54	MG	DA	3209	1/1	0.90	0.09	45,45,45,45	0
54	MG	BB	201	1/1	0.90	0.32	67,67,67,67	0
54	MG	BA	3299	1/1	0.90	0.09	44,44,44,44	0
54	MG	DA	3226	1/1	0.90	0.10	41,41,41,41	0
54	MG	CA	1799	1/1	0.90	0.15	99,99,99,99	0
54	MG	BA	3091	1/1	0.90	0.15	34,34,34,34	0
54	MG	BB	213	1/1	0.90	0.08	46,46,46,46	0
54	MG	BB	216	1/1	0.90	0.14	59,59,59,59	0
54	MG	BA	3307	1/1	0.90	0.12	46,46,46,46	0
54	MG	BE	301	1/1	0.90	0.21	43,43,43,43	0
54	MG	AA	1628	1/1	0.90	0.15	81,81,81,81	0
54	MG	AA	1741	1/1	0.90	0.16	58,58,58,58	0
54	MG	DA	3275	1/1	0.90	0.09	69,69,69,69	0
54	MG	AI	201	1/1	0.90	0.13	67,67,67,67	0
54	MG	CA	1689	1/1	0.90	0.07	90,90,90,90	0
54	MG	DA	3280	1/1	0.90	0.11	52,52,52,52	0
54	MG	DA	3550	1/1	0.90	0.09	51,51,51,51	0
54	MG	AA	1647	1/1	0.90	0.29	73,73,73,73	0
54	MG	DA	3024	1/1	0.90	0.23	64,64,64,64	0
54	MG	BA	3333	1/1	0.90	0.10	54,54,54,54	0
54	MG	DA	3556	1/1	0.90	0.16	87,87,87,87	0
54	MG	BA	3108	1/1	0.90	0.24	51,51,51,51	0
54	MG	BA	3005	1/1	0.90	0.08	56,56,56,56	0
54	MG	DA	3563	1/1	0.90	0.20	57,57,57,57	0
54	MG	CA	1698	1/1	0.90	0.15	62,62,62,62	0
54	MG	DA	3569	1/1	0.90	0.11	60,60,60,60	0
54	MG	BT	202	1/1	0.90	0.18	52,52,52,52	0
54	MG	CA	1706	1/1	0.90	0.13	76,76,76,76	0
54	MG	DA	3575	1/1	0.90	0.11	98,98,98,98	0
54	MG	BA	3623	1/1	0.90	0.11	85,85,85,85	0
54	MG	BA	3112	1/1	0.90	0.17	52,52,52,52	0
54	MG	CA	1711	1/1	0.90	0.14	55,55,55,55	0
54	MG	DA	3054	1/1	0.90	0.13	46,46,46,46	0
54	MG	BA	3219	1/1	0.90	0.12	67,67,67,67	0
54	MG	DA	3591	1/1	0.90	0.16	39,39,39,39	0
54	MG	AA	1656	1/1	0.90	0.14	69,69,69,69	0
54	MG	DA	3077	1/1	0.90	0.08	42,42,42,42	0
54	MG	DA	3312	1/1	0.90	0.09	52,52,52,52	0
54	MG	BA	3633	1/1	0.90	0.19	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3081	1/1	0.90	0.12	60,60,60,60	0
54	MG	BA	3635	1/1	0.90	0.10	72,72,72,72	0
54	MG	DA	3084	1/1	0.90	0.09	45,45,45,45	0
54	MG	BA	3375	1/1	0.90	0.13	61,61,61,61	0
54	MG	DA	3335	1/1	0.90	0.14	68,68,68,68	0
54	MG	DA	3616	1/1	0.90	0.08	63,63,63,63	0
54	MG	AA	1601	1/1	0.90	0.28	52,52,52,52	0
54	MG	DA	3091	1/1	0.90	0.43	38,38,38,38	0
54	MG	CA	1723	1/1	0.90	0.09	66,66,66,66	0
54	MG	DA	3625	1/1	0.90	0.14	76,76,76,76	0
54	MG	BA	3643	1/1	0.90	0.29	28,28,28,28	0
54	MG	BA	3653	1/1	0.90	0.09	58,58,58,58	0
54	MG	DA	3630	1/1	0.90	0.12	76,76,76,76	0
54	MG	DA	3095	1/1	0.90	0.23	65,65,65,65	0
54	MG	BA	3655	1/1	0.90	0.19	68,68,68,68	0
54	MG	CA	1609	1/1	0.90	0.38	77,77,77,77	0
54	MG	BA	3534	1/1	0.90	0.12	69,69,69,69	0
54	MG	DB	205	1/1	0.90	0.10	92,92,92,92	0
54	MG	BA	3657	1/1	0.90	0.09	91,91,91,91	0
54	MG	BA	3120	1/1	0.90	0.07	54,54,54,54	0
54	MG	BA	3387	1/1	0.90	0.13	27,27,27,27	0
54	MG	DA	3384	1/1	0.90	0.19	49,49,49,49	0
54	MG	DF	302	1/1	0.90	0.15	63,63,63,63	0
54	MG	CA	1749	1/1	0.90	0.16	69,69,69,69	0
54	MG	CA	1621	1/1	0.90	0.21	87,87,87,87	0
54	MG	DA	3121	1/1	0.90	0.19	62,62,62,62	0
54	MG	DA	3122	1/1	0.90	0.16	58,58,58,58	0
54	MG	BA	3539	1/1	0.90	0.09	58,58,58,58	0
54	MG	CA	1756	1/1	0.90	0.11	77,77,77,77	0
54	MG	DA	3400	1/1	0.90	0.09	41,41,41,41	0
54	MG	AA	1689	1/1	0.90	0.17	56,56,56,56	0
54	MG	CA	1771	1/1	0.91	0.14	71,71,71,71	0
54	MG	CA	1773	1/1	0.91	0.10	89,89,89,89	0
54	MG	AA	1719	1/1	0.91	0.20	66,66,66,66	0
54	MG	DA	3418	1/1	0.91	0.07	48,48,48,48	0
54	MG	DA	3420	1/1	0.91	0.10	52,52,52,52	0
54	MG	DA	3424	1/1	0.91	0.12	49,49,49,49	0
54	MG	AA	1650	1/1	0.91	0.09	74,74,74,74	0
54	MG	BA	3571	1/1	0.91	0.10	74,74,74,74	0
54	MG	AA	1625	1/1	0.91	0.21	42,42,42,42	0
54	MG	BA	3576	1/1	0.91	0.08	55,55,55,55	0
54	MG	BA	3021	1/1	0.91	0.34	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3026	1/1	0.91	0.16	50,50,50,50	0
54	MG	DA	3441	1/1	0.91	0.18	63,63,63,63	0
54	MG	DA	3443	1/1	0.91	0.11	51,51,51,51	0
54	MG	DA	3444	1/1	0.91	0.20	73,73,73,73	0
54	MG	BA	3454	1/1	0.91	0.15	55,55,55,55	0
54	MG	CA	1651	1/1	0.91	0.09	55,55,55,55	0
54	MG	DA	3451	1/1	0.91	0.09	60,60,60,60	0
54	MG	DA	3454	1/1	0.91	0.10	42,42,42,42	0
54	MG	DA	3170	1/1	0.91	0.16	31,31,31,31	0
54	MG	BA	3134	1/1	0.91	0.09	50,50,50,50	0
54	MG	BA	3136	1/1	0.91	0.10	24,24,24,24	0
54	MG	BA	3029	1/1	0.91	0.14	38,38,38,38	0
54	MG	CA	1792	1/1	0.91	0.16	65,65,65,65	0
54	MG	BA	3276	1/1	0.91	0.11	47,47,47,47	0
54	MG	DA	3477	1/1	0.91	0.07	63,63,63,63	0
54	MG	DA	3195	1/1	0.91	0.14	33,33,33,33	0
54	MG	CA	1796	1/1	0.91	0.12	85,85,85,85	0
54	MG	AA	1724	1/1	0.91	0.15	93,93,93,93	0
54	MG	BA	3279	1/1	0.91	0.13	38,38,38,38	0
54	MG	DA	3205	1/1	0.91	0.06	44,44,44,44	0
54	MG	BB	210	1/1	0.91	0.15	62,62,62,62	0
54	MG	CA	1661	1/1	0.91	0.12	55,55,55,55	0
54	MG	BA	3478	1/1	0.91	0.14	50,50,50,50	0
54	MG	BA	3603	1/1	0.91	0.19	39,39,39,39	0
54	MG	AA	1618	1/1	0.91	0.31	57,57,57,57	0
54	MG	DA	3006	1/1	0.91	0.09	42,42,42,42	0
54	MG	DA	3010	1/1	0.91	0.20	48,48,48,48	0
54	MG	AA	1685	1/1	0.91	0.16	57,57,57,57	0
54	MG	BA	3151	1/1	0.91	0.12	34,34,34,34	0
54	MG	DA	3249	1/1	0.91	0.10	47,47,47,47	0
54	MG	CA	1682	1/1	0.91	0.20	60,60,60,60	0
54	MG	DA	3255	1/1	0.91	0.09	51,51,51,51	0
54	MG	BE	303	1/1	0.91	0.17	47,47,47,47	0
54	MG	DA	3524	1/1	0.91	0.10	61,61,61,61	0
54	MG	DA	3525	1/1	0.91	0.15	57,57,57,57	0
54	MG	DA	3017	1/1	0.91	0.16	48,48,48,48	0
54	MG	DA	3018	1/1	0.91	0.22	54,54,54,54	0
54	MG	CA	1685	1/1	0.91	0.20	62,62,62,62	0
54	MG	DA	3539	1/1	0.91	0.14	54,54,54,54	0
54	MG	BA	3040	1/1	0.91	0.12	52,52,52,52	0
54	MG	BA	3493	1/1	0.91	0.14	65,65,65,65	0
54	MG	DA	3546	1/1	0.91	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3027	1/1	0.91	0.10	47,47,47,47	0
54	MG	DA	3549	1/1	0.91	0.15	39,39,39,39	0
54	MG	BG	201	1/1	0.91	0.13	56,56,56,56	0
54	MG	AA	1663	1/1	0.91	0.14	62,62,62,62	0
54	MG	DA	3553	1/1	0.91	0.12	64,64,64,64	0
54	MG	BA	3496	1/1	0.91	0.24	56,56,56,56	0
54	MG	BA	3161	1/1	0.91	0.17	20,20,20,20	0
54	MG	AA	1688	1/1	0.91	0.15	62,62,62,62	0
54	MG	BA	3168	1/1	0.91	0.11	68,68,68,68	0
54	MG	CA	1703	1/1	0.91	0.13	46,46,46,46	0
54	MG	AA	1803	1/1	0.91	0.17	81,81,81,81	0
54	MG	BA	3308	1/1	0.91	0.12	51,51,51,51	0
54	MG	BW	201	1/1	0.91	0.09	44,44,44,44	0
54	MG	DA	3570	1/1	0.91	0.12	63,63,63,63	0
54	MG	DA	3298	1/1	0.91	0.09	51,51,51,51	0
54	MG	AA	1636	1/1	0.91	0.07	49,49,49,49	0
54	MG	AA	1772	1/1	0.91	0.08	71,71,71,71	0
54	MG	DA	3076	1/1	0.91	0.32	54,54,54,54	0
54	MG	BA	3315	1/1	0.91	0.11	63,63,63,63	0
54	MG	B3	102	1/1	0.91	0.10	52,52,52,52	0
54	MG	DA	3315	1/1	0.91	0.08	49,49,49,49	0
54	MG	BA	3074	1/1	0.91	0.07	32,32,32,32	0
54	MG	B9	103	1/1	0.91	0.14	52,52,52,52	0
54	MG	AA	1806	1/1	0.91	0.13	60,60,60,60	0
54	MG	BA	3527	1/1	0.91	0.10	51,51,51,51	0
54	MG	AA	1776	1/1	0.91	0.24	68,68,68,68	0
54	MG	AA	1746	1/1	0.91	0.08	63,63,63,63	0
54	MG	CA	1605	1/1	0.91	0.29	63,63,63,63	0
54	MG	AA	1778	1/1	0.91	0.10	74,74,74,74	0
54	MG	AA	1690	1/1	0.91	0.11	60,60,60,60	0
54	MG	BA	3659	1/1	0.91	0.08	61,61,61,61	0
54	MG	AA	1615	1/1	0.91	0.26	76,76,76,76	0
54	MG	DA	3098	1/1	0.91	0.36	52,52,52,52	0
54	MG	BA	3347	1/1	0.91	0.12	44,44,44,44	0
54	MG	DA	3352	1/1	0.91	0.10	82,82,82,82	0
54	MG	DA	3619	1/1	0.91	0.11	57,57,57,57	0
54	MG	DA	3623	1/1	0.91	0.07	42,42,42,42	0
54	MG	DA	3353	1/1	0.91	0.10	79,79,79,79	0
54	MG	CA	1744	1/1	0.91	0.11	69,69,69,69	0
54	MG	DA	3103	1/1	0.91	0.17	48,48,48,48	0
54	MG	DA	3369	1/1	0.91	0.06	85,85,85,85	0
54	MG	BA	3217	1/1	0.91	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AL	201	1/1	0.91	0.10	65,65,65,65	0
54	MG	BA	3546	1/1	0.91	0.10	46,46,46,46	0
54	MG	CA	1752	1/1	0.91	0.10	91,91,91,91	0
54	MG	DA	3385	1/1	0.91	0.19	59,59,59,59	0
54	MG	CA	1622	1/1	0.91	0.20	65,65,65,65	0
54	MG	AA	1610	1/1	0.91	0.13	64,64,64,64	0
54	MG	DA	3390	1/1	0.91	0.15	73,73,73,73	0
54	MG	BA	3676	1/1	0.91	0.17	46,46,46,46	0
54	MG	BA	3229	1/1	0.91	0.07	61,61,61,61	0
54	MG	DA	3397	1/1	0.91	0.11	59,59,59,59	0
54	MG	BA	3234	1/1	0.91	0.16	61,61,61,61	0
54	MG	DO	202	1/1	0.91	0.11	60,60,60,60	0
54	MG	BA	3419	1/1	0.91	0.08	29,29,29,29	0
54	MG	DQ	203	1/1	0.91	0.10	62,62,62,62	0
54	MG	AA	1786	1/1	0.91	0.08	89,89,89,89	0
54	MG	DT	202	1/1	0.91	0.08	62,62,62,62	0
54	MG	DA	3403	1/1	0.91	0.09	56,56,56,56	0
54	MG	CA	1763	1/1	0.91	0.07	66,66,66,66	0
54	MG	DA	3408	1/1	0.91	0.07	54,54,54,54	0
54	MG	DA	3135	1/1	0.91	0.23	59,59,59,59	0
54	MG	BA	3687	1/1	0.91	0.08	53,53,53,53	0
54	MG	DA	3382	1/1	0.92	0.13	57,57,57,57	0
54	MG	BB	217	1/1	0.92	0.08	66,66,66,66	0
54	MG	BB	219	1/1	0.92	0.09	54,54,54,54	0
54	MG	BD	301	1/1	0.92	0.11	51,51,51,51	0
54	MG	BA	3445	1/1	0.92	0.09	60,60,60,60	0
54	MG	BA	3582	1/1	0.92	0.13	66,66,66,66	0
54	MG	BA	3583	1/1	0.92	0.08	63,63,63,63	0
54	MG	BA	3587	1/1	0.92	0.06	60,60,60,60	0
54	MG	CA	1714	1/1	0.92	0.20	67,67,67,67	0
54	MG	DA	3101	1/1	0.92	0.20	60,60,60,60	0
54	MG	BF	301	1/1	0.92	0.12	40,40,40,40	0
54	MG	BA	3447	1/1	0.92	0.08	53,53,53,53	0
54	MG	DA	3401	1/1	0.92	0.12	56,56,56,56	0
54	MG	BA	3142	1/1	0.92	0.20	36,36,36,36	0
54	MG	AA	1676	1/1	0.92	0.10	86,86,86,86	0
54	MG	DA	3405	1/1	0.92	0.08	56,56,56,56	0
54	MG	BA	3145	1/1	0.92	0.10	33,33,33,33	0
54	MG	BA	3261	1/1	0.92	0.10	21,21,21,21	0
54	MG	DA	3111	1/1	0.92	0.10	44,44,44,44	0
54	MG	DA	3112	1/1	0.92	0.12	48,48,48,48	0
54	MG	BA	3263	1/1	0.92	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3596	1/1	0.92	0.10	59,59,59,59	0
54	MG	BA	3460	1/1	0.92	0.10	51,51,51,51	0
54	MG	BA	3146	1/1	0.92	0.13	34,34,34,34	0
54	MG	DA	3421	1/1	0.92	0.15	44,44,44,44	0
54	MG	CA	1740	1/1	0.92	0.20	72,72,72,72	0
54	MG	BV	204	1/1	0.92	0.08	67,67,67,67	0
54	MG	BA	3266	1/1	0.92	0.21	66,66,66,66	0
54	MG	BA	3465	1/1	0.92	0.10	24,24,24,24	0
54	MG	AD	303	1/1	0.92	0.11	84,84,84,84	0
54	MG	B2	101	1/1	0.92	0.15	46,46,46,46	0
54	MG	BA	3067	1/1	0.92	0.19	55,55,55,55	0
54	MG	BA	3476	1/1	0.92	0.15	55,55,55,55	0
54	MG	AE	201	1/1	0.92	0.21	62,62,62,62	0
54	MG	AF	201	1/1	0.92	0.11	53,53,53,53	0
54	MG	DA	3145	1/1	0.92	0.16	60,60,60,60	0
54	MG	AA	1735	1/1	0.92	0.18	62,62,62,62	0
54	MG	AA	1716	1/1	0.92	0.07	62,62,62,62	0
54	MG	BA	3286	1/1	0.92	0.08	42,42,42,42	0
54	MG	DA	3458	1/1	0.92	0.10	58,58,58,58	0
54	MG	AM	201	1/1	0.92	0.25	78,78,78,78	0
54	MG	BA	3492	1/1	0.92	0.07	57,57,57,57	0
54	MG	DA	3163	1/1	0.92	0.10	39,39,39,39	0
54	MG	AM	202	1/1	0.92	0.14	59,59,59,59	0
54	MG	DA	3166	1/1	0.92	0.09	56,56,56,56	0
54	MG	DA	3167	1/1	0.92	0.06	30,30,30,30	0
54	MG	DA	3472	1/1	0.92	0.10	73,73,73,73	0
54	MG	CA	1764	1/1	0.92	0.12	90,90,90,90	0
54	MG	CA	1766	1/1	0.92	0.13	65,65,65,65	0
54	MG	BA	3628	1/1	0.92	0.10	46,46,46,46	0
54	MG	DA	3176	1/1	0.92	0.18	37,37,37,37	0
54	MG	CA	1608	1/1	0.92	0.14	54,54,54,54	0
54	MG	DA	3489	1/1	0.92	0.08	48,48,48,48	0
54	MG	DA	3179	1/1	0.92	0.14	43,43,43,43	0
54	MG	CA	1772	1/1	0.92	0.10	61,61,61,61	0
54	MG	DA	3184	1/1	0.92	0.10	33,33,33,33	0
54	MG	BA	3167	1/1	0.92	0.12	45,45,45,45	0
54	MG	DA	3190	1/1	0.92	0.12	43,43,43,43	0
54	MG	AA	1687	1/1	0.92	0.20	79,79,79,79	0
54	MG	BA	3297	1/1	0.92	0.09	52,52,52,52	0
54	MG	BA	3298	1/1	0.92	0.09	43,43,43,43	0
54	MG	DA	3506	1/1	0.92	0.08	57,57,57,57	0
54	MG	BA	3101	1/1	0.92	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3508	1/1	0.92	0.08	73,73,73,73	0
54	MG	BA	3646	1/1	0.92	0.11	38,38,38,38	0
54	MG	CA	1780	1/1	0.92	0.20	74,74,74,74	0
54	MG	DA	3516	1/1	0.92	0.10	56,56,56,56	0
54	MG	BA	3305	1/1	0.92	0.08	67,67,67,67	0
54	MG	CA	1623	1/1	0.92	0.23	60,60,60,60	0
54	MG	DA	3217	1/1	0.92	0.11	54,54,54,54	0
54	MG	BA	3509	1/1	0.92	0.09	77,77,77,77	0
54	MG	BA	3172	1/1	0.92	0.07	65,65,65,65	0
54	MG	AA	1718	1/1	0.92	0.11	59,59,59,59	0
54	MG	DA	3532	1/1	0.92	0.10	58,58,58,58	0
54	MG	DA	3533	1/1	0.92	0.08	79,79,79,79	0
54	MG	DA	3535	1/1	0.92	0.09	67,67,67,67	0
54	MG	BA	3179	1/1	0.92	0.21	31,31,31,31	0
54	MG	BA	3104	1/1	0.92	0.20	27,27,27,27	0
54	MG	DA	3236	1/1	0.92	0.07	40,40,40,40	0
54	MG	DA	3540	1/1	0.92	0.09	48,48,48,48	0
54	MG	AA	1742	1/1	0.92	0.09	78,78,78,78	0
54	MG	AA	1703	1/1	0.92	0.14	64,64,64,64	0
54	MG	AA	1602	1/1	0.92	0.15	70,70,70,70	0
54	MG	BA	3204	1/1	0.92	0.13	47,47,47,47	0
54	MG	BA	3329	1/1	0.92	0.07	30,30,30,30	0
54	MG	DA	3262	1/1	0.92	0.09	55,55,55,55	0
54	MG	DA	3263	1/1	0.92	0.12	54,54,54,54	0
54	MG	BA	3331	1/1	0.92	0.10	47,47,47,47	0
54	MG	CA	1642	1/1	0.92	0.27	64,64,64,64	0
54	MG	DA	3274	1/1	0.92	0.07	51,51,51,51	0
54	MG	BA	3110	1/1	0.92	0.22	60,60,60,60	0
54	MG	AA	1706	1/1	0.92	0.21	59,59,59,59	0
54	MG	CE	201	1/1	0.92	0.11	78,78,78,78	0
54	MG	DA	3561	1/1	0.92	0.09	65,65,65,65	0
54	MG	CA	1646	1/1	0.92	0.17	71,71,71,71	0
54	MG	AA	1683	1/1	0.92	0.07	69,69,69,69	0
54	MG	DA	3566	1/1	0.92	0.14	70,70,70,70	0
54	MG	AA	1634	1/1	0.92	0.33	58,58,58,58	0
54	MG	BA	3540	1/1	0.92	0.13	64,64,64,64	0
54	MG	DA	3284	1/1	0.92	0.11	70,70,70,70	0
54	MG	BA	3544	1/1	0.92	0.09	60,60,60,60	0
54	MG	AA	1811	1/1	0.92	0.12	65,65,65,65	0
54	MG	BA	3705	1/1	0.92	0.08	57,57,57,57	0
54	MG	BA	3118	1/1	0.92	0.12	59,59,59,59	0
54	MG	BA	3547	1/1	0.92	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3550	1/1	0.92	0.08	50,50,50,50	0
54	MG	DA	3581	1/1	0.92	0.08	46,46,46,46	0
54	MG	DA	3295	1/1	0.92	0.13	58,58,58,58	0
54	MG	BA	3220	1/1	0.92	0.11	62,62,62,62	0
54	MG	AA	1726	1/1	0.92	0.10	75,75,75,75	0
54	MG	BA	3121	1/1	0.92	0.20	26,26,26,26	0
54	MG	BA	3382	1/1	0.92	0.13	39,39,39,39	0
54	MG	DA	3305	1/1	0.92	0.17	66,66,66,66	0
54	MG	DA	3030	1/1	0.92	0.37	63,63,63,63	0
54	MG	CA	1673	1/1	0.92	0.16	73,73,73,73	0
54	MG	DA	3036	1/1	0.92	0.12	62,62,62,62	0
54	MG	DA	3309	1/1	0.92	0.12	45,45,45,45	0
54	MG	DA	3611	1/1	0.92	0.15	57,57,57,57	0
54	MG	AA	1727	1/1	0.92	0.12	82,82,82,82	0
54	MG	DA	3314	1/1	0.92	0.07	31,31,31,31	0
54	MG	BA	3722	1/1	0.92	0.09	71,71,71,71	0
54	MG	CA	1680	1/1	0.92	0.10	92,92,92,92	0
54	MG	DA	3317	1/1	0.92	0.13	55,55,55,55	0
54	MG	DA	3622	1/1	0.92	0.11	80,80,80,80	0
54	MG	BA	3723	1/1	0.92	0.07	70,70,70,70	0
54	MG	DA	3319	1/1	0.92	0.08	53,53,53,53	0
54	MG	DA	3321	1/1	0.92	0.08	74,74,74,74	0
54	MG	DA	3046	1/1	0.92	0.08	58,58,58,58	0
54	MG	DA	3324	1/1	0.92	0.09	86,86,86,86	0
54	MG	DA	3325	1/1	0.92	0.06	72,72,72,72	0
54	MG	BA	3724	1/1	0.92	0.12	97,97,97,97	0
54	MG	BA	3725	1/1	0.92	0.07	57,57,57,57	0
54	MG	AA	1728	1/1	0.92	0.17	68,68,68,68	0
54	MG	DA	3636	1/1	0.92	0.09	66,66,66,66	0
54	MG	BA	3408	1/1	0.92	0.08	24,24,24,24	0
54	MG	DA	3060	1/1	0.92	0.08	57,57,57,57	0
54	MG	BA	3052	1/1	0.92	0.08	38,38,38,38	0
54	MG	DA	3066	1/1	0.92	0.21	51,51,51,51	0
54	MG	DA	3344	1/1	0.92	0.07	56,56,56,56	0
54	MG	BB	202	1/1	0.92	0.12	45,45,45,45	0
54	MG	DF	301	1/1	0.92	0.09	51,51,51,51	0
54	MG	DA	3074	1/1	0.92	0.21	46,46,46,46	0
54	MG	CA	1690	1/1	0.92	0.09	75,75,75,75	0
54	MG	BB	203	1/1	0.92	0.16	48,48,48,48	0
54	MG	BA	3573	1/1	0.92	0.08	54,54,54,54	0
54	MG	BA	3423	1/1	0.92	0.08	46,46,46,46	0
54	MG	DA	3362	1/1	0.92	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3055	1/1	0.92	0.14	44,44,44,44	0
54	MG	BA	3240	1/1	0.92	0.12	66,66,66,66	0
54	MG	DA	3370	1/1	0.92	0.13	87,87,87,87	0
54	MG	CA	1702	1/1	0.92	0.10	55,55,55,55	0
54	MG	DA	3089	1/1	0.92	0.17	50,50,50,50	0
54	MG	BA	3138	1/1	0.92	0.08	64,64,64,64	0
55	ZN	D4	101	1/1	0.92	0.09	173,173,173,173	0
54	MG	BA	3524	1/1	0.93	0.12	35,35,35,35	0
54	MG	CA	1691	1/1	0.93	0.15	74,74,74,74	0
54	MG	DA	3251	1/1	0.93	0.10	41,41,41,41	0
54	MG	BA	3525	1/1	0.93	0.13	47,47,47,47	0
54	MG	BH	201	1/1	0.93	0.16	60,60,60,60	0
54	MG	BA	3350	1/1	0.93	0.09	28,28,28,28	0
54	MG	BN	202	1/1	0.93	0.10	57,57,57,57	0
54	MG	DA	3039	1/1	0.93	0.10	57,57,57,57	0
54	MG	DA	3266	1/1	0.93	0.07	40,40,40,40	0
54	MG	BA	3035	1/1	0.93	0.08	23,23,23,23	0
54	MG	CA	1699	1/1	0.93	0.18	73,73,73,73	0
54	MG	BA	3371	1/1	0.93	0.10	26,26,26,26	0
54	MG	BA	3636	1/1	0.93	0.18	25,25,25,25	0
54	MG	BA	3637	1/1	0.93	0.15	81,81,81,81	0
54	MG	BS	201	1/1	0.93	0.16	63,63,63,63	0
54	MG	DA	3053	1/1	0.93	0.16	28,28,28,28	0
54	MG	BA	3638	1/1	0.93	0.09	82,82,82,82	0
54	MG	BA	3038	1/1	0.93	0.11	34,34,34,34	0
54	MG	DA	3063	1/1	0.93	0.22	47,47,47,47	0
54	MG	AA	1730	1/1	0.93	0.07	70,70,70,70	0
54	MG	BA	3642	1/1	0.93	0.09	46,46,46,46	0
54	MG	DA	3068	1/1	0.93	0.12	38,38,38,38	0
54	MG	DA	3503	1/1	0.93	0.07	59,59,59,59	0
54	MG	DA	3504	1/1	0.93	0.16	52,52,52,52	0
54	MG	DA	3291	1/1	0.93	0.14	64,64,64,64	0
54	MG	BA	3533	1/1	0.93	0.10	24,24,24,24	0
54	MG	BA	3644	1/1	0.93	0.12	35,35,35,35	0
54	MG	BA	3171	1/1	0.93	0.08	49,49,49,49	0
54	MG	BA	3650	1/1	0.93	0.11	53,53,53,53	0
54	MG	BA	3652	1/1	0.93	0.09	51,51,51,51	0
54	MG	B5	101	1/1	0.93	0.09	49,49,49,49	0
54	MG	DA	3517	1/1	0.93	0.14	52,52,52,52	0
54	MG	AA	1745	1/1	0.93	0.10	63,63,63,63	0
54	MG	CA	1725	1/1	0.93	0.13	91,91,91,91	0
54	MG	BA	3654	1/1	0.93	0.22	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3053	1/1	0.93	0.08	33,33,33,33	0
54	MG	CA	1730	1/1	0.93	0.08	65,65,65,65	0
54	MG	DA	3529	1/1	0.93	0.10	65,65,65,65	0
54	MG	BA	3392	1/1	0.93	0.17	29,29,29,29	0
54	MG	BA	3278	1/1	0.93	0.11	39,39,39,39	0
54	MG	AA	1731	1/1	0.93	0.17	72,72,72,72	0
54	MG	BA	3280	1/1	0.93	0.08	57,57,57,57	0
54	MG	BA	3186	1/1	0.93	0.12	30,30,30,30	0
54	MG	DA	3537	1/1	0.93	0.07	49,49,49,49	0
54	MG	BA	3283	1/1	0.93	0.09	36,36,36,36	0
54	MG	AA	1691	1/1	0.93	0.09	57,57,57,57	0
54	MG	AA	1765	1/1	0.93	0.13	57,57,57,57	0
54	MG	CA	1748	1/1	0.93	0.13	57,57,57,57	0
54	MG	BA	3557	1/1	0.93	0.08	25,25,25,25	0
54	MG	DA	3544	1/1	0.93	0.07	67,67,67,67	0
54	MG	DA	3322	1/1	0.93	0.22	61,61,61,61	0
54	MG	BA	3675	1/1	0.93	0.10	48,48,48,48	0
54	MG	DA	3104	1/1	0.93	0.19	51,51,51,51	0
54	MG	BA	3196	1/1	0.93	0.12	52,52,52,52	0
54	MG	CA	1615	1/1	0.93	0.17	42,42,42,42	0
54	MG	BA	3061	1/1	0.93	0.15	44,44,44,44	0
54	MG	DA	3330	1/1	0.93	0.09	56,56,56,56	0
54	MG	DA	3334	1/1	0.93	0.09	45,45,45,45	0
54	MG	CA	1620	1/1	0.93	0.27	74,74,74,74	0
54	MG	BA	3064	1/1	0.93	0.24	54,54,54,54	0
54	MG	BA	3292	1/1	0.93	0.07	36,36,36,36	0
54	MG	BA	3202	1/1	0.93	0.09	67,67,67,67	0
54	MG	DA	3562	1/1	0.93	0.09	65,65,65,65	0
54	MG	BA	3457	1/1	0.93	0.11	53,53,53,53	0
54	MG	DA	3342	1/1	0.93	0.09	40,40,40,40	0
54	MG	BA	3691	1/1	0.93	0.09	57,57,57,57	0
54	MG	BA	3294	1/1	0.93	0.06	32,32,32,32	0
54	MG	AA	1766	1/1	0.93	0.15	57,57,57,57	0
54	MG	DA	3571	1/1	0.93	0.10	53,53,53,53	0
54	MG	CA	1767	1/1	0.93	0.11	86,86,86,86	0
54	MG	BA	3130	1/1	0.93	0.14	79,79,79,79	0
54	MG	AA	1807	1/1	0.93	0.11	73,73,73,73	0
54	MG	BA	3710	1/1	0.93	0.10	63,63,63,63	0
54	MG	BA	3712	1/1	0.93	0.09	49,49,49,49	0
54	MG	DA	3137	1/1	0.93	0.19	45,45,45,45	0
54	MG	BA	3301	1/1	0.93	0.09	61,61,61,61	0
54	MG	CA	1638	1/1	0.93	0.39	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3582	1/1	0.93	0.10	83,83,83,83	0
54	MG	BA	3302	1/1	0.93	0.15	47,47,47,47	0
54	MG	DA	3586	1/1	0.93	0.06	142,142,142,142	0
54	MG	DA	3373	1/1	0.93	0.18	58,58,58,58	0
54	MG	BA	3070	1/1	0.93	0.16	39,39,39,39	0
54	MG	DA	3593	1/1	0.93	0.08	58,58,58,58	0
54	MG	BA	3137	1/1	0.93	0.10	45,45,45,45	0
54	MG	DA	3378	1/1	0.93	0.15	65,65,65,65	0
54	MG	DA	3380	1/1	0.93	0.07	47,47,47,47	0
54	MG	BA	3013	1/1	0.93	0.18	24,24,24,24	0
54	MG	BA	3139	1/1	0.93	0.07	55,55,55,55	0
54	MG	CA	1782	1/1	0.93	0.14	63,63,63,63	0
54	MG	DA	3386	1/1	0.93	0.12	64,64,64,64	0
54	MG	AA	1809	1/1	0.93	0.21	79,79,79,79	0
54	MG	DA	3612	1/1	0.93	0.20	49,49,49,49	0
54	MG	CA	1784	1/1	0.93	0.10	53,53,53,53	0
54	MG	BA	3480	1/1	0.93	0.10	58,58,58,58	0
54	MG	CA	1648	1/1	0.93	0.14	72,72,72,72	0
54	MG	DA	3165	1/1	0.93	0.07	36,36,36,36	0
54	MG	AA	1810	1/1	0.93	0.15	67,67,67,67	0
54	MG	BA	3080	1/1	0.93	0.17	42,42,42,42	0
54	MG	BA	3318	1/1	0.93	0.09	64,64,64,64	0
54	MG	BA	3016	1/1	0.93	0.07	44,44,44,44	0
54	MG	AA	1788	1/1	0.93	0.08	76,76,76,76	0
54	MG	BA	3597	1/1	0.93	0.08	36,36,36,36	0
54	MG	BA	3092	1/1	0.93	0.09	40,40,40,40	0
54	MG	BA	3330	1/1	0.93	0.10	45,45,45,45	0
54	MG	BA	3498	1/1	0.93	0.06	45,45,45,45	0
54	MG	AA	1669	1/1	0.93	0.14	80,80,80,80	0
54	MG	CA	1662	1/1	0.93	0.07	54,54,54,54	0
54	MG	DA	3188	1/1	0.93	0.08	51,51,51,51	0
54	MG	AA	1768	1/1	0.93	0.09	79,79,79,79	0
54	MG	AA	1648	1/1	0.93	0.20	73,73,73,73	0
54	MG	CA	1665	1/1	0.93	0.12	60,60,60,60	0
54	MG	CA	1666	1/1	0.93	0.08	71,71,71,71	0
54	MG	DA	3009	1/1	0.93	0.15	27,27,27,27	0
54	MG	BA	3610	1/1	0.93	0.12	36,36,36,36	0
54	MG	AA	1631	1/1	0.93	0.14	64,64,64,64	0
54	MG	BA	3614	1/1	0.93	0.23	47,47,47,47	0
54	MG	DF	305	1/1	0.93	0.10	74,74,74,74	0
54	MG	BA	3339	1/1	0.93	0.16	34,34,34,34	0
54	MG	DA	3015	1/1	0.93	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3340	1/1	0.93	0.07	38,38,38,38	0
54	MG	BA	3341	1/1	0.93	0.13	44,44,44,44	0
54	MG	AA	1627	1/1	0.93	0.11	58,58,58,58	0
54	MG	DA	3229	1/1	0.93	0.13	76,76,76,76	0
54	MG	DW	201	1/1	0.93	0.10	63,63,63,63	0
54	MG	BA	3163	1/1	0.93	0.27	30,30,30,30	0
54	MG	BE	305	1/1	0.93	0.10	35,35,35,35	0
54	MG	DA	3447	1/1	0.93	0.13	58,58,58,58	0
54	MG	AA	1758	1/1	0.93	0.14	48,48,48,48	0
54	MG	D9	102	1/1	0.93	0.17	51,51,51,51	0
54	MG	DA	3450	1/1	0.93	0.06	70,70,70,70	0
54	MG	BF	304	1/1	0.93	0.11	47,47,47,47	0
54	MG	CA	1649	1/1	0.94	0.23	67,67,67,67	0
54	MG	AA	1751	1/1	0.94	0.20	54,54,54,54	0
54	MG	BA	3184	1/1	0.94	0.13	37,37,37,37	0
54	MG	AA	1697	1/1	0.94	0.09	50,50,50,50	0
54	MG	DA	3174	1/1	0.94	0.06	24,24,24,24	0
54	MG	CA	1790	1/1	0.94	0.07	48,48,48,48	0
54	MG	BA	3125	1/1	0.94	0.08	39,39,39,39	0
54	MG	DA	3425	1/1	0.94	0.23	42,42,42,42	0
54	MG	AA	1815	1/1	0.94	0.13	72,72,72,72	0
54	MG	BA	3018	1/1	0.94	0.24	52,52,52,52	0
54	MG	DA	3434	1/1	0.94	0.10	60,60,60,60	0
54	MG	AA	1624	1/1	0.94	0.22	49,49,49,49	0
54	MG	AA	1754	1/1	0.94	0.07	49,49,49,49	0
54	MG	BA	3025	1/1	0.94	0.08	34,34,34,34	0
54	MG	BA	3077	1/1	0.94	0.07	43,43,43,43	0
54	MG	BA	3618	1/1	0.94	0.08	67,67,67,67	0
54	MG	DA	3442	1/1	0.94	0.16	59,59,59,59	0
54	MG	DA	3191	1/1	0.94	0.17	56,56,56,56	0
54	MG	BA	3522	1/1	0.94	0.17	53,53,53,53	0
54	MG	DA	3445	1/1	0.94	0.10	45,45,45,45	0
54	MG	DA	3194	1/1	0.94	0.10	22,22,22,22	0
54	MG	AA	1739	1/1	0.94	0.16	72,72,72,72	0
54	MG	BA	3395	1/1	0.94	0.05	37,37,37,37	0
54	MG	BD	305	1/1	0.94	0.06	46,46,46,46	0
54	MG	CA	1668	1/1	0.94	0.11	65,65,65,65	0
54	MG	CA	1669	1/1	0.94	0.09	71,71,71,71	0
54	MG	CA	1672	1/1	0.94	0.11	74,74,74,74	0
54	MG	BD	306	1/1	0.94	0.17	30,30,30,30	0
54	MG	CA	1674	1/1	0.94	0.11	80,80,80,80	0
54	MG	DA	3220	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3401	1/1	0.94	0.16	34,34,34,34	0
54	MG	DA	3224	1/1	0.94	0.08	60,60,60,60	0
54	MG	CA	1676	1/1	0.94	0.10	64,64,64,64	0
54	MG	DA	3227	1/1	0.94	0.06	39,39,39,39	0
54	MG	DA	3474	1/1	0.94	0.08	41,41,41,41	0
54	MG	DA	3476	1/1	0.94	0.07	95,95,95,95	0
54	MG	BA	3290	1/1	0.94	0.05	27,27,27,27	0
54	MG	BA	3418	1/1	0.94	0.13	28,28,28,28	0
54	MG	BA	3084	1/1	0.94	0.15	43,43,43,43	0
54	MG	DA	3481	1/1	0.94	0.12	51,51,51,51	0
54	MG	DA	3482	1/1	0.94	0.07	69,69,69,69	0
54	MG	DA	3483	1/1	0.94	0.08	63,63,63,63	0
54	MG	DA	3232	1/1	0.94	0.08	45,45,45,45	0
54	MG	DA	3019	1/1	0.94	0.10	46,46,46,46	0
54	MG	BA	3531	1/1	0.94	0.08	25,25,25,25	0
54	MG	BA	3140	1/1	0.94	0.11	44,44,44,44	0
54	MG	BA	3431	1/1	0.94	0.17	28,28,28,28	0
54	MG	BA	3141	1/1	0.94	0.08	67,67,67,67	0
54	MG	BA	3434	1/1	0.94	0.11	56,56,56,56	0
54	MG	DA	3498	1/1	0.94	0.10	39,39,39,39	0
54	MG	AA	1607	1/1	0.94	0.18	57,57,57,57	0
54	MG	BA	3538	1/1	0.94	0.12	55,55,55,55	0
54	MG	DA	3256	1/1	0.94	0.17	57,57,57,57	0
54	MG	DA	3257	1/1	0.94	0.17	40,40,40,40	0
54	MG	DA	3033	1/1	0.94	0.16	48,48,48,48	0
54	MG	DA	3035	1/1	0.94	0.07	43,43,43,43	0
54	MG	AA	1708	1/1	0.94	0.13	61,61,61,61	0
54	MG	AA	1713	1/1	0.94	0.10	61,61,61,61	0
54	MG	BA	3221	1/1	0.94	0.13	51,51,51,51	0
54	MG	DA	3273	1/1	0.94	0.07	93,93,93,93	0
54	MG	DA	3513	1/1	0.94	0.11	52,52,52,52	0
54	MG	BQ	204	1/1	0.94	0.08	46,46,46,46	0
54	MG	DA	3515	1/1	0.94	0.09	54,54,54,54	0
54	MG	BR	201	1/1	0.94	0.13	39,39,39,39	0
54	MG	BA	3227	1/1	0.94	0.15	55,55,55,55	0
54	MG	DA	3518	1/1	0.94	0.12	53,53,53,53	0
54	MG	DA	3043	1/1	0.94	0.15	64,64,64,64	0
54	MG	BA	3648	1/1	0.94	0.13	42,42,42,42	0
54	MG	BA	3094	1/1	0.94	0.22	33,33,33,33	0
54	MG	DA	3049	1/1	0.94	0.17	49,49,49,49	0
54	MG	BA	3303	1/1	0.94	0.10	40,40,40,40	0
54	MG	AA	1743	1/1	0.94	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3052	1/1	0.94	0.09	35,35,35,35	0
54	MG	BV	203	1/1	0.94	0.07	56,56,56,56	0
54	MG	BA	3551	1/1	0.94	0.11	60,60,60,60	0
54	MG	DA	3057	1/1	0.94	0.18	53,53,53,53	0
54	MG	BA	3232	1/1	0.94	0.09	24,24,24,24	0
54	MG	AA	1744	1/1	0.94	0.14	74,74,74,74	0
54	MG	BA	3037	1/1	0.94	0.13	33,33,33,33	0
54	MG	AA	1761	1/1	0.94	0.12	65,65,65,65	0
54	MG	BA	3661	1/1	0.94	0.09	40,40,40,40	0
54	MG	B3	101	1/1	0.94	0.12	54,54,54,54	0
54	MG	DA	3070	1/1	0.94	0.17	51,51,51,51	0
54	MG	DA	3300	1/1	0.94	0.06	29,29,29,29	0
54	MG	DA	3545	1/1	0.94	0.07	53,53,53,53	0
54	MG	DA	3072	1/1	0.94	0.26	60,60,60,60	0
54	MG	CA	1716	1/1	0.94	0.12	49,49,49,49	0
54	MG	DA	3075	1/1	0.94	0.07	48,48,48,48	0
54	MG	CA	1718	1/1	0.94	0.08	76,76,76,76	0
54	MG	BA	3561	1/1	0.94	0.07	46,46,46,46	0
54	MG	DA	3552	1/1	0.94	0.18	56,56,56,56	0
54	MG	BA	3665	1/1	0.94	0.09	72,72,72,72	0
54	MG	DA	3310	1/1	0.94	0.16	47,47,47,47	0
54	MG	DA	3311	1/1	0.94	0.07	31,31,31,31	0
54	MG	DA	3080	1/1	0.94	0.13	48,48,48,48	0
54	MG	BA	3562	1/1	0.94	0.06	34,34,34,34	0
54	MG	AA	1629	1/1	0.94	0.30	59,59,59,59	0
54	MG	CA	1724	1/1	0.94	0.13	60,60,60,60	0
54	MG	B9	104	1/1	0.94	0.11	52,52,52,52	0
54	MG	DA	3087	1/1	0.94	0.14	52,52,52,52	0
54	MG	BA	3670	1/1	0.94	0.09	65,65,65,65	0
54	MG	BA	3042	1/1	0.94	0.13	27,27,27,27	0
54	MG	DA	3568	1/1	0.94	0.06	62,62,62,62	0
54	MG	BA	3107	1/1	0.94	0.20	47,47,47,47	0
54	MG	CA	1731	1/1	0.94	0.10	62,62,62,62	0
54	MG	BA	3673	1/1	0.94	0.10	69,69,69,69	0
54	MG	BA	3468	1/1	0.94	0.18	63,63,63,63	0
54	MG	BA	3321	1/1	0.94	0.13	77,77,77,77	0
54	MG	DA	3327	1/1	0.94	0.07	66,66,66,66	0
54	MG	BA	3471	1/1	0.94	0.07	50,50,50,50	0
54	MG	DA	3097	1/1	0.94	0.08	30,30,30,30	0
54	MG	BA	3474	1/1	0.94	0.12	63,63,63,63	0
54	MG	BA	3244	1/1	0.94	0.10	49,49,49,49	0
54	MG	BA	3682	1/1	0.94	0.06	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3323	1/1	0.94	0.16	57,57,57,57	0
54	MG	BA	3578	1/1	0.94	0.08	49,49,49,49	0
54	MG	BA	3685	1/1	0.94	0.15	69,69,69,69	0
54	MG	DA	3105	1/1	0.94	0.21	54,54,54,54	0
54	MG	DA	3343	1/1	0.94	0.09	54,54,54,54	0
54	MG	BA	3044	1/1	0.94	0.27	53,53,53,53	0
54	MG	DA	3346	1/1	0.94	0.10	57,57,57,57	0
54	MG	CA	1618	1/1	0.94	0.17	61,61,61,61	0
54	MG	CA	1753	1/1	0.94	0.21	74,74,74,74	0
54	MG	DA	3349	1/1	0.94	0.07	55,55,55,55	0
54	MG	BA	3002	1/1	0.94	0.10	60,60,60,60	0
54	MG	BA	3692	1/1	0.94	0.06	38,38,38,38	0
54	MG	BA	3701	1/1	0.94	0.07	34,34,34,34	0
54	MG	DA	3357	1/1	0.94	0.07	45,45,45,45	0
54	MG	DA	3114	1/1	0.94	0.08	36,36,36,36	0
54	MG	DA	3361	1/1	0.94	0.13	40,40,40,40	0
54	MG	BA	3252	1/1	0.94	0.08	52,52,52,52	0
54	MG	DA	3363	1/1	0.94	0.08	51,51,51,51	0
54	MG	BA	3483	1/1	0.94	0.13	31,31,31,31	0
54	MG	DA	3367	1/1	0.94	0.09	67,67,67,67	0
54	MG	BA	3586	1/1	0.94	0.11	39,39,39,39	0
54	MG	BA	3484	1/1	0.94	0.05	41,41,41,41	0
54	MG	BA	3256	1/1	0.94	0.10	38,38,38,38	0
54	MG	DA	3372	1/1	0.94	0.15	79,79,79,79	0
54	MG	DA	3126	1/1	0.94	0.23	56,56,56,56	0
54	MG	BA	3711	1/1	0.94	0.14	52,52,52,52	0
54	MG	DA	3629	1/1	0.94	0.07	80,80,80,80	0
54	MG	DA	3376	1/1	0.94	0.07	73,73,73,73	0
54	MG	DA	3131	1/1	0.94	0.19	25,25,25,25	0
54	MG	DA	3132	1/1	0.94	0.13	54,54,54,54	0
54	MG	AA	1679	1/1	0.94	0.14	58,58,58,58	0
54	MG	DA	3381	1/1	0.94	0.08	55,55,55,55	0
54	MG	BA	3713	1/1	0.94	0.06	35,35,35,35	0
54	MG	CA	1633	1/1	0.94	0.15	50,50,50,50	0
54	MG	CA	1769	1/1	0.94	0.06	58,58,58,58	0
54	MG	BA	3490	1/1	0.94	0.07	74,74,74,74	0
54	MG	CA	1636	1/1	0.94	0.23	58,58,58,58	0
54	MG	DD	301	1/1	0.94	0.06	61,61,61,61	0
54	MG	AA	1749	1/1	0.94	0.09	58,58,58,58	0
54	MG	DD	304	1/1	0.94	0.08	39,39,39,39	0
54	MG	DE	301	1/1	0.94	0.06	29,29,29,29	0
54	MG	BA	3593	1/1	0.94	0.26	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1775	1/1	0.94	0.14	78,78,78,78	0
54	MG	DF	304	1/1	0.94	0.07	41,41,41,41	0
54	MG	DA	3394	1/1	0.94	0.09	59,59,59,59	0
54	MG	BA	3007	1/1	0.94	0.08	41,41,41,41	0
54	MG	DA	3146	1/1	0.94	0.18	55,55,55,55	0
54	MG	CA	1640	1/1	0.94	0.15	63,63,63,63	0
54	MG	BA	3116	1/1	0.94	0.09	50,50,50,50	0
54	MG	BA	3012	1/1	0.94	0.13	37,37,37,37	0
54	MG	DA	3151	1/1	0.94	0.08	31,31,31,31	0
54	MG	BA	3720	1/1	0.94	0.07	64,64,64,64	0
54	MG	DA	3157	1/1	0.94	0.08	33,33,33,33	0
54	MG	AA	1789	1/1	0.94	0.10	78,78,78,78	0
54	MG	DA	3406	1/1	0.94	0.10	54,54,54,54	0
54	MG	BA	3599	1/1	0.94	0.11	63,63,63,63	0
54	MG	BA	3269	1/1	0.94	0.18	51,51,51,51	0
54	MG	BA	3601	1/1	0.94	0.12	43,43,43,43	0
54	MG	DA	3411	1/1	0.94	0.07	89,89,89,89	0
54	MG	BR	205	1/1	0.95	0.10	45,45,45,45	0
54	MG	BA	3541	1/1	0.95	0.11	21,21,21,21	0
54	MG	AA	1670	1/1	0.95	0.12	56,56,56,56	0
54	MG	BV	201	1/1	0.95	0.25	30,30,30,30	0
54	MG	DA	3239	1/1	0.95	0.07	46,46,46,46	0
54	MG	DA	3240	1/1	0.95	0.06	56,56,56,56	0
54	MG	DA	3241	1/1	0.95	0.08	47,47,47,47	0
54	MG	DA	3242	1/1	0.95	0.06	36,36,36,36	0
54	MG	DA	3044	1/1	0.95	0.16	55,55,55,55	0
54	MG	DA	3245	1/1	0.95	0.08	37,37,37,37	0
54	MG	BA	3218	1/1	0.95	0.07	56,56,56,56	0
54	MG	DA	3453	1/1	0.95	0.05	49,49,49,49	0
54	MG	BA	3103	1/1	0.95	0.23	33,33,33,33	0
54	MG	DA	3250	1/1	0.95	0.14	38,38,38,38	0
54	MG	AA	1673	1/1	0.95	0.11	76,76,76,76	0
54	MG	DA	3252	1/1	0.95	0.06	45,45,45,45	0
54	MG	BA	3549	1/1	0.95	0.09	22,22,22,22	0
54	MG	DA	3254	1/1	0.95	0.19	39,39,39,39	0
54	MG	AA	1614	1/1	0.95	0.07	42,42,42,42	0
54	MG	DA	3468	1/1	0.95	0.10	66,66,66,66	0
54	MG	BA	3224	1/1	0.95	0.05	28,28,28,28	0
54	MG	B0	104	1/1	0.95	0.06	49,49,49,49	0
54	MG	DA	3258	1/1	0.95	0.10	35,35,35,35	0
54	MG	DA	3260	1/1	0.95	0.13	57,57,57,57	0
54	MG	B1	101	1/1	0.95	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3448	1/1	0.95	0.11	46,46,46,46	0
54	MG	BA	3226	1/1	0.95	0.11	49,49,49,49	0
54	MG	BA	3058	1/1	0.95	0.24	57,57,57,57	0
54	MG	DA	3268	1/1	0.95	0.08	54,54,54,54	0
54	MG	DA	3271	1/1	0.95	0.06	42,42,42,42	0
54	MG	DA	3064	1/1	0.95	0.12	36,36,36,36	0
54	MG	AA	1709	1/1	0.95	0.12	57,57,57,57	0
54	MG	DA	3488	1/1	0.95	0.12	46,46,46,46	0
54	MG	B3	103	1/1	0.95	0.11	38,38,38,38	0
54	MG	DA	3490	1/1	0.95	0.07	60,60,60,60	0
54	MG	DA	3492	1/1	0.95	0.12	59,59,59,59	0
54	MG	DA	3067	1/1	0.95	0.29	58,58,58,58	0
54	MG	BA	3060	1/1	0.95	0.14	49,49,49,49	0
54	MG	AA	1710	1/1	0.95	0.17	52,52,52,52	0
54	MG	B7	101	1/1	0.95	0.09	45,45,45,45	0
54	MG	B8	101	1/1	0.95	0.14	45,45,45,45	0
54	MG	BA	3156	1/1	0.95	0.09	28,28,28,28	0
54	MG	BA	3566	1/1	0.95	0.11	48,48,48,48	0
54	MG	CA	1727	1/1	0.95	0.16	63,63,63,63	0
54	MG	BA	3459	1/1	0.95	0.20	57,57,57,57	0
54	MG	BA	3568	1/1	0.95	0.11	35,35,35,35	0
54	MG	BA	3022	1/1	0.95	0.07	38,38,38,38	0
54	MG	BA	3237	1/1	0.95	0.07	41,41,41,41	0
54	MG	CA	1733	1/1	0.95	0.09	89,89,89,89	0
54	MG	CA	1735	1/1	0.95	0.09	85,85,85,85	0
54	MG	BA	3678	1/1	0.95	0.23	47,47,47,47	0
54	MG	BA	3312	1/1	0.95	0.06	32,32,32,32	0
54	MG	BA	3463	1/1	0.95	0.08	38,38,38,38	0
54	MG	AA	1775	1/1	0.95	0.07	63,63,63,63	0
54	MG	AA	1692	1/1	0.95	0.11	66,66,66,66	0
54	MG	DA	3299	1/1	0.95	0.06	33,33,33,33	0
54	MG	BA	3317	1/1	0.95	0.10	69,69,69,69	0
54	MG	CA	1743	1/1	0.95	0.13	65,65,65,65	0
54	MG	DA	3520	1/1	0.95	0.04	74,74,74,74	0
54	MG	BA	3027	1/1	0.95	0.06	32,32,32,32	0
54	MG	BA	3688	1/1	0.95	0.07	72,72,72,72	0
54	MG	CA	1614	1/1	0.95	0.13	70,70,70,70	0
54	MG	BA	3689	1/1	0.95	0.07	55,55,55,55	0
54	MG	DA	3528	1/1	0.95	0.07	36,36,36,36	0
54	MG	BA	3690	1/1	0.95	0.06	42,42,42,42	0
54	MG	BA	3071	1/1	0.95	0.14	46,46,46,46	0
54	MG	DA	3531	1/1	0.95	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1619	1/1	0.95	0.25	56,56,56,56	0
54	MG	AA	1653	1/1	0.95	0.16	64,64,64,64	0
54	MG	BA	3581	1/1	0.95	0.09	42,42,42,42	0
54	MG	BA	3245	1/1	0.95	0.08	29,29,29,29	0
54	MG	BA	3247	1/1	0.95	0.09	45,45,45,45	0
54	MG	BA	3585	1/1	0.95	0.11	65,65,65,65	0
54	MG	DA	3107	1/1	0.95	0.18	38,38,38,38	0
54	MG	CA	1760	1/1	0.95	0.18	93,93,93,93	0
54	MG	DA	3320	1/1	0.95	0.06	54,54,54,54	0
54	MG	BA	3328	1/1	0.95	0.06	49,49,49,49	0
54	MG	BA	3170	1/1	0.95	0.07	38,38,38,38	0
54	MG	BA	3119	1/1	0.95	0.10	57,57,57,57	0
54	MG	CA	1628	1/1	0.95	0.11	71,71,71,71	0
54	MG	DA	3113	1/1	0.95	0.20	56,56,56,56	0
54	MG	BA	3589	1/1	0.95	0.06	41,41,41,41	0
54	MG	AA	1701	1/1	0.95	0.09	68,68,68,68	0
54	MG	BA	3173	1/1	0.95	0.07	63,63,63,63	0
54	MG	DA	3329	1/1	0.95	0.13	34,34,34,34	0
54	MG	AA	1729	1/1	0.95	0.09	55,55,55,55	0
54	MG	CA	1770	1/1	0.95	0.12	71,71,71,71	0
54	MG	BA	3122	1/1	0.95	0.08	46,46,46,46	0
54	MG	BA	3338	1/1	0.95	0.10	49,49,49,49	0
54	MG	DA	3557	1/1	0.95	0.26	55,55,55,55	0
54	MG	DA	3128	1/1	0.95	0.16	47,47,47,47	0
54	MG	DA	3339	1/1	0.95	0.06	53,53,53,53	0
54	MG	DA	3560	1/1	0.95	0.09	57,57,57,57	0
54	MG	AA	1702	1/1	0.95	0.10	67,67,67,67	0
54	MG	BA	3264	1/1	0.95	0.07	86,86,86,86	0
54	MG	BA	3079	1/1	0.95	0.16	45,45,45,45	0
54	MG	BA	3494	1/1	0.95	0.10	52,52,52,52	0
54	MG	BA	3187	1/1	0.95	0.20	69,69,69,69	0
54	MG	DA	3567	1/1	0.95	0.07	57,57,57,57	0
54	MG	DA	3345	1/1	0.95	0.12	56,56,56,56	0
54	MG	BA	3344	1/1	0.95	0.09	41,41,41,41	0
54	MG	BA	3188	1/1	0.95	0.11	47,47,47,47	0
54	MG	CA	1644	1/1	0.95	0.23	63,63,63,63	0
54	MG	DA	3572	1/1	0.95	0.05	45,45,45,45	0
54	MG	DA	3138	1/1	0.95	0.29	49,49,49,49	0
54	MG	DA	3139	1/1	0.95	0.21	53,53,53,53	0
54	MG	BA	3604	1/1	0.95	0.14	43,43,43,43	0
54	MG	BA	3268	1/1	0.95	0.08	52,52,52,52	0
54	MG	DA	3356	1/1	0.95	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1781	1/1	0.95	0.14	71,71,71,71	0
54	MG	BA	3729	1/1	0.95	0.13	42,42,42,42	0
54	MG	DA	3360	1/1	0.95	0.07	36,36,36,36	0
54	MG	BA	3353	1/1	0.95	0.07	51,51,51,51	0
54	MG	BA	3505	1/1	0.95	0.08	38,38,38,38	0
54	MG	DA	3584	1/1	0.95	0.07	37,37,37,37	0
54	MG	BA	3355	1/1	0.95	0.13	51,51,51,51	0
54	MG	DA	3364	1/1	0.95	0.08	54,54,54,54	0
54	MG	BA	3611	1/1	0.95	0.07	32,32,32,32	0
54	MG	BA	3359	1/1	0.95	0.16	19,19,19,19	0
54	MG	AA	1784	1/1	0.95	0.26	63,63,63,63	0
54	MG	DA	3595	1/1	0.95	0.11	90,90,90,90	0
54	MG	BA	3363	1/1	0.95	0.16	48,48,48,48	0
54	MG	BB	215	1/1	0.95	0.09	57,57,57,57	0
54	MG	CA	1794	1/1	0.95	0.09	57,57,57,57	0
54	MG	DA	3161	1/1	0.95	0.09	47,47,47,47	0
54	MG	BA	3365	1/1	0.95	0.10	33,33,33,33	0
54	MG	AA	1747	1/1	0.95	0.16	60,60,60,60	0
54	MG	DA	3610	1/1	0.95	0.12	79,79,79,79	0
54	MG	AA	1638	1/1	0.95	0.11	64,64,64,64	0
54	MG	BA	3519	1/1	0.95	0.07	26,26,26,26	0
54	MG	DA	3379	1/1	0.95	0.10	69,69,69,69	0
54	MG	BD	304	1/1	0.95	0.07	19,19,19,19	0
54	MG	BA	3520	1/1	0.95	0.14	29,29,29,29	0
54	MG	AA	1750	1/1	0.95	0.14	55,55,55,55	0
54	MG	DA	3173	1/1	0.95	0.06	34,34,34,34	0
54	MG	BA	3625	1/1	0.95	0.13	52,52,52,52	0
54	MG	DA	3001	1/1	0.95	0.07	38,38,38,38	0
54	MG	DA	3003	1/1	0.95	0.18	34,34,34,34	0
54	MG	CA	1667	1/1	0.95	0.19	66,66,66,66	0
54	MG	AA	1812	1/1	0.95	0.07	82,82,82,82	0
54	MG	DA	3391	1/1	0.95	0.17	62,62,62,62	0
54	MG	DA	3392	1/1	0.95	0.08	43,43,43,43	0
54	MG	DA	3007	1/1	0.95	0.23	59,59,59,59	0
54	MG	BE	302	1/1	0.95	0.15	29,29,29,29	0
54	MG	CA	1671	1/1	0.95	0.07	78,78,78,78	0
54	MG	DA	3187	1/1	0.95	0.09	44,44,44,44	0
54	MG	BA	3203	1/1	0.95	0.15	39,39,39,39	0
54	MG	DA	3637	1/1	0.95	0.14	63,63,63,63	0
54	MG	BA	3096	1/1	0.95	0.07	36,36,36,36	0
54	MG	DB	204	1/1	0.95	0.15	65,65,65,65	0
54	MG	BA	3284	1/1	0.95	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3097	1/1	0.95	0.06	40,40,40,40	0
54	MG	BA	3099	1/1	0.95	0.16	47,47,47,47	0
54	MG	DB	209	1/1	0.95	0.14	67,67,67,67	0
54	MG	BA	3047	1/1	0.95	0.06	30,30,30,30	0
54	MG	BF	306	1/1	0.95	0.08	61,61,61,61	0
54	MG	DD	302	1/1	0.95	0.06	32,32,32,32	0
54	MG	BA	3409	1/1	0.95	0.07	26,26,26,26	0
54	MG	BA	3415	1/1	0.95	0.11	26,26,26,26	0
54	MG	DD	305	1/1	0.95	0.08	56,56,56,56	0
54	MG	DA	3201	1/1	0.95	0.06	29,29,29,29	0
54	MG	DA	3203	1/1	0.95	0.07	36,36,36,36	0
54	MG	CA	1683	1/1	0.95	0.08	71,71,71,71	0
54	MG	DF	303	1/1	0.95	0.09	56,56,56,56	0
54	MG	DA	3412	1/1	0.95	0.13	75,75,75,75	0
54	MG	DA	3207	1/1	0.95	0.09	27,27,27,27	0
54	MG	DA	3208	1/1	0.95	0.07	31,31,31,31	0
54	MG	AA	1664	1/1	0.95	0.10	74,74,74,74	0
54	MG	BA	3535	1/1	0.95	0.08	58,58,58,58	0
54	MG	DP	202	1/1	0.95	0.07	53,53,53,53	0
54	MG	DP	203	1/1	0.95	0.12	61,61,61,61	0
54	MG	BA	3289	1/1	0.95	0.13	58,58,58,58	0
54	MG	CA	1687	1/1	0.95	0.13	68,68,68,68	0
54	MG	DA	3422	1/1	0.95	0.06	71,71,71,71	0
54	MG	BA	3215	1/1	0.95	0.10	41,41,41,41	0
54	MG	DA	3223	1/1	0.95	0.07	39,39,39,39	0
54	MG	BA	3645	1/1	0.95	0.10	59,59,59,59	0
54	MG	DA	3225	1/1	0.95	0.08	53,53,53,53	0
54	MG	BA	3425	1/1	0.95	0.15	38,38,38,38	0
54	MG	D8	102	1/1	0.95	0.10	66,66,66,66	0
54	MG	BR	202	1/1	0.95	0.11	35,35,35,35	0
54	MG	BA	3428	1/1	0.95	0.13	23,23,23,23	0
54	MG	BA	3216	1/1	0.95	0.20	64,64,64,64	0
54	MG	CA	1700	1/1	0.96	0.08	56,56,56,56	0
54	MG	DA	3448	1/1	0.96	0.19	53,53,53,53	0
54	MG	CA	1701	1/1	0.96	0.09	74,74,74,74	0
54	MG	DA	3248	1/1	0.96	0.09	59,59,59,59	0
54	MG	DA	3048	1/1	0.96	0.18	50,50,50,50	0
54	MG	DA	3452	1/1	0.96	0.17	45,45,45,45	0
54	MG	BA	3647	1/1	0.96	0.07	59,59,59,59	0
54	MG	BT	203	1/1	0.96	0.04	51,51,51,51	0
54	MG	DA	3455	1/1	0.96	0.10	34,34,34,34	0
54	MG	DA	3456	1/1	0.96	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3457	1/1	0.96	0.05	59,59,59,59	0
54	MG	CA	1704	1/1	0.96	0.17	71,71,71,71	0
54	MG	AA	1657	1/1	0.96	0.12	51,51,51,51	0
54	MG	BA	3422	1/1	0.96	0.05	33,33,33,33	0
54	MG	BA	3651	1/1	0.96	0.15	34,34,34,34	0
54	MG	DA	3056	1/1	0.96	0.04	31,31,31,31	0
54	MG	CA	1708	1/1	0.96	0.10	73,73,73,73	0
54	MG	DA	3058	1/1	0.96	0.06	38,38,38,38	0
54	MG	DA	3059	1/1	0.96	0.09	43,43,43,43	0
54	MG	BA	3296	1/1	0.96	0.15	40,40,40,40	0
54	MG	CA	1710	1/1	0.96	0.16	55,55,55,55	0
54	MG	DA	3475	1/1	0.96	0.07	60,60,60,60	0
54	MG	AA	1684	1/1	0.96	0.06	43,43,43,43	0
54	MG	BY	202	1/1	0.96	0.16	49,49,49,49	0
54	MG	AA	1640	1/1	0.96	0.15	70,70,70,70	0
54	MG	BZ	302	1/1	0.96	0.17	45,45,45,45	0
54	MG	AA	1763	1/1	0.96	0.12	73,73,73,73	0
54	MG	BA	3542	1/1	0.96	0.06	33,33,33,33	0
54	MG	BA	3300	1/1	0.96	0.11	54,54,54,54	0
54	MG	BA	3658	1/1	0.96	0.12	61,61,61,61	0
54	MG	DA	3485	1/1	0.96	0.10	33,33,33,33	0
54	MG	AA	1637	1/1	0.96	0.15	64,64,64,64	0
54	MG	DA	3487	1/1	0.96	0.16	65,65,65,65	0
54	MG	DA	3277	1/1	0.96	0.07	60,60,60,60	0
54	MG	DA	3278	1/1	0.96	0.07	71,71,71,71	0
54	MG	BA	3435	1/1	0.96	0.05	40,40,40,40	0
54	MG	BA	3662	1/1	0.96	0.08	26,26,26,26	0
54	MG	AA	1798	1/1	0.96	0.06	67,67,67,67	0
54	MG	DA	3078	1/1	0.96	0.16	41,41,41,41	0
54	MG	BA	3441	1/1	0.96	0.08	58,58,58,58	0
54	MG	CA	1726	1/1	0.96	0.10	77,77,77,77	0
54	MG	BA	3023	1/1	0.96	0.07	43,43,43,43	0
54	MG	BA	3668	1/1	0.96	0.06	60,60,60,60	0
54	MG	BA	3231	1/1	0.96	0.07	35,35,35,35	0
54	MG	DA	3289	1/1	0.96	0.09	44,44,44,44	0
54	MG	DA	3085	1/1	0.96	0.22	60,60,60,60	0
54	MG	BA	3552	1/1	0.96	0.09	26,26,26,26	0
54	MG	BA	3554	1/1	0.96	0.05	41,41,41,41	0
54	MG	CA	1732	1/1	0.96	0.15	63,63,63,63	0
54	MG	BA	3555	1/1	0.96	0.07	23,23,23,23	0
54	MG	CA	1734	1/1	0.96	0.16	79,79,79,79	0
54	MG	BA	3446	1/1	0.96	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3510	1/1	0.96	0.08	46,46,46,46	0
54	MG	DA	3512	1/1	0.96	0.08	43,43,43,43	0
54	MG	BA	3157	1/1	0.96	0.11	36,36,36,36	0
54	MG	BA	3159	1/1	0.96	0.12	44,44,44,44	0
54	MG	CA	1738	1/1	0.96	0.10	52,52,52,52	0
54	MG	BA	3063	1/1	0.96	0.09	31,31,31,31	0
54	MG	DA	3303	1/1	0.96	0.06	46,46,46,46	0
54	MG	DA	3304	1/1	0.96	0.04	39,39,39,39	0
54	MG	BA	3450	1/1	0.96	0.05	24,24,24,24	0
54	MG	BA	3236	1/1	0.96	0.06	27,27,27,27	0
54	MG	DA	3521	1/1	0.96	0.06	43,43,43,43	0
54	MG	DA	3099	1/1	0.96	0.05	54,54,54,54	0
54	MG	AA	1642	1/1	0.96	0.09	53,53,53,53	0
54	MG	BA	3565	1/1	0.96	0.08	57,57,57,57	0
54	MG	BA	3066	1/1	0.96	0.05	41,41,41,41	0
54	MG	DA	3526	1/1	0.96	0.06	42,42,42,42	0
54	MG	CA	1745	1/1	0.96	0.19	52,52,52,52	0
54	MG	CA	1611	1/1	0.96	0.20	56,56,56,56	0
54	MG	DA	3313	1/1	0.96	0.07	34,34,34,34	0
54	MG	CA	1747	1/1	0.96	0.07	63,63,63,63	0
54	MG	BA	3455	1/1	0.96	0.05	41,41,41,41	0
54	MG	AA	1661	1/1	0.96	0.13	62,62,62,62	0
54	MG	DA	3534	1/1	0.96	0.11	53,53,53,53	0
54	MG	AA	1782	1/1	0.96	0.06	59,59,59,59	0
54	MG	BA	3241	1/1	0.96	0.16	56,56,56,56	0
54	MG	BA	3028	1/1	0.96	0.05	34,34,34,34	0
54	MG	CA	1617	1/1	0.96	0.27	63,63,63,63	0
54	MG	BA	3572	1/1	0.96	0.07	44,44,44,44	0
54	MG	BA	3243	1/1	0.96	0.09	31,31,31,31	0
54	MG	BA	3114	1/1	0.96	0.06	39,39,39,39	0
54	MG	DA	3116	1/1	0.96	0.16	26,26,26,26	0
54	MG	BA	3700	1/1	0.96	0.07	41,41,41,41	0
54	MG	DA	3120	1/1	0.96	0.15	47,47,47,47	0
54	MG	AA	1783	1/1	0.96	0.20	71,71,71,71	0
54	MG	BA	3464	1/1	0.96	0.05	28,28,28,28	0
54	MG	DA	3548	1/1	0.96	0.06	54,54,54,54	0
54	MG	DA	3123	1/1	0.96	0.15	48,48,48,48	0
54	MG	AA	1668	1/1	0.96	0.06	52,52,52,52	0
54	MG	DA	3333	1/1	0.96	0.07	54,54,54,54	0
54	MG	BA	3466	1/1	0.96	0.13	78,78,78,78	0
54	MG	BA	3707	1/1	0.96	0.07	49,49,49,49	0
54	MG	AP	101	1/1	0.96	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1720	1/1	0.96	0.13	74,74,74,74	0
54	MG	BA	3177	1/1	0.96	0.08	41,41,41,41	0
54	MG	BA	3076	1/1	0.96	0.20	58,58,58,58	0
54	MG	BA	3473	1/1	0.96	0.09	54,54,54,54	0
54	MG	BA	3257	1/1	0.96	0.07	21,21,21,21	0
54	MG	CA	1634	1/1	0.96	0.08	40,40,40,40	0
54	MG	BA	3180	1/1	0.96	0.10	42,42,42,42	0
54	MG	BA	3034	1/1	0.96	0.17	40,40,40,40	0
54	MG	BA	3185	1/1	0.96	0.06	44,44,44,44	0
54	MG	DA	3564	1/1	0.96	0.13	61,61,61,61	0
54	MG	BA	3078	1/1	0.96	0.10	45,45,45,45	0
54	MG	BA	3123	1/1	0.96	0.10	48,48,48,48	0
54	MG	BA	3342	1/1	0.96	0.05	43,43,43,43	0
54	MG	DA	3142	1/1	0.96	0.16	48,48,48,48	0
54	MG	AA	1643	1/1	0.96	0.07	56,56,56,56	0
54	MG	AA	1787	1/1	0.96	0.10	54,54,54,54	0
54	MG	DA	3355	1/1	0.96	0.09	67,67,67,67	0
54	MG	BA	3190	1/1	0.96	0.13	36,36,36,36	0
54	MG	BA	3081	1/1	0.96	0.10	38,38,38,38	0
54	MG	DA	3358	1/1	0.96	0.06	59,59,59,59	0
54	MG	BA	3270	1/1	0.96	0.06	51,51,51,51	0
54	MG	BA	3351	1/1	0.96	0.06	49,49,49,49	0
54	MG	BA	3352	1/1	0.96	0.06	37,37,37,37	0
54	MG	BA	3274	1/1	0.96	0.13	48,48,48,48	0
54	MG	BA	3602	1/1	0.96	0.05	43,43,43,43	0
54	MG	DA	3154	1/1	0.96	0.08	47,47,47,47	0
54	MG	CA	1788	1/1	0.96	0.07	51,51,51,51	0
54	MG	DA	3366	1/1	0.96	0.14	41,41,41,41	0
54	MG	BA	3275	1/1	0.96	0.12	31,31,31,31	0
54	MG	DA	3585	1/1	0.96	0.14	36,36,36,36	0
54	MG	BA	3357	1/1	0.96	0.16	40,40,40,40	0
54	MG	DA	3590	1/1	0.96	0.09	59,59,59,59	0
54	MG	DA	3162	1/1	0.96	0.11	33,33,33,33	0
54	MG	BA	3358	1/1	0.96	0.14	22,22,22,22	0
54	MG	BB	206	1/1	0.96	0.13	34,34,34,34	0
54	MG	BA	3194	1/1	0.96	0.21	52,52,52,52	0
54	MG	AA	1680	1/1	0.96	0.15	54,54,54,54	0
54	MG	BA	3361	1/1	0.96	0.08	30,30,30,30	0
54	MG	BA	3503	1/1	0.96	0.10	23,23,23,23	0
54	MG	BA	3362	1/1	0.96	0.06	30,30,30,30	0
54	MG	DA	3603	1/1	0.96	0.07	44,44,44,44	0
54	MG	DA	3604	1/1	0.96	0.07	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3172	1/1	0.96	0.05	30,30,30,30	0
54	MG	BA	3133	1/1	0.96	0.09	30,30,30,30	0
54	MG	DA	3607	1/1	0.96	0.06	65,65,65,65	0
54	MG	BA	3364	1/1	0.96	0.05	24,24,24,24	0
54	MG	BA	3087	1/1	0.96	0.14	36,36,36,36	0
54	MG	BD	303	1/1	0.96	0.10	33,33,33,33	0
54	MG	BA	3616	1/1	0.96	0.15	26,26,26,26	0
54	MG	CQ	201	1/1	0.96	0.08	76,76,76,76	0
54	MG	DA	3387	1/1	0.96	0.08	72,72,72,72	0
54	MG	BA	3370	1/1	0.96	0.09	23,23,23,23	0
54	MG	BA	3039	1/1	0.96	0.16	58,58,58,58	0
54	MG	BA	3089	1/1	0.96	0.09	32,32,32,32	0
54	MG	DA	3620	1/1	0.96	0.06	65,65,65,65	0
54	MG	DA	3005	1/1	0.96	0.18	53,53,53,53	0
54	MG	BA	3620	1/1	0.96	0.19	40,40,40,40	0
54	MG	CA	1670	1/1	0.96	0.18	80,80,80,80	0
54	MG	DA	3008	1/1	0.96	0.13	44,44,44,44	0
54	MG	BA	3514	1/1	0.96	0.06	29,29,29,29	0
54	MG	DA	3627	1/1	0.96	0.10	58,58,58,58	0
54	MG	DA	3396	1/1	0.96	0.06	48,48,48,48	0
54	MG	BA	3516	1/1	0.96	0.07	54,54,54,54	0
54	MG	BA	3376	1/1	0.96	0.10	37,37,37,37	0
54	MG	DA	3631	1/1	0.96	0.08	54,54,54,54	0
54	MG	BA	3518	1/1	0.96	0.10	28,28,28,28	0
54	MG	DA	3633	1/1	0.96	0.11	49,49,49,49	0
54	MG	BA	3090	1/1	0.96	0.20	30,30,30,30	0
54	MG	BF	302	1/1	0.96	0.42	31,31,31,31	0
54	MG	DA	3402	1/1	0.96	0.07	53,53,53,53	0
54	MG	BF	303	1/1	0.96	0.07	43,43,43,43	0
54	MG	BA	3009	1/1	0.96	0.15	23,23,23,23	0
54	MG	BA	3521	1/1	0.96	0.07	35,35,35,35	0
54	MG	BA	3629	1/1	0.96	0.17	34,34,34,34	0
54	MG	BA	3011	1/1	0.96	0.21	47,47,47,47	0
54	MG	DB	207	1/1	0.96	0.08	82,82,82,82	0
54	MG	DA	3022	1/1	0.96	0.10	37,37,37,37	0
54	MG	DA	3210	1/1	0.96	0.10	47,47,47,47	0
54	MG	BA	3043	1/1	0.96	0.08	30,30,30,30	0
54	MG	DA	3213	1/1	0.96	0.05	33,33,33,33	0
54	MG	DA	3216	1/1	0.96	0.07	43,43,43,43	0
54	MG	DA	3414	1/1	0.96	0.08	66,66,66,66	0
54	MG	BA	3390	1/1	0.96	0.09	33,33,33,33	0
54	MG	DA	3218	1/1	0.96	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3209	1/1	0.96	0.10	19,19,19,19	0
54	MG	DE	303	1/1	0.96	0.16	31,31,31,31	0
54	MG	DA	3419	1/1	0.96	0.05	51,51,51,51	0
54	MG	BO	201	1/1	0.96	0.07	53,53,53,53	0
54	MG	DA	3029	1/1	0.96	0.14	37,37,37,37	0
54	MG	AA	1748	1/1	0.96	0.11	57,57,57,57	0
54	MG	DA	3031	1/1	0.96	0.20	46,46,46,46	0
54	MG	BA	3398	1/1	0.96	0.14	30,30,30,30	0
54	MG	DA	3426	1/1	0.96	0.11	55,55,55,55	0
54	MG	DO	203	1/1	0.96	0.07	75,75,75,75	0
54	MG	BQ	203	1/1	0.96	0.07	38,38,38,38	0
54	MG	DA	3034	1/1	0.96	0.09	34,34,34,34	0
54	MG	DA	3433	1/1	0.96	0.09	34,34,34,34	0
54	MG	BA	3400	1/1	0.96	0.04	39,39,39,39	0
54	MG	BA	3641	1/1	0.96	0.08	47,47,47,47	0
54	MG	CA	1693	1/1	0.96	0.06	73,73,73,73	0
54	MG	DA	3233	1/1	0.96	0.10	42,42,42,42	0
54	MG	DA	3438	1/1	0.96	0.08	54,54,54,54	0
54	MG	D5	102	1/1	0.96	0.05	44,44,44,44	0
54	MG	BA	3143	1/1	0.96	0.12	23,23,23,23	0
54	MG	AA	1790	1/1	0.96	0.14	63,63,63,63	0
54	MG	CA	1696	1/1	0.96	0.08	71,71,71,71	0
54	MG	D8	101	1/1	0.96	0.10	52,52,52,52	0
54	MG	BA	3098	1/1	0.96	0.06	39,39,39,39	0
54	MG	AA	1773	1/1	0.96	0.07	52,52,52,52	0
55	ZN	AN	101	1/1	0.96	0.10	118,118,118,118	0
54	MG	BA	3147	1/1	0.96	0.10	33,33,33,33	0
54	MG	DA	3045	1/1	0.96	0.13	48,48,48,48	0
54	MG	BB	204	1/1	0.97	0.06	47,47,47,47	0
54	MG	DA	3511	1/1	0.97	0.07	44,44,44,44	0
54	MG	BA	3214	1/1	0.97	0.05	39,39,39,39	0
54	MG	BA	3440	1/1	0.97	0.07	50,50,50,50	0
54	MG	CA	1632	1/1	0.97	0.07	57,57,57,57	0
54	MG	BB	207	1/1	0.97	0.17	49,49,49,49	0
54	MG	DA	3350	1/1	0.97	0.08	40,40,40,40	0
54	MG	DA	3055	1/1	0.97	0.12	25,25,25,25	0
54	MG	BB	208	1/1	0.97	0.09	33,33,33,33	0
54	MG	BA	3160	1/1	0.97	0.04	32,32,32,32	0
54	MG	DA	3354	1/1	0.97	0.13	39,39,39,39	0
54	MG	BA	3335	1/1	0.97	0.07	43,43,43,43	0
54	MG	BA	3273	1/1	0.97	0.06	60,60,60,60	0
54	MG	BA	3630	1/1	0.97	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3061	1/1	0.97	0.08	45,45,45,45	0
54	MG	DA	3062	1/1	0.97	0.17	43,43,43,43	0
54	MG	BA	3632	1/1	0.97	0.14	29,29,29,29	0
54	MG	DA	3527	1/1	0.97	0.07	38,38,38,38	0
54	MG	AA	1711	1/1	0.97	0.05	35,35,35,35	0
54	MG	BB	218	1/1	0.97	0.06	69,69,69,69	0
54	MG	BA	3032	1/1	0.97	0.09	25,25,25,25	0
54	MG	AA	1682	1/1	0.97	0.14	48,48,48,48	0
54	MG	DA	3211	1/1	0.97	0.07	38,38,38,38	0
54	MG	BD	302	1/1	0.97	0.07	37,37,37,37	0
54	MG	AA	1792	1/1	0.97	0.10	51,51,51,51	0
54	MG	DA	3214	1/1	0.97	0.06	32,32,32,32	0
54	MG	AA	1672	1/1	0.97	0.06	50,50,50,50	0
54	MG	DA	3071	1/1	0.97	0.08	39,39,39,39	0
54	MG	BA	3543	1/1	0.97	0.10	29,29,29,29	0
54	MG	DA	3219	1/1	0.97	0.04	32,32,32,32	0
54	MG	DA	3073	1/1	0.97	0.09	41,41,41,41	0
54	MG	DA	3541	1/1	0.97	0.06	46,46,46,46	0
54	MG	DA	3375	1/1	0.97	0.04	60,60,60,60	0
54	MG	BA	3451	1/1	0.97	0.04	49,49,49,49	0
54	MG	BA	3065	1/1	0.97	0.06	36,36,36,36	0
54	MG	BA	3222	1/1	0.97	0.04	34,34,34,34	0
54	MG	BA	3132	1/1	0.97	0.06	45,45,45,45	0
54	MG	BA	3548	1/1	0.97	0.08	32,32,32,32	0
54	MG	CA	1765	1/1	0.97	0.05	87,87,87,87	0
54	MG	BA	3346	1/1	0.97	0.06	43,43,43,43	0
54	MG	DA	3383	1/1	0.97	0.11	59,59,59,59	0
54	MG	AA	1771	1/1	0.97	0.07	67,67,67,67	0
54	MG	DA	3230	1/1	0.97	0.07	31,31,31,31	0
54	MG	BA	3019	1/1	0.97	0.07	23,23,23,23	0
54	MG	BA	3135	1/1	0.97	0.06	50,50,50,50	0
54	MG	BA	3649	1/1	0.97	0.19	30,30,30,30	0
54	MG	BA	3553	1/1	0.97	0.07	27,27,27,27	0
54	MG	AA	1677	1/1	0.97	0.06	50,50,50,50	0
54	MG	DA	3237	1/1	0.97	0.07	51,51,51,51	0
54	MG	DA	3238	1/1	0.97	0.10	44,44,44,44	0
54	MG	DA	3088	1/1	0.97	0.07	39,39,39,39	0
54	MG	AA	1734	1/1	0.97	0.07	50,50,50,50	0
54	MG	BA	3354	1/1	0.97	0.05	24,24,24,24	0
54	MG	BA	3178	1/1	0.97	0.13	23,23,23,23	0
54	MG	BA	3356	1/1	0.97	0.07	55,55,55,55	0
54	MG	BA	3233	1/1	0.97	0.05	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3246	1/1	0.97	0.06	41,41,41,41	0
54	MG	BA	3041	1/1	0.97	0.05	29,29,29,29	0
54	MG	BP	201	1/1	0.97	0.10	44,44,44,44	0
54	MG	AA	1774	1/1	0.97	0.07	78,78,78,78	0
54	MG	BA	3181	1/1	0.97	0.06	41,41,41,41	0
54	MG	BQ	202	1/1	0.97	0.07	47,47,47,47	0
54	MG	BA	3660	1/1	0.97	0.07	39,39,39,39	0
54	MG	AA	1612	1/1	0.97	0.07	61,61,61,61	0
54	MG	BQ	205	1/1	0.97	0.09	42,42,42,42	0
54	MG	BA	3024	1/1	0.97	0.12	44,44,44,44	0
54	MG	BA	3295	1/1	0.97	0.18	52,52,52,52	0
54	MG	BA	3075	1/1	0.97	0.09	36,36,36,36	0
54	MG	BA	3475	1/1	0.97	0.09	45,45,45,45	0
54	MG	BA	3045	1/1	0.97	0.10	35,35,35,35	0
54	MG	DA	3580	1/1	0.97	0.06	39,39,39,39	0
54	MG	DA	3261	1/1	0.97	0.05	37,37,37,37	0
54	MG	BA	3366	1/1	0.97	0.09	36,36,36,36	0
54	MG	BA	3367	1/1	0.97	0.10	34,34,34,34	0
54	MG	BA	3369	1/1	0.97	0.04	27,27,27,27	0
54	MG	BU	202	1/1	0.97	0.15	34,34,34,34	0
54	MG	DA	3267	1/1	0.97	0.06	34,34,34,34	0
54	MG	DA	3588	1/1	0.97	0.07	38,38,38,38	0
54	MG	DA	3589	1/1	0.97	0.07	42,42,42,42	0
54	MG	CA	1795	1/1	0.97	0.06	66,66,66,66	0
54	MG	DA	3269	1/1	0.97	0.06	36,36,36,36	0
54	MG	BA	3109	1/1	0.97	0.06	37,37,37,37	0
54	MG	BA	3575	1/1	0.97	0.06	59,59,59,59	0
54	MG	BA	3481	1/1	0.97	0.06	22,22,22,22	0
54	MG	DA	3115	1/1	0.97	0.15	33,33,33,33	0
54	MG	DA	3430	1/1	0.97	0.09	28,28,28,28	0
54	MG	AA	1799	1/1	0.97	0.08	44,44,44,44	0
54	MG	DA	3117	1/1	0.97	0.21	69,69,69,69	0
54	MG	DA	3599	1/1	0.97	0.04	45,45,45,45	0
54	MG	BA	3372	1/1	0.97	0.10	32,32,32,32	0
54	MG	DA	3119	1/1	0.97	0.11	38,38,38,38	0
54	MG	BA	3373	1/1	0.97	0.10	46,46,46,46	0
54	MG	BA	3048	1/1	0.97	0.05	35,35,35,35	0
54	MG	BA	3050	1/1	0.97	0.28	54,54,54,54	0
54	MG	B0	101	1/1	0.97	0.16	40,40,40,40	0
54	MG	DA	3609	1/1	0.97	0.05	42,42,42,42	0
54	MG	BA	3193	1/1	0.97	0.08	46,46,46,46	0
54	MG	DA	3002	1/1	0.97	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3380	1/1	0.97	0.06	37,37,37,37	0
54	MG	DA	3127	1/1	0.97	0.18	24,24,24,24	0
54	MG	DA	3287	1/1	0.97	0.12	52,52,52,52	0
54	MG	BA	3381	1/1	0.97	0.08	41,41,41,41	0
54	MG	DA	3129	1/1	0.97	0.25	38,38,38,38	0
54	MG	BA	3246	1/1	0.97	0.10	46,46,46,46	0
54	MG	BA	3051	1/1	0.97	0.13	33,33,33,33	0
54	MG	DA	3621	1/1	0.97	0.08	41,41,41,41	0
54	MG	BA	3006	1/1	0.97	0.05	67,67,67,67	0
54	MG	BA	3389	1/1	0.97	0.08	30,30,30,30	0
54	MG	BA	3250	1/1	0.97	0.06	39,39,39,39	0
54	MG	BA	3115	1/1	0.97	0.06	35,35,35,35	0
54	MG	BA	3083	1/1	0.97	0.06	32,32,32,32	0
54	MG	DA	3012	1/1	0.97	0.17	34,34,34,34	0
54	MG	BA	3695	1/1	0.97	0.07	52,52,52,52	0
54	MG	BA	3696	1/1	0.97	0.04	38,38,38,38	0
54	MG	DA	3301	1/1	0.97	0.06	31,31,31,31	0
54	MG	BA	3502	1/1	0.97	0.09	34,34,34,34	0
54	MG	DA	3461	1/1	0.97	0.06	76,76,76,76	0
54	MG	BA	3310	1/1	0.97	0.05	19,19,19,19	0
54	MG	BA	3504	1/1	0.97	0.10	53,53,53,53	0
54	MG	DA	3465	1/1	0.97	0.10	63,63,63,63	0
54	MG	BA	3399	1/1	0.97	0.10	42,42,42,42	0
54	MG	BA	3253	1/1	0.97	0.08	39,39,39,39	0
54	MG	AA	1626	1/1	0.97	0.16	32,32,32,32	0
54	MG	DB	202	1/1	0.97	0.19	67,67,67,67	0
54	MG	DB	203	1/1	0.97	0.09	61,61,61,61	0
54	MG	DA	3021	1/1	0.97	0.11	32,32,32,32	0
54	MG	DA	3470	1/1	0.97	0.05	50,50,50,50	0
54	MG	DA	3471	1/1	0.97	0.04	41,41,41,41	0
54	MG	BA	3708	1/1	0.97	0.08	49,49,49,49	0
54	MG	DA	3473	1/1	0.97	0.08	34,34,34,34	0
54	MG	AA	1801	1/1	0.97	0.05	87,87,87,87	0
54	MG	BA	3259	1/1	0.97	0.07	20,20,20,20	0
54	MG	DA	3150	1/1	0.97	0.13	29,29,29,29	0
54	MG	DA	3026	1/1	0.97	0.12	47,47,47,47	0
54	MG	BA	3410	1/1	0.97	0.22	56,56,56,56	0
54	MG	DA	3153	1/1	0.97	0.04	32,32,32,32	0
54	MG	BA	3411	1/1	0.97	0.07	24,24,24,24	0
54	MG	DA	3155	1/1	0.97	0.08	53,53,53,53	0
54	MG	DE	302	1/1	0.97	0.05	37,37,37,37	0
54	MG	DA	3156	1/1	0.97	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3414	1/1	0.97	0.12	23,23,23,23	0
54	MG	DA	3158	1/1	0.97	0.09	49,49,49,49	0
54	MG	BA	3515	1/1	0.97	0.06	35,35,35,35	0
54	MG	CA	1721	1/1	0.97	0.06	53,53,53,53	0
54	MG	BA	3154	1/1	0.97	0.07	47,47,47,47	0
54	MG	BA	3155	1/1	0.97	0.05	37,37,37,37	0
54	MG	BA	3262	1/1	0.97	0.06	51,51,51,51	0
54	MG	DA	3491	1/1	0.97	0.06	42,42,42,42	0
54	MG	AA	1616	1/1	0.97	0.12	55,55,55,55	0
54	MG	DA	3493	1/1	0.97	0.11	33,33,33,33	0
54	MG	BA	3325	1/1	0.97	0.07	28,28,28,28	0
54	MG	DQ	201	1/1	0.97	0.11	52,52,52,52	0
54	MG	DQ	202	1/1	0.97	0.14	39,39,39,39	0
54	MG	BA	3424	1/1	0.97	0.09	25,25,25,25	0
54	MG	BA	3326	1/1	0.97	0.05	46,46,46,46	0
54	MG	DR	201	1/1	0.97	0.09	40,40,40,40	0
54	MG	DR	202	1/1	0.97	0.10	45,45,45,45	0
54	MG	DT	201	1/1	0.97	0.14	52,52,52,52	0
54	MG	BA	3523	1/1	0.97	0.10	43,43,43,43	0
54	MG	BA	3207	1/1	0.97	0.04	57,57,57,57	0
54	MG	DA	3499	1/1	0.97	0.07	55,55,55,55	0
54	MG	D1	101	1/1	0.97	0.07	59,59,59,59	0
54	MG	BA	3429	1/1	0.97	0.08	59,59,59,59	0
54	MG	BA	3430	1/1	0.97	0.15	27,27,27,27	0
54	MG	BA	3057	1/1	0.97	0.26	29,29,29,29	0
54	MG	BA	3158	1/1	0.97	0.11	22,22,22,22	0
54	MG	BA	3433	1/1	0.97	0.11	31,31,31,31	0
54	MG	BA	3622	1/1	0.97	0.09	31,31,31,31	0
54	MG	DA	3180	1/1	0.97	0.04	29,29,29,29	0
55	ZN	AD	301	1/1	0.97	0.18	76,76,76,76	0
54	MG	AA	1681	1/1	0.97	0.06	44,44,44,44	0
55	ZN	B4	101	1/1	0.97	0.04	117,117,117,117	0
54	MG	DA	3183	1/1	0.97	0.08	36,36,36,36	0
54	MG	BA	3211	1/1	0.97	0.09	49,49,49,49	0
54	MG	DA	3331	1/1	0.98	0.04	48,48,48,48	0
54	MG	DA	3332	1/1	0.98	0.06	28,28,28,28	0
54	MG	BA	3337	1/1	0.98	0.04	27,27,27,27	0
54	MG	BA	3388	1/1	0.98	0.09	20,20,20,20	0
54	MG	BA	3198	1/1	0.98	0.13	35,35,35,35	0
54	MG	DA	3336	1/1	0.98	0.06	53,53,53,53	0
54	MG	BA	3199	1/1	0.98	0.06	46,46,46,46	0
54	MG	BA	3680	1/1	0.98	0.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3681	1/1	0.98	0.10	31,31,31,31	0
54	MG	AA	1722	1/1	0.98	0.08	48,48,48,48	0
54	MG	BA	3175	1/1	0.98	0.05	31,31,31,31	0
54	MG	BA	3396	1/1	0.98	0.06	39,39,39,39	0
54	MG	BA	3397	1/1	0.98	0.06	36,36,36,36	0
54	MG	DA	3025	1/1	0.98	0.28	35,35,35,35	0
54	MG	DA	3464	1/1	0.98	0.04	35,35,35,35	0
54	MG	BA	3686	1/1	0.98	0.04	43,43,43,43	0
54	MG	BA	3609	1/1	0.98	0.05	37,37,37,37	0
54	MG	BA	3176	1/1	0.98	0.05	27,27,27,27	0
54	MG	DA	3234	1/1	0.98	0.15	52,52,52,52	0
54	MG	BA	3069	1/1	0.98	0.04	42,42,42,42	0
54	MG	DA	3587	1/1	0.98	0.14	49,49,49,49	0
54	MG	AA	1814	1/1	0.98	0.07	66,66,66,66	0
54	MG	BA	3613	1/1	0.98	0.04	50,50,50,50	0
54	MG	BA	3470	1/1	0.98	0.05	33,33,33,33	0
54	MG	BA	3004	1/1	0.98	0.09	53,53,53,53	0
54	MG	BA	3403	1/1	0.98	0.08	35,35,35,35	0
54	MG	BA	3699	1/1	0.98	0.04	43,43,43,43	0
54	MG	BA	3404	1/1	0.98	0.06	27,27,27,27	0
54	MG	BT	201	1/1	0.98	0.15	49,49,49,49	0
54	MG	BA	3406	1/1	0.98	0.10	25,25,25,25	0
54	MG	CA	1751	1/1	0.98	0.09	89,89,89,89	0
54	MG	DA	3480	1/1	0.98	0.04	57,57,57,57	0
54	MG	BA	3304	1/1	0.98	0.05	33,33,33,33	0
54	MG	DA	3600	1/1	0.98	0.04	33,33,33,33	0
54	MG	DA	3602	1/1	0.98	0.04	53,53,53,53	0
54	MG	DA	3041	1/1	0.98	0.10	34,34,34,34	0
54	MG	BU	201	1/1	0.98	0.17	30,30,30,30	0
54	MG	BA	3703	1/1	0.98	0.03	26,26,26,26	0
54	MG	CA	1755	1/1	0.98	0.10	79,79,79,79	0
54	MG	BU	203	1/1	0.98	0.22	31,31,31,31	0
54	MG	AA	1655	1/1	0.98	0.06	64,64,64,64	0
54	MG	BA	3348	1/1	0.98	0.06	44,44,44,44	0
54	MG	BA	3706	1/1	0.98	0.06	44,44,44,44	0
54	MG	BA	3271	1/1	0.98	0.06	66,66,66,66	0
54	MG	BA	3272	1/1	0.98	0.04	40,40,40,40	0
54	MG	BA	3046	1/1	0.98	0.09	35,35,35,35	0
54	MG	DA	3615	1/1	0.98	0.04	67,67,67,67	0
54	MG	BA	3482	1/1	0.98	0.10	21,21,21,21	0
54	MG	BA	3416	1/1	0.98	0.06	22,22,22,22	0
54	MG	BA	3417	1/1	0.98	0.05	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	B0	102	1/1	0.98	0.06	50,50,50,50	0
54	MG	BA	3182	1/1	0.98	0.05	30,30,30,30	0
54	MG	BA	3486	1/1	0.98	0.06	25,25,25,25	0
54	MG	BA	3183	1/1	0.98	0.05	37,37,37,37	0
54	MG	CA	1679	1/1	0.98	0.08	53,53,53,53	0
54	MG	BA	3631	1/1	0.98	0.19	35,35,35,35	0
54	MG	BA	3558	1/1	0.98	0.05	60,60,60,60	0
54	MG	BA	3488	1/1	0.98	0.04	20,20,20,20	0
54	MG	BA	3634	1/1	0.98	0.05	63,63,63,63	0
54	MG	BA	3420	1/1	0.98	0.06	23,23,23,23	0
54	MG	BA	3311	1/1	0.98	0.07	34,34,34,34	0
54	MG	BA	3036	1/1	0.98	0.09	41,41,41,41	0
54	MG	BA	3563	1/1	0.98	0.06	59,59,59,59	0
54	MG	BA	3313	1/1	0.98	0.06	23,23,23,23	0
54	MG	B9	102	1/1	0.98	0.19	29,29,29,29	0
54	MG	AA	1705	1/1	0.98	0.04	46,46,46,46	0
54	MG	BA	3093	1/1	0.98	0.15	28,28,28,28	0
54	MG	BA	3316	1/1	0.98	0.05	43,43,43,43	0
54	MG	BA	3497	1/1	0.98	0.08	29,29,29,29	0
54	MG	DA	3171	1/1	0.98	0.04	28,28,28,28	0
54	MG	BA	3062	1/1	0.98	0.06	32,32,32,32	0
54	MG	BA	3166	1/1	0.98	0.08	53,53,53,53	0
54	MG	BA	3320	1/1	0.98	0.06	42,42,42,42	0
54	MG	BA	3095	1/1	0.98	0.05	39,39,39,39	0
54	MG	BA	3131	1/1	0.98	0.07	28,28,28,28	0
54	MG	DA	3290	1/1	0.98	0.07	47,47,47,47	0
54	MG	DA	3177	1/1	0.98	0.07	32,32,32,32	0
54	MG	BA	3249	1/1	0.98	0.08	20,20,20,20	0
54	MG	BA	3324	1/1	0.98	0.06	48,48,48,48	0
54	MG	BA	3437	1/1	0.98	0.07	28,28,28,28	0
54	MG	DA	3181	1/1	0.98	0.05	50,50,50,50	0
54	MG	DA	3082	1/1	0.98	0.13	34,34,34,34	0
54	MG	BA	3438	1/1	0.98	0.06	31,31,31,31	0
54	MG	BA	3508	1/1	0.98	0.06	33,33,33,33	0
54	MG	BA	3439	1/1	0.98	0.04	30,30,30,30	0
54	MG	BB	214	1/1	0.98	0.07	38,38,38,38	0
54	MG	BA	3191	1/1	0.98	0.15	43,43,43,43	0
54	MG	DA	3189	1/1	0.98	0.07	36,36,36,36	0
54	MG	BA	3049	1/1	0.98	0.14	26,26,26,26	0
54	MG	BA	3442	1/1	0.98	0.10	24,24,24,24	0
54	MG	DA	3417	1/1	0.98	0.07	59,59,59,59	0
54	MG	DA	3192	1/1	0.98	0.03	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3443	1/1	0.98	0.06	31,31,31,31	0
54	MG	AA	1712	1/1	0.98	0.10	43,43,43,43	0
54	MG	CA	1802	1/1	0.98	0.05	60,60,60,60	0
54	MG	BA	3223	1/1	0.98	0.06	24,24,24,24	0
54	MG	DA	3423	1/1	0.98	0.03	37,37,37,37	0
54	MG	DA	3197	1/1	0.98	0.06	28,28,28,28	0
54	MG	BA	3254	1/1	0.98	0.05	36,36,36,36	0
54	MG	DA	3199	1/1	0.98	0.09	29,29,29,29	0
54	MG	BA	3374	1/1	0.98	0.10	27,27,27,27	0
54	MG	DA	3429	1/1	0.98	0.10	26,26,26,26	0
54	MG	BA	3663	1/1	0.98	0.04	53,53,53,53	0
54	MG	DA	3431	1/1	0.98	0.08	27,27,27,27	0
54	MG	DA	3202	1/1	0.98	0.06	29,29,29,29	0
54	MG	AA	1738	1/1	0.98	0.04	62,62,62,62	0
54	MG	DA	3204	1/1	0.98	0.06	32,32,32,32	0
54	MG	BA	3225	1/1	0.98	0.07	19,19,19,19	0
54	MG	CA	1717	1/1	0.98	0.07	85,85,85,85	0
54	MG	BA	3332	1/1	0.98	0.05	37,37,37,37	0
54	MG	BA	3378	1/1	0.98	0.06	24,24,24,24	0
54	MG	BA	3379	1/1	0.98	0.06	30,30,30,30	0
54	MG	DA	3440	1/1	0.98	0.09	65,65,65,65	0
54	MG	BA	3258	1/1	0.98	0.09	18,18,18,18	0
54	MG	BA	3195	1/1	0.98	0.06	46,46,46,46	0
54	MG	AA	1671	1/1	0.98	0.06	64,64,64,64	0
54	MG	BE	306	1/1	0.98	0.11	24,24,24,24	0
54	MG	DA	3215	1/1	0.98	0.03	30,30,30,30	0
54	MG	BA	3456	1/1	0.98	0.05	37,37,37,37	0
54	MG	BA	3383	1/1	0.98	0.04	26,26,26,26	0
54	MG	BA	3001	1/1	0.98	0.14	45,45,45,45	0
55	ZN	D5	101	1/1	0.98	0.03	53,53,53,53	0
54	MG	BA	3213	1/1	0.99	0.06	28,28,28,28	0
54	MG	DA	3270	1/1	0.99	0.03	24,24,24,24	0
54	MG	DA	3160	1/1	0.99	0.02	42,42,42,42	0
54	MG	BA	3402	1/1	0.99	0.04	31,31,31,31	0
54	MG	BA	3506	1/1	0.99	0.03	33,33,33,33	0
54	MG	BA	3085	1/1	0.99	0.15	23,23,23,23	0
54	MG	BA	3472	1/1	0.99	0.07	34,34,34,34	0
54	MG	BA	3086	1/1	0.99	0.14	21,21,21,21	0
54	MG	BA	3584	1/1	0.99	0.04	48,48,48,48	0
54	MG	BA	3008	1/1	0.99	0.07	20,20,20,20	0
54	MG	DA	3221	1/1	0.99	0.06	27,27,27,27	0
54	MG	CA	1678	1/1	0.99	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3169	1/1	0.99	0.05	32,32,32,32	0
54	MG	BA	3200	1/1	0.99	0.07	24,24,24,24	0
54	MG	AA	1737	1/1	0.99	0.06	41,41,41,41	0
54	MG	BA	3255	1/1	0.99	0.02	25,25,25,25	0
54	MG	DA	3460	1/1	0.99	0.06	32,32,32,32	0
54	MG	BA	3667	1/1	0.99	0.04	22,22,22,22	0
54	MG	BA	3010	1/1	0.99	0.11	27,27,27,27	0
54	MG	BA	3412	1/1	0.99	0.08	19,19,19,19	0
54	MG	BA	3413	1/1	0.99	0.09	24,24,24,24	0
54	MG	AA	1808	1/1	0.99	0.06	43,43,43,43	0
54	MG	BA	3017	1/1	0.99	0.12	27,27,27,27	0
54	MG	BA	3384	1/1	0.99	0.09	29,29,29,29	0
54	MG	DA	3407	1/1	0.99	0.07	51,51,51,51	0
54	MG	BA	3385	1/1	0.99	0.06	31,31,31,31	0
54	MG	BA	3082	1/1	0.99	0.03	26,26,26,26	0
54	MG	BA	3319	1/1	0.99	0.10	26,26,26,26	0
54	MG	BA	3598	1/1	0.99	0.06	34,34,34,34	0
54	MG	BA	3162	1/1	0.99	0.09	22,22,22,22	0
54	MG	BA	3421	1/1	0.99	0.09	34,34,34,34	0
54	MG	DA	3186	1/1	0.99	0.04	27,27,27,27	0
54	MG	BA	3489	1/1	0.99	0.03	57,57,57,57	0
54	MG	BA	3054	1/1	0.99	0.05	31,31,31,31	0
54	MG	DA	3243	1/1	0.99	0.02	32,32,32,32	0
54	MG	BA	3124	1/1	0.99	0.07	24,24,24,24	0
54	MG	BA	3528	1/1	0.99	0.08	27,27,27,27	0
54	MG	BA	3728	1/1	0.99	0.03	47,47,47,47	0
54	MG	BA	3391	1/1	0.99	0.09	24,24,24,24	0
54	MG	BA	3282	1/1	0.99	0.05	29,29,29,29	0
54	MG	BA	3426	1/1	0.99	0.05	28,28,28,28	0
54	MG	BA	3427	1/1	0.99	0.06	28,28,28,28	0
54	MG	BA	3393	1/1	0.99	0.08	29,29,29,29	0
54	MG	CA	1656	1/1	0.99	0.02	66,66,66,66	0
54	MG	DA	3427	1/1	0.99	0.07	24,24,24,24	0
54	MG	DA	3368	1/1	0.99	0.03	56,56,56,56	0
54	MG	DA	3613	1/1	0.99	0.05	45,45,45,45	0
54	MG	BA	3394	1/1	0.99	0.03	27,27,27,27	0
54	MG	CA	1658	1/1	0.99	0.08	64,64,64,64	0
54	MG	AA	1733	1/1	0.99	0.06	59,59,59,59	0
54	MG	BA	3126	1/1	0.99	0.10	30,30,30,30	0
54	MG	BA	3127	1/1	0.99	0.05	30,30,30,30	0
54	MG	BB	209	1/1	0.99	0.05	45,45,45,45	0
54	MG	DA	3259	1/1	0.99	0.05	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3693	1/1	0.99	0.04	36,36,36,36	0
54	MG	BA	3694	1/1	0.99	0.07	21,21,21,21	0
54	MG	DA	3206	1/1	0.99	0.04	34,34,34,34	0
54	MG	BB	212	1/1	0.99	0.03	49,49,49,49	0
54	MG	BA	3212	1/1	0.99	0.04	52,52,52,52	0
55	ZN	B5	102	1/1	0.99	0.02	42,42,42,42	0
55	ZN	B9	101	1/1	0.99	0.02	49,49,49,49	0
54	MG	BA	3349	1/1	0.99	0.04	30,30,30,30	0
55	ZN	CN	101	1/1	0.99	0.04	108,108,108,108	0
55	ZN	DY	201	1/1	0.99	0.03	77,77,77,77	0
54	MG	BA	3698	1/1	0.99	0.08	24,24,24,24	0
54	MG	BA	3230	1/1	0.99	0.09	29,29,29,29	0
55	ZN	D6	101	1/1	0.99	0.06	66,66,66,66	0
55	ZN	D9	101	1/1	0.99	0.03	68,68,68,68	0
55	ZN	B6	101	1/1	1.00	0.04	42,42,42,42	0
54	MG	BA	3405	1/1	1.00	0.04	22,22,22,22	0
54	MG	BA	3164	1/1	1.00	0.09	39,39,39,39	0
54	MG	BA	3407	1/1	1.00	0.03	24,24,24,24	0
54	MG	DA	3601	1/1	1.00	0.03	32,32,32,32	0
54	MG	DA	3265	1/1	1.00	0.05	34,34,34,34	0
55	ZN	BY	201	1/1	1.00	0.02	54,54,54,54	0
54	MG	BA	3368	1/1	1.00	0.03	27,27,27,27	0
54	MG	BA	3697	1/1	1.00	0.06	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.