



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 01:03 AM UTC

PDB ID : 4V8H / pdb_00004v8h
Title : Crystal structure of HPF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

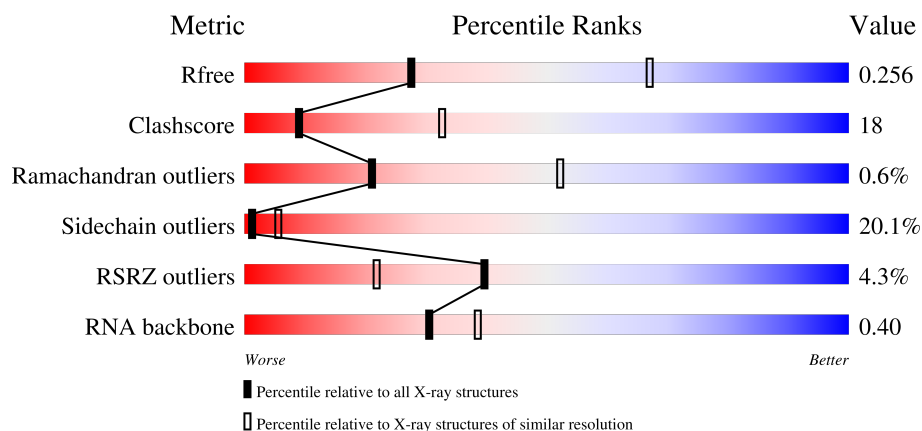
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	2% 30% 50% 18% .
1	CA	1522	2% 29% 51% 19% .
2	AB	256	5% 34% 42% 14% 10%
2	CB	256	10% 34% 41% 14% . 11%

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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	AX	101	
22	CX	101	
23	BA	2913	
23	DA	2913	
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	BA	3301	-	-	-	X
54	MG	DA	3218	-	-	-	X
54	MG	DA	3276	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286308 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	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			
1	CA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	230	Total	C	N	O	S	0	0	0
			1787	1141	319	322	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	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
			1450	906	279	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
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	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
			1105	699	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
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	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
			1164	726	224	208	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
			1045	665	188	190	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
			852	533	163	156			

- 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
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			663	410	132	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
			905	567	178	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
			804	497	164	142	1			
13	CM	114	Total	C	N	O	S	0	0	0
			804	497	164	142	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 478	C 303	N 99	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
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			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	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	87	Total	C	N	O	S	0	0	0
			665	410	142	111	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

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

- Molecule 22 is a protein called Probable sigma(54) modulation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AX	95	Total	C	N	O	S	0	0	0
			631	396	116	118	1			
22	CX	95	Total	C	N	O	S	0	0	0
			601	378	108	114	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	96	HIS	-	expression tag	UNP P0AFX0
AX	97	HIS	-	expression tag	UNP P0AFX0
AX	98	HIS	-	expression tag	UNP P0AFX0
AX	99	HIS	-	expression tag	UNP P0AFX0
AX	100	HIS	-	expression tag	UNP P0AFX0
AX	101	HIS	-	expression tag	UNP P0AFX0
CX	96	HIS	-	expression tag	UNP P0AFX0
CX	97	HIS	-	expression tag	UNP P0AFX0
CX	98	HIS	-	expression tag	UNP P0AFX0
CX	99	HIS	-	expression tag	UNP P0AFX0
CX	100	HIS	-	expression tag	UNP P0AFX0
CX	101	HIS	-	expression tag	UNP P0AFX0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2837	Total	C	N	O	P	0	0	0
			61112	27197	11440	19639	2836			
23	DA	2814	Total	C	N	O	P	0	0	0
			60621	26978	11351	19479	2813			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	?	-	U	deletion	GB AP008226.1
BA	?	-	U	deletion	GB AP008226.1
DA	?	-	U	deletion	GB AP008226.1

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	?	-	U	deletion	GB AP008226.1

- 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			
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
			2135	1349	422	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
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	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
			1037	666	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			953	608	168	176	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	0	0	0
			865	544	172	149			
36	DS	110	Total	C	N	O	0	0	0
			865	544	172	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	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	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			
40	DW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	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
			742	483	134	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
			785	503	145	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	201	Total	C	N	O	S	0	0	0
			1536	980	272	282	2			
43	DZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- 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	76	Total	C	N	O	S	0	0	0
			594	368	125	100	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	70	Total	C	N	O	S	0	0	0
			588	365	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
			458	293	87	78			

- 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
			455	286	90	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
			449	278	90	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
			418	257	104	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	135	Total	Mg	0	0
			135	135		
54	AC	1	Total	Mg	0	0
			1	1		
54	AD	1	Total	Mg	0	0
			1	1		
54	AF	1	Total	Mg	0	0
			1	1		
54	AQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	660	Total 660	Mg 660	0	0
54	BB	23	Total 23	Mg 23	0	0
54	BD	3	Total 3	Mg 3	0	0
54	BE	5	Total 5	Mg 5	0	0
54	BF	2	Total 2	Mg 2	0	0
54	BG	1	Total 1	Mg 1	0	0
54	BP	1	Total 1	Mg 1	0	0
54	BQ	4	Total 4	Mg 4	0	0
54	BR	1	Total 1	Mg 1	0	0
54	BS	1	Total 1	Mg 1	0	0
54	BT	2	Total 2	Mg 2	0	0
54	BV	1	Total 1	Mg 1	0	0
54	BW	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	B0	3	Total 3	Mg 3	0	0
54	B1	1	Total 1	Mg 1	0	0
54	B2	1	Total 1	Mg 1	0	0
54	B3	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	B8	2	Total 2	Mg 2	0	0
54	B9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CA	162	Total 162	Mg 162	0	0
54	CE	1	Total 1	Mg 1	0	0
54	CQ	1	Total 1	Mg 1	0	0
54	DA	598	Total 598	Mg 598	0	0
54	DB	8	Total 8	Mg 8	0	0
54	DD	2	Total 2	Mg 2	0	0
54	DE	4	Total 4	Mg 4	0	0
54	DF	1	Total 1	Mg 1	0	0
54	DO	2	Total 2	Mg 2	0	0
54	DP	1	Total 1	Mg 1	0	0
54	DQ	2	Total 2	Mg 2	0	0
54	DR	3	Total 3	Mg 3	0	0
54	D0	2	Total 2	Mg 2	0	0
54	D1	1	Total 1	Mg 1	0	0
54	D5	1	Total 1	Mg 1	0	0
54	D8	2	Total 2	Mg 2	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	268	Total 268	O 268	0	0
56	AE	1	Total 1	O 1	0	0
56	AL	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	AT	1	Total 1	O 1	0	0
56	AX	1	Total 1	O 1	0	0
56	BA	1694	Total 1694	O 1694	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	57	Total 57	O 57	0	0
56	BD	20	Total 20	O 20	0	0
56	BE	11	Total 11	O 11	0	0
56	BF	6	Total 6	O 6	0	0
56	BH	1	Total 1	O 1	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	2	Total 2	O 2	0	0
56	BP	11	Total 11	O 11	0	0
56	BQ	5	Total 5	O 5	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	3	Total 3	O 3	0	0
56	BV	3	Total 3	O 3	0	0
56	BW	3	Total 3	O 3	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	4	Total 4	O 4	0	0
56	B0	8	Total 8	O 8	0	0
56	B1	2	Total 2	O 2	0	0
56	B3	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B6	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B7	5	Total 5	O 5	0	0
56	B8	10	Total 10	O 10	0	0
56	B9	1	Total 1	O 1	0	0
56	CA	265	Total 265	O 265	0	0
56	CC	1	Total 1	O 1	0	0
56	CD	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	1	Total 1	O 1	0	0
56	CP	1	Total 1	O 1	0	0
56	CQ	1	Total 1	O 1	0	0
56	CT	1	Total 1	O 1	0	0
56	CX	1	Total 1	O 1	0	0
56	DA	1174	Total 1174	O 1174	0	0
56	DB	17	Total 17	O 17	0	0
56	DD	8	Total 8	O 8	0	0
56	DE	11	Total 11	O 11	0	0
56	DF	7	Total 7	O 7	0	0
56	DN	1	Total 1	O 1	0	0
56	DO	5	Total 5	O 5	0	0

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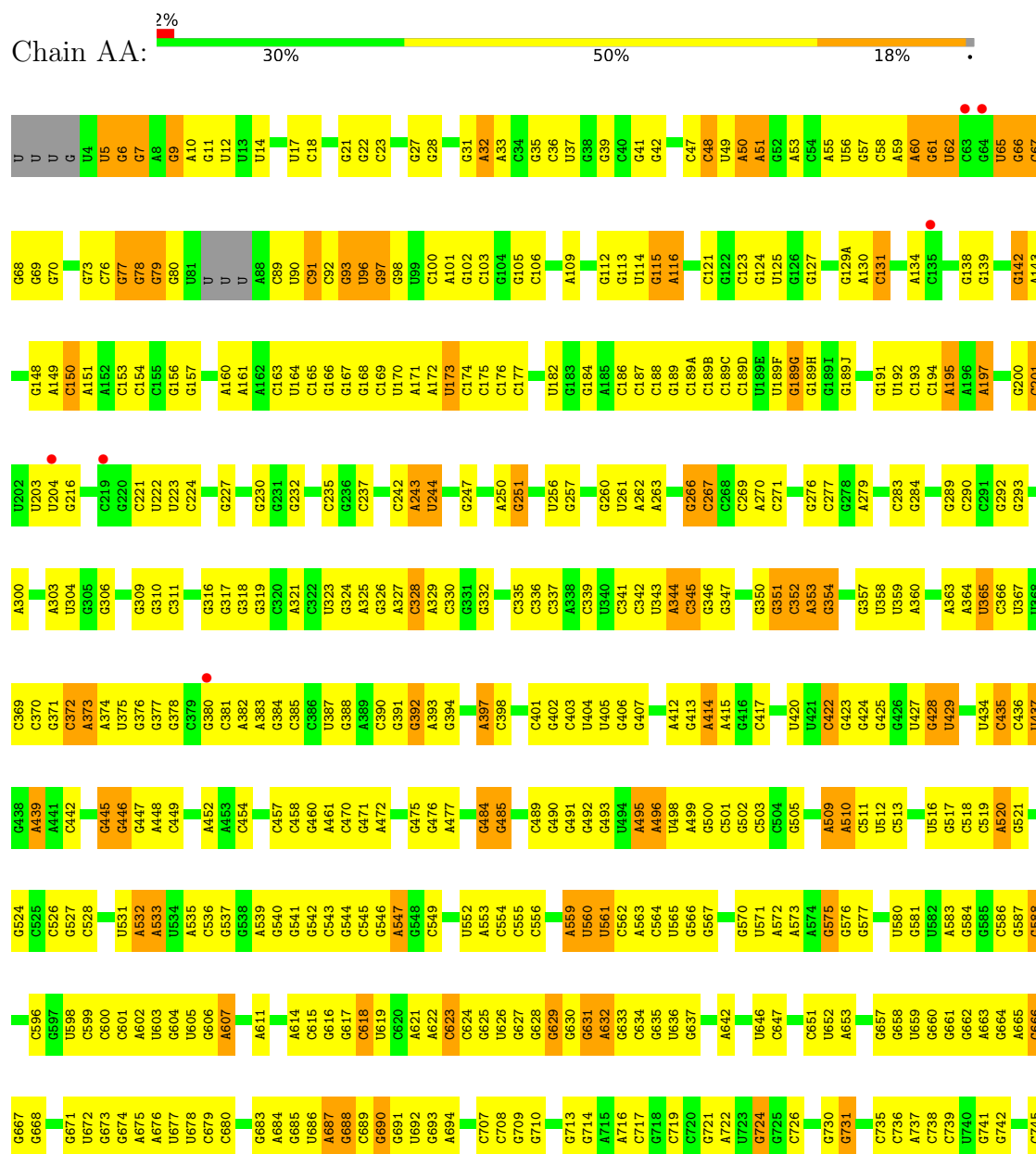
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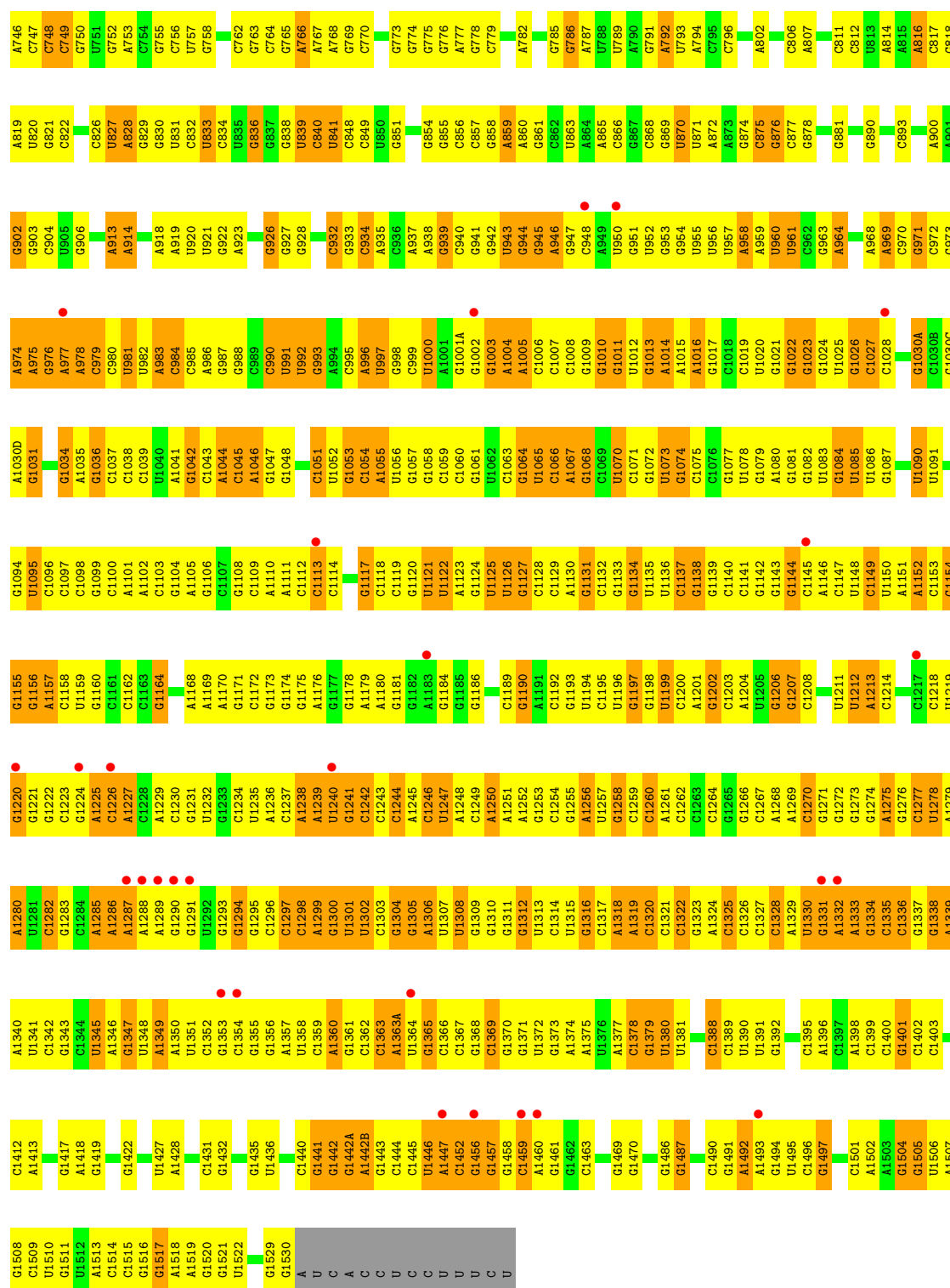
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DP	10	Total	O	0	0
			10	10		
56	DQ	3	Total	O	0	0
			3	3		
56	DR	2	Total	O	0	0
			2	2		
56	DT	2	Total	O	0	0
			2	2		
56	DU	5	Total	O	0	0
			5	5		
56	DV	2	Total	O	0	0
			2	2		
56	DW	2	Total	O	0	0
			2	2		
56	DX	1	Total	O	0	0
			1	1		
56	DY	2	Total	O	0	0
			2	2		
56	D0	1	Total	O	0	0
			1	1		
56	D1	5	Total	O	0	0
			5	5		
56	D3	1	Total	O	0	0
			1	1		
56	D4	1	Total	O	0	0
			1	1		
56	D7	3	Total	O	0	0
			3	3		
56	D8	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 1: 16S Ribosomal RNA

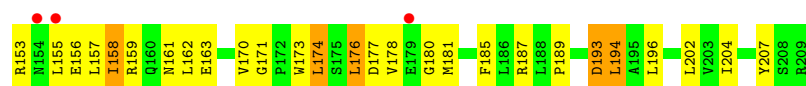
Chain CA: 29% 51% 19%



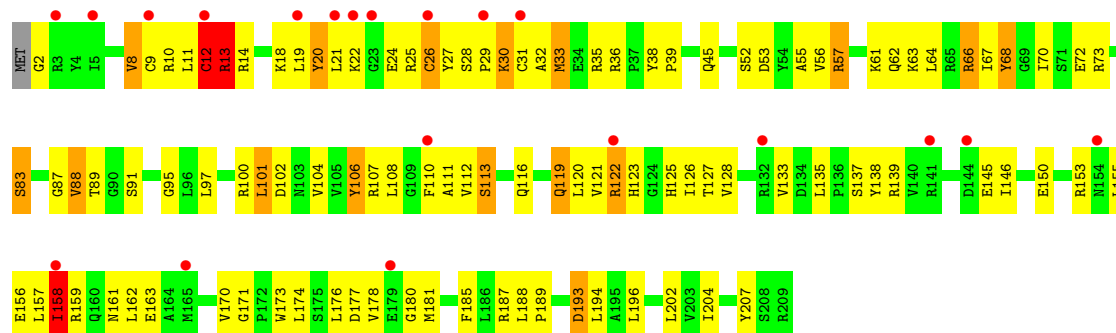
G1108	G1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	U1121	U1122	U1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	C1150	C1151	C1152	C1153																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U1048	U1049	U1050	C1051	U1052	U1053	U1054	A1055	U1056	U1057	U1058	C1059	U1060	A1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G993	A994	C995	A996	C997	C998	C999	C1000	A1001	U1001A	G1002	G1003	A1004	A1005	C1006	C1007	C1008	U1009	G1010	G1011	U1012	G1013	G1014	U1015	A1016	G1017	C1018	C1019	U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	C1029	C1030	C1030A	C1030B	C1030C	A1030D	G1031	G1032	G1033	G1034	A1035	G1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043	A1044	C1045	A1046	G1047																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G851	A765	A766	A767	G768	G769	G770	G771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A163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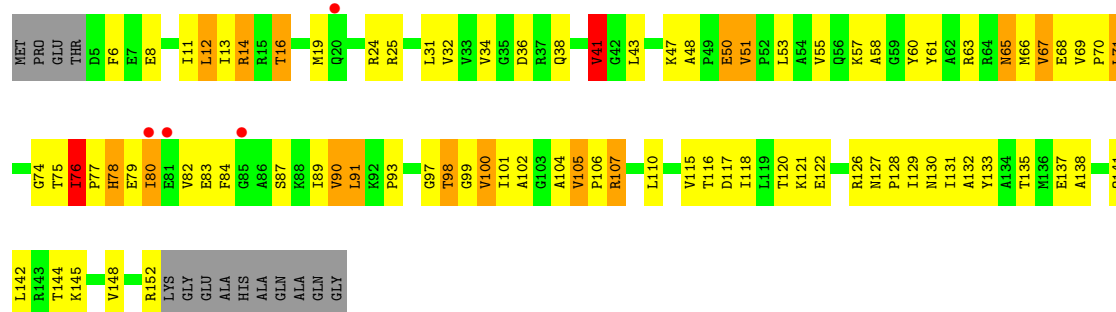




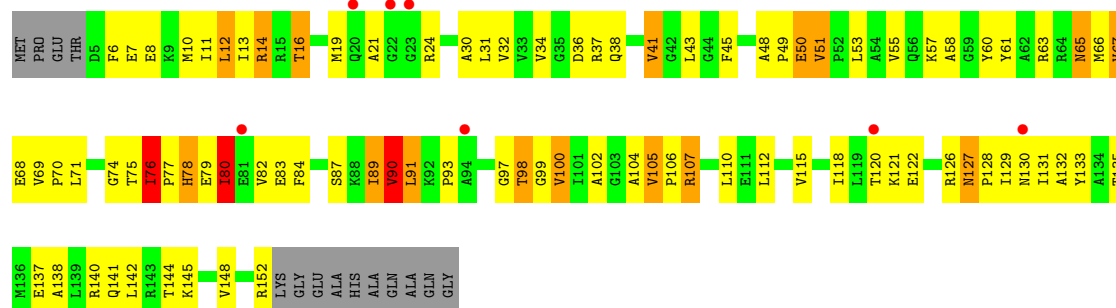
• Molecule 4: 30S Ribosomal Protein S4



• Molecule 5: 30S Ribosomal Protein S5

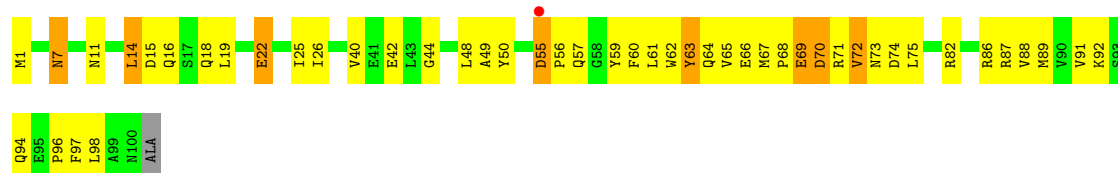


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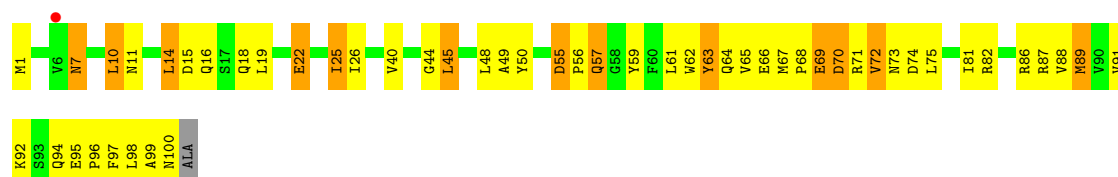


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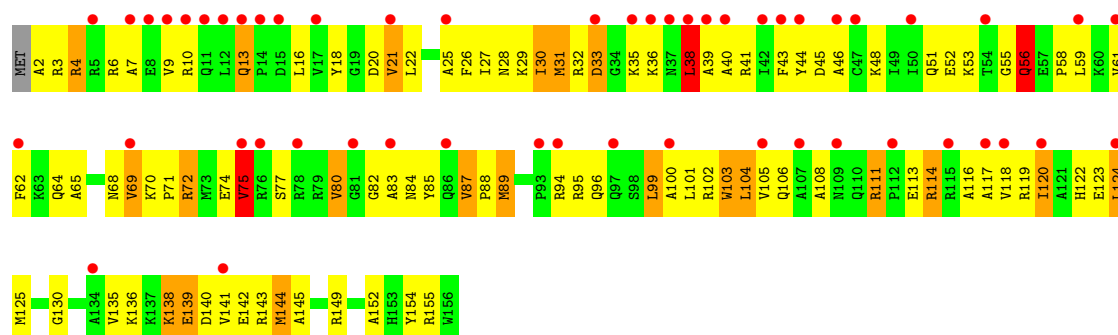




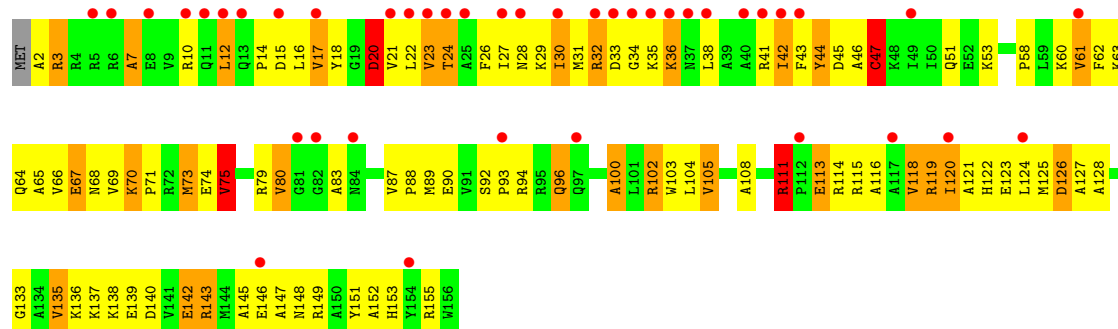
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• Molecule 7: 30S Ribosomal Protein S7

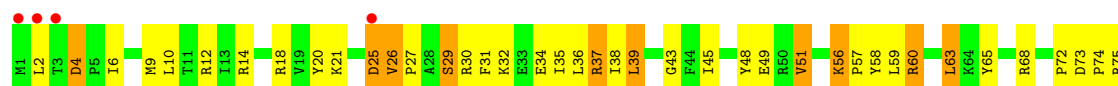


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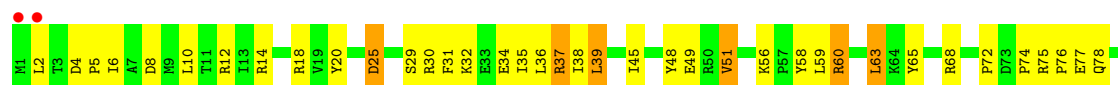


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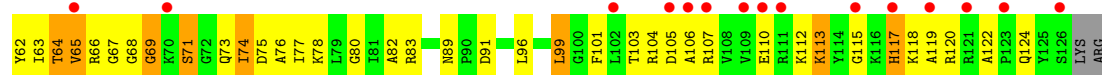
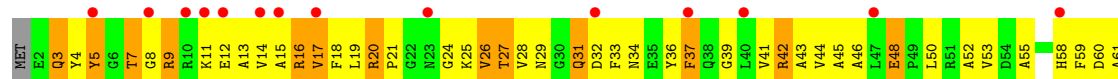




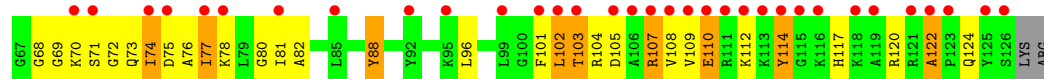
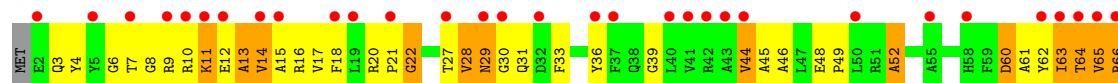
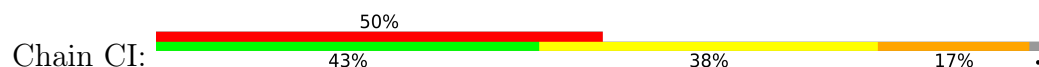
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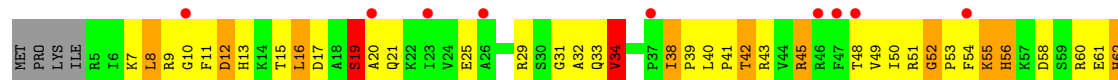
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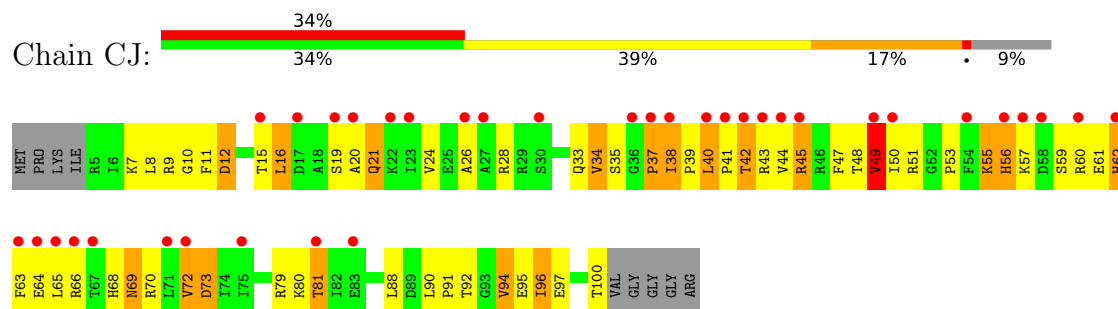
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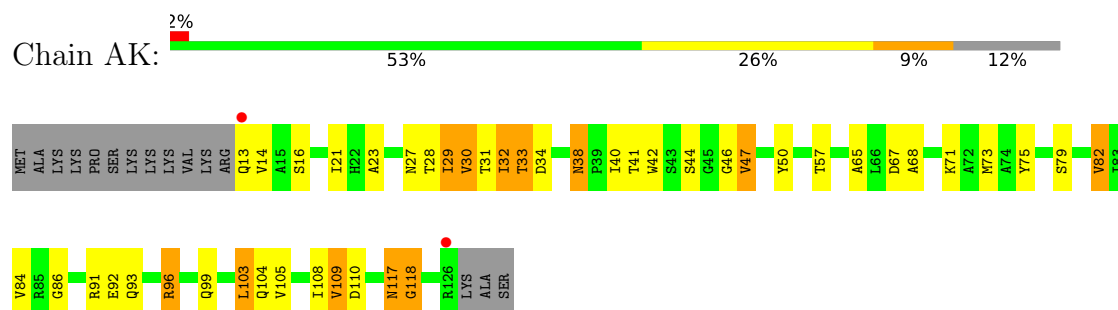
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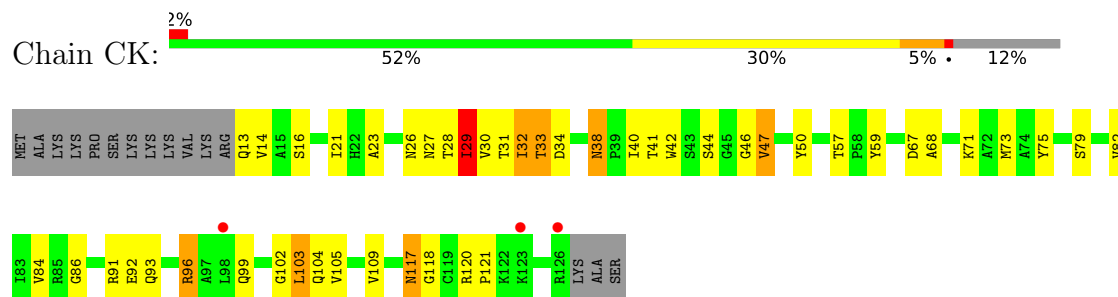
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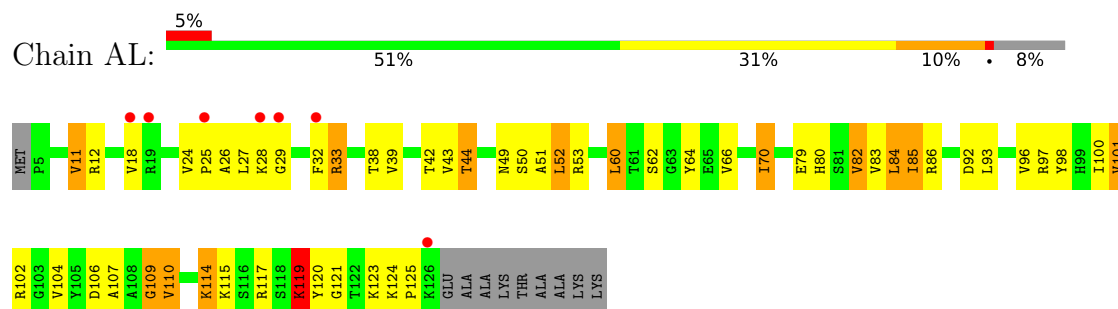
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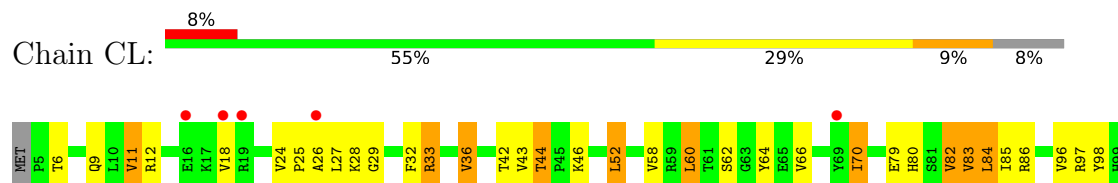
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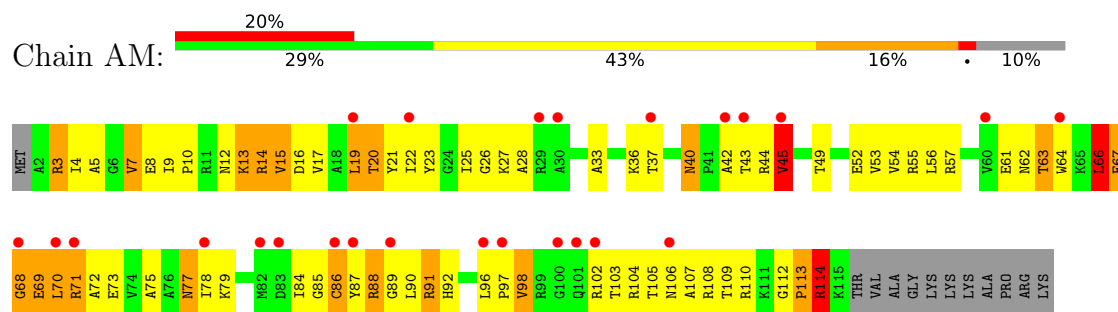
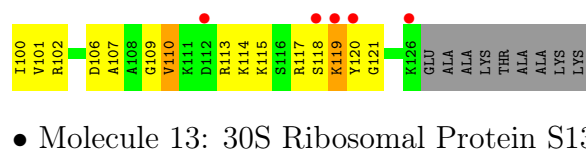


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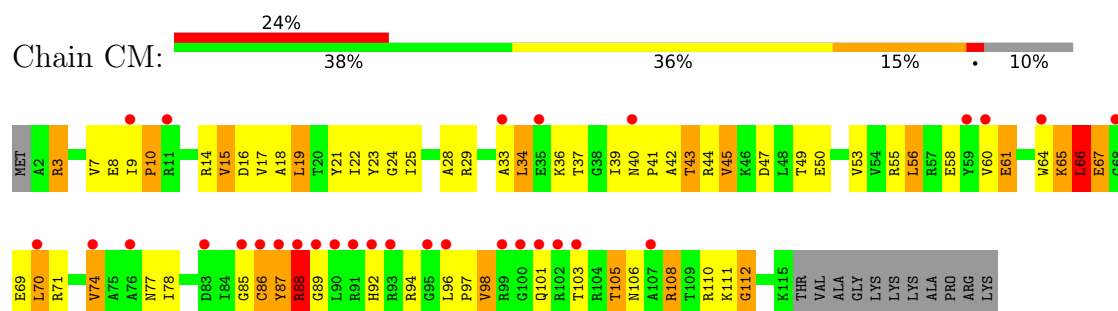


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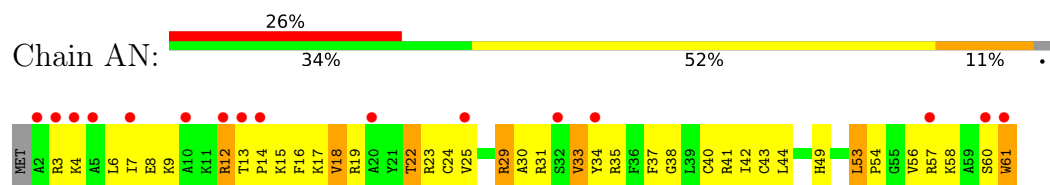




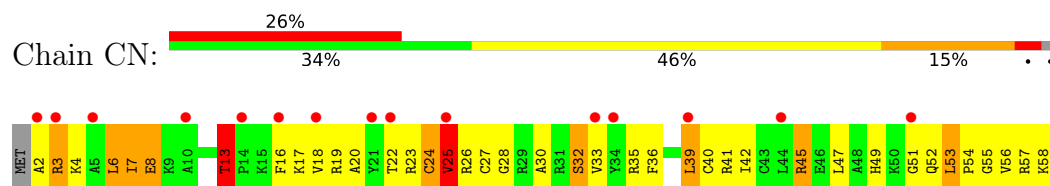
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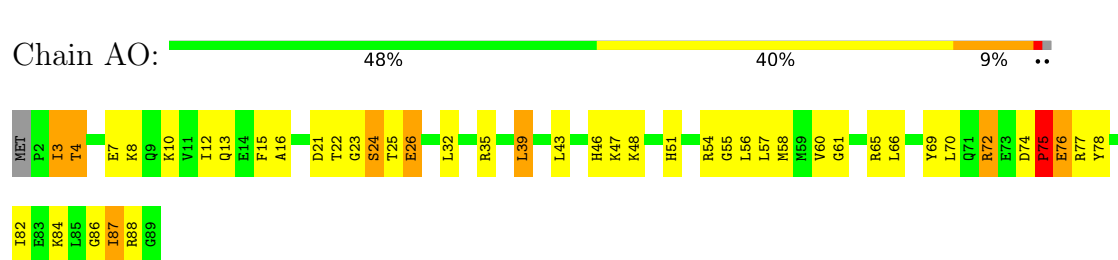
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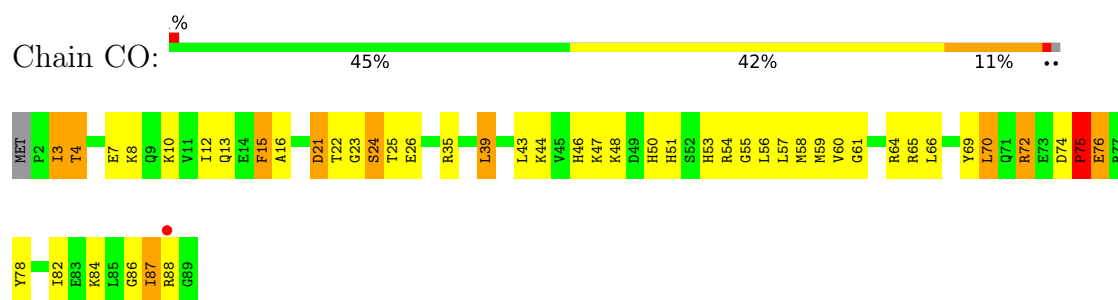
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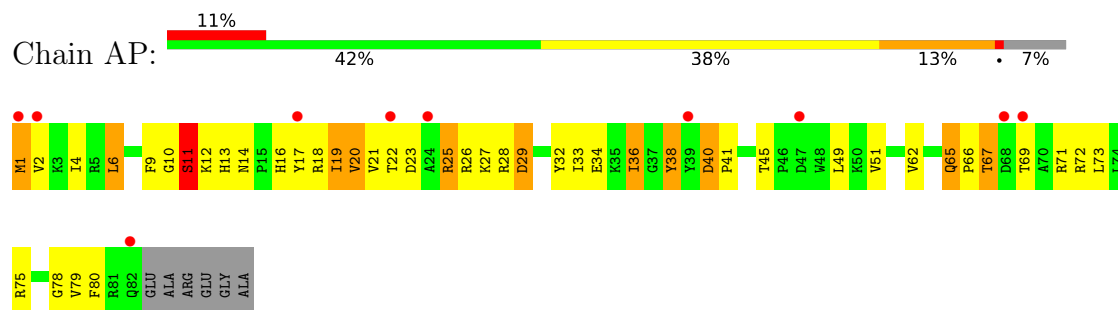
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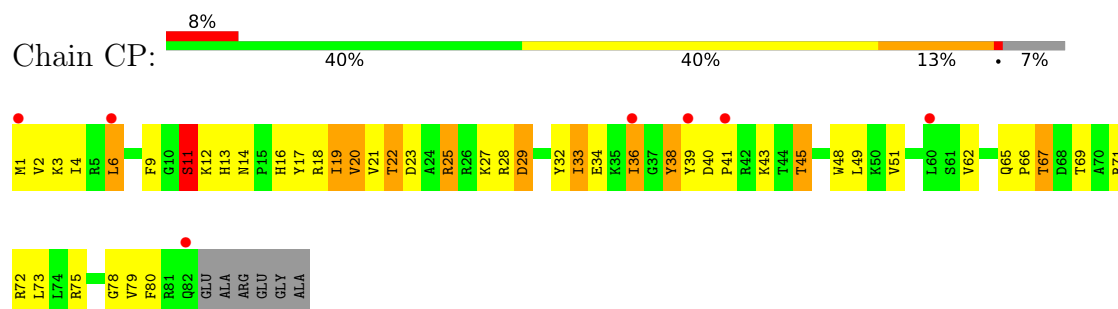
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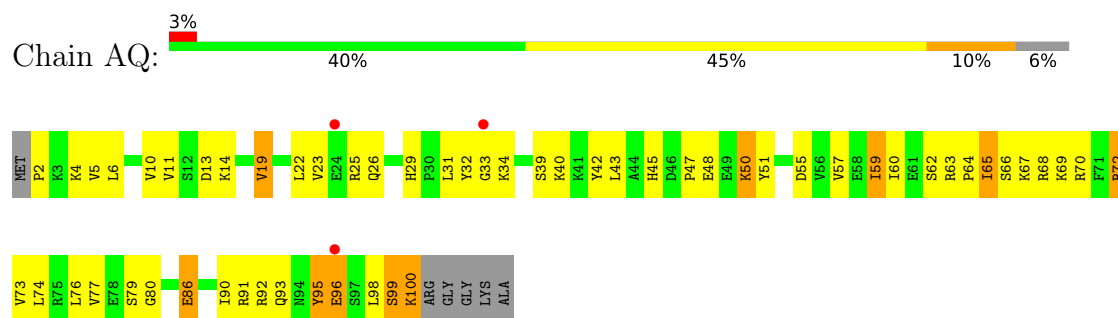
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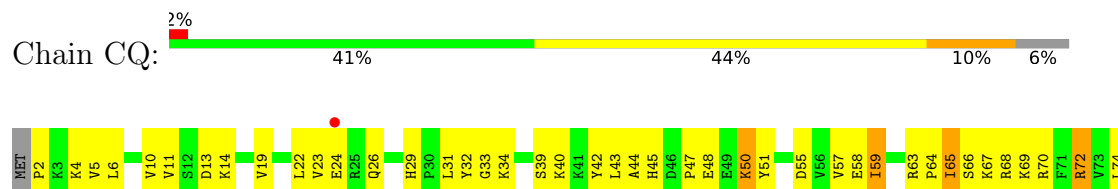
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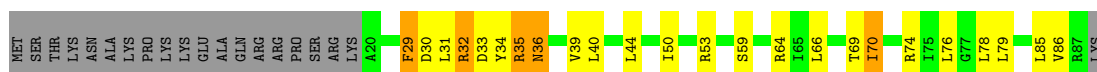
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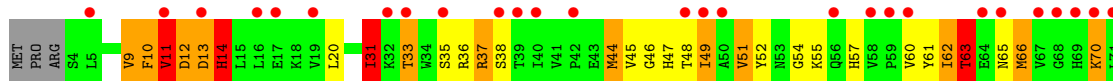
- Molecule 18: 30S Ribosomal Protein S18



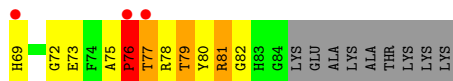
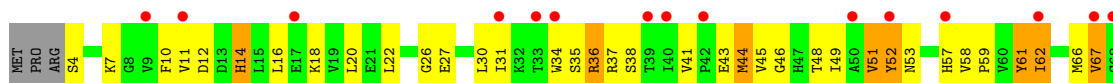
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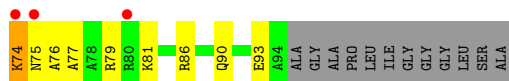
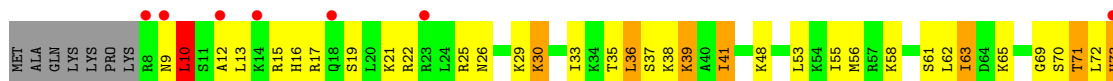
- Molecule 19: 30S Ribosomal Protein S19



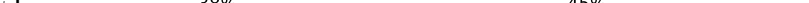
- Molecule 19: 30S Ribosomal Protein S19



- Molecule 20: 30S Ribosomal Protein S20

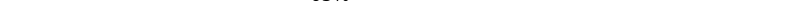


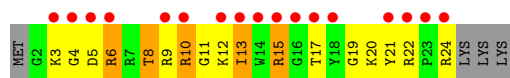
- Molecule 20: 30S Ribosomal Protein S20

Chain CT: 



- Molecule 21: 30S Ribosomal Protein THX

Chain AU: 

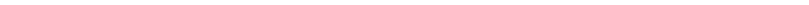


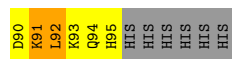
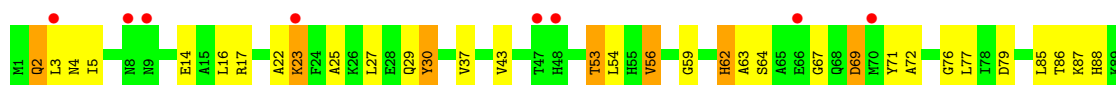
- Molecule 21: 30S Ribosomal Protein THX

Chain CU: 

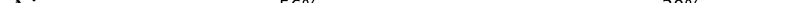


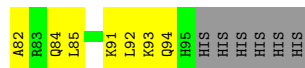
- Molecule 22: Probable sigma(54) modulation protein

Chain AX: 

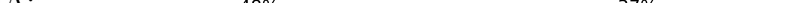


- Molecule 22: Probable sigma(54) modulation protein

Chain CX: 



- Molecule 23: 23S Ribosomal RNA

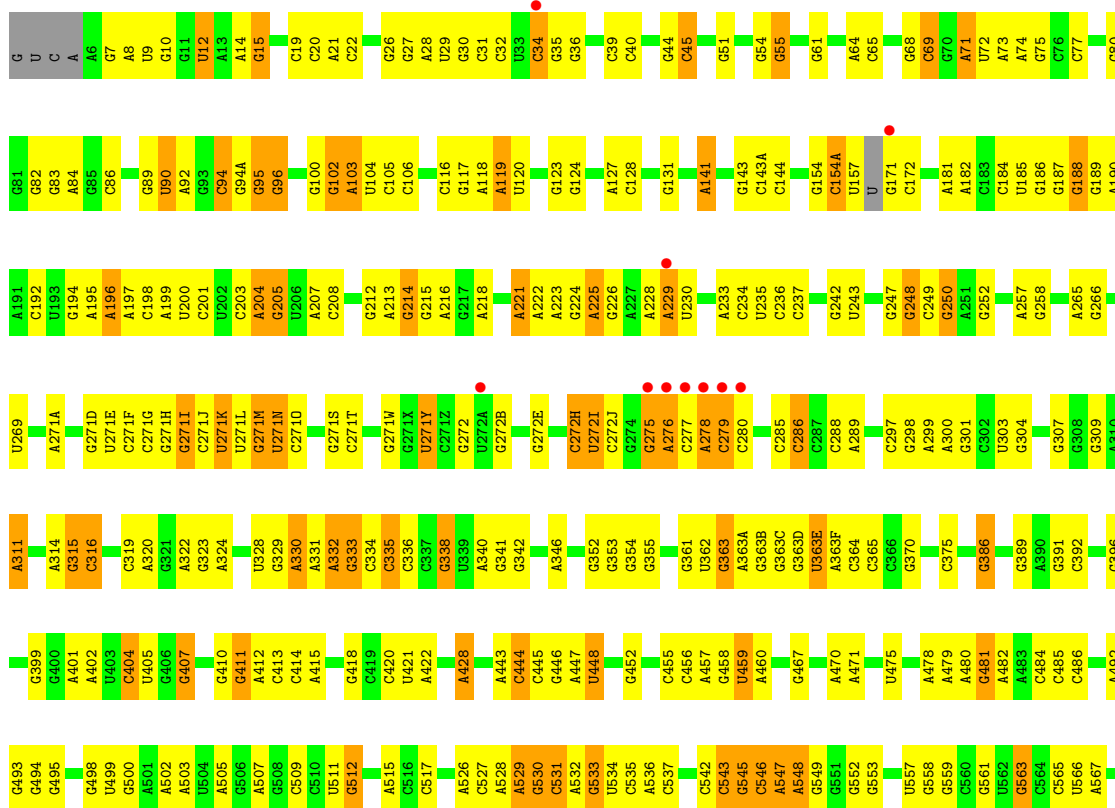
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G1144	U	G1015	C924	U848	U762	C659	C605	A515	A432	G329	U271K	G96
G1151	C	G1016	U	A849	A764	G662	U607	C516	G438	A330	U271L	G100
G1152	U	G1017	G928	G853	G765	C665	U614A	C517	U	A331	U271M	G102
G1153	U	U1018	G932	U	G769	G666	G614B	C527	A443	A332	C271O	A103
G1154	U	U1019	A933	U	U769	G667	G614C	A528	A444	G333	G271S	U104
A1155	A	A1020	U	C856	G770	U667	A614C	A529	C444	C334	C271T	C105
A1156	A	G1022	G938	C857	G771	G668	G615	G530	C445	C335	G271U	U
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G1162	A	G1025	G942	U860	G775	G674	G624	G533	A449	G341	G271X	A118
G1163	G	U1026	U943	A861	G776	U675	U	U534	G450	G342	U271Y	U120
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U1166	G	U1030	U	U865	A782	A685	G630	C541	A454	G353	G272C	C129
G1169	U	G1031	A953	U866	A783	G686	A631	C542	C455	G354	G272D	G131
G1170	A	U1033	G954	C869	A784	U	A632	C543	C456	G355	U	A141
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G1172	U	U1035	G956	A879	C786	U	A634	C545	U458	G361	C272F	C143A
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C1178	C	G1042	C961	C883	G792	G704	U639	U557	U	G363D	G274	G240
C1179	A	C1043	G962	C884	C796	A705	C640	G558	G467	U362	G275	A241
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G1184	U	A1045	G968	C886	C797	G707	A644	G560	A470	U363F	A276	U243
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G1186	A	A1048	C973	C889	U803	G710	A646	G562	A472	U	C279	U
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A1194	A	U	G979	U895	U810	A718	A652A	G570	A483	G386	C296	U185
C1201	G	G	A980	A896	U811	C719	A652B	A571	C484	U387	C297	G186
A1204	G	U	A983	C897	C812	U	G652C	A572	C485	U	G247	G187
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G1235	C	C	A917	A918	U831	A746	G	C582	U	U269	G269	C197
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U1141	G	G	U921	U922	U833	G748	G652J	U584	A503	G307	G308	C201
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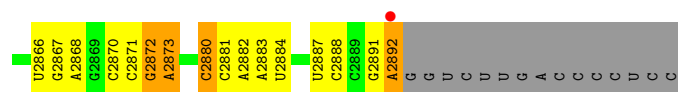
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- Molecule 23: 23S Ribosomal RNA

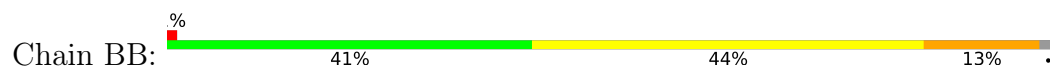




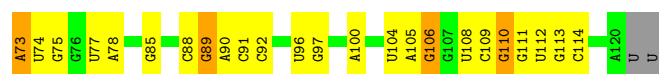
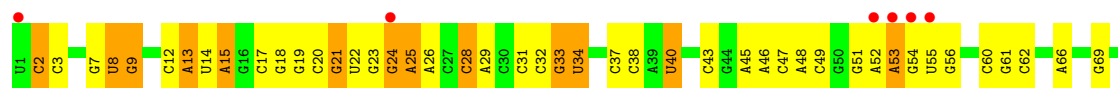
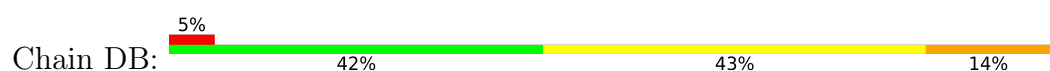
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G2791	A2713	A2632	G2545	C2442	A2289	C2201	G2060	A1969	C1893	U1798	A1700
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• Molecule 24: 5S Ribosomal RNA



• Molecule 24: 5S Ribosomal RNA



• Molecule 25: 50S Ribosomal Protein L2

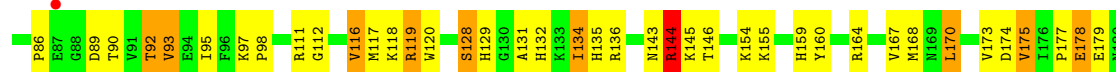
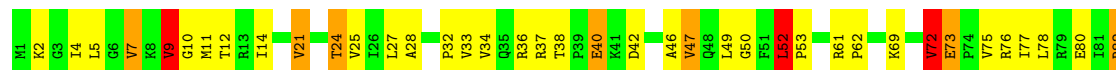


• Molecule 25: 50S Ribosomal Protein L2

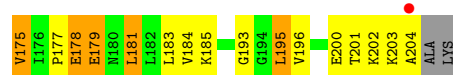
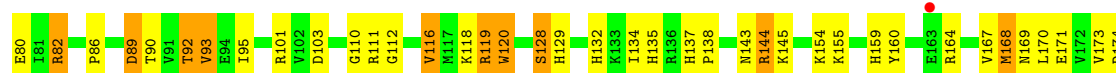
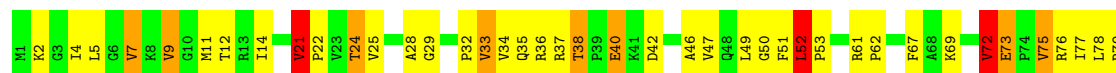




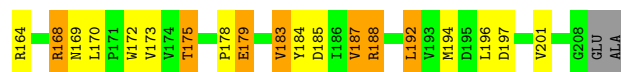
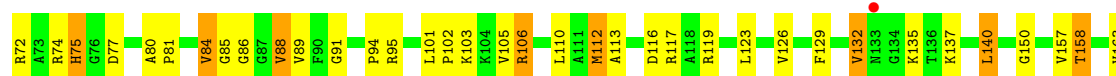
• Molecule 26: 50S Ribosomal Protein L3



• Molecule 26: 50S Ribosomal Protein L3

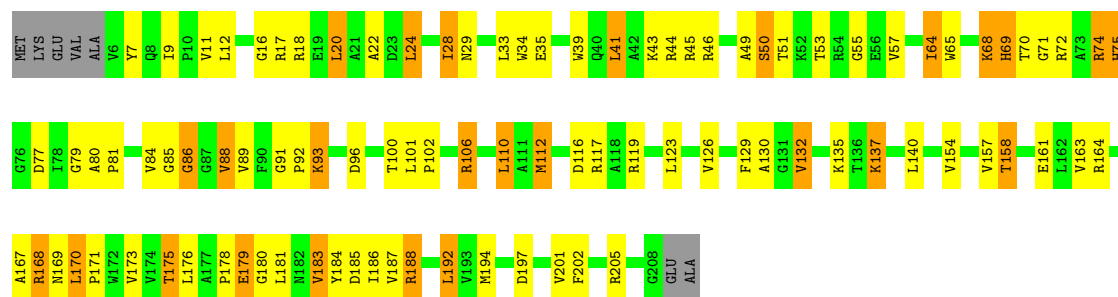


• Molecule 27: 50S Ribosomal Protein L4



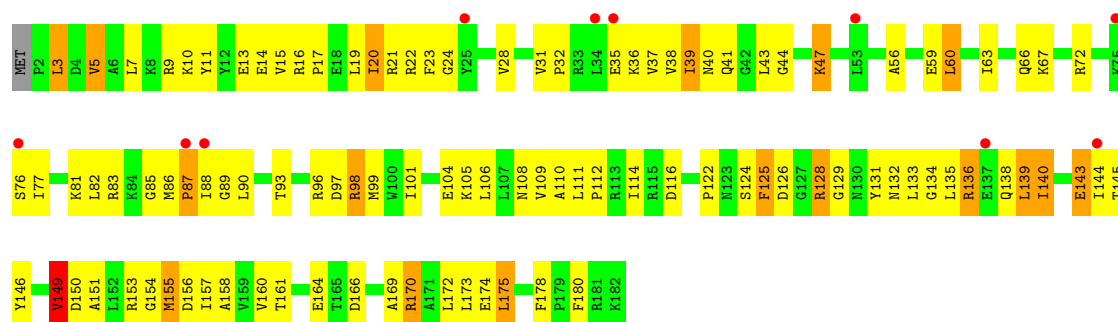
• Molecule 27: 50S Ribosomal Protein L4





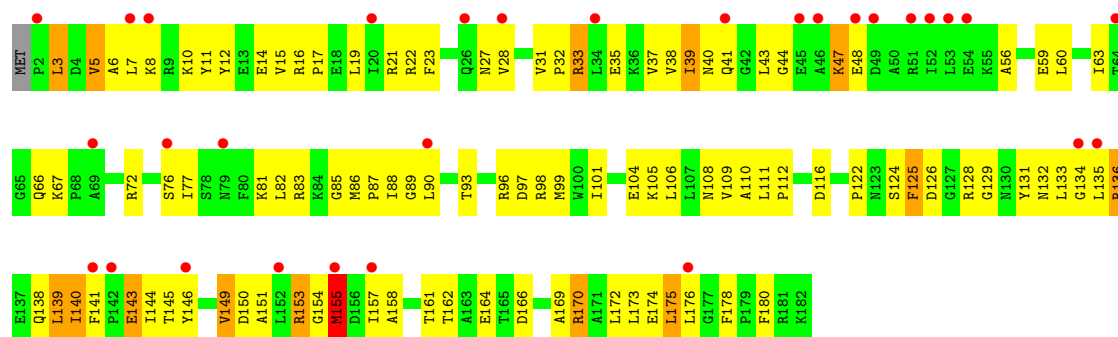
• Molecule 28: 50S Ribosomal Protein L5

Chain BG: 5% 42% 47% 9% ..



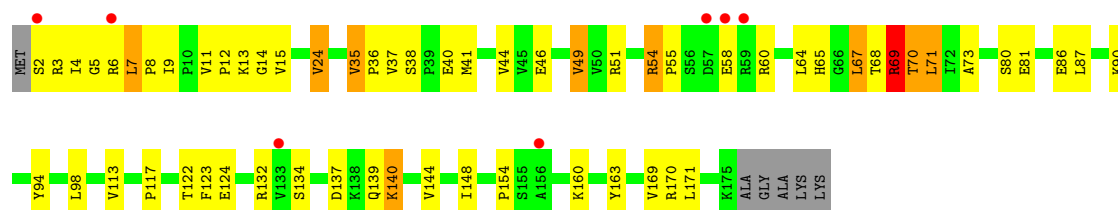
• Molecule 28: 50S Ribosomal Protein L5

Chain DG: 16% 42% 49% 8% ..

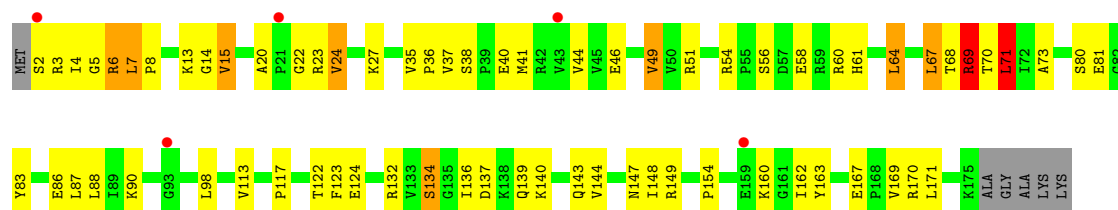


• Molecule 29: 50S Ribosomal Protein L6

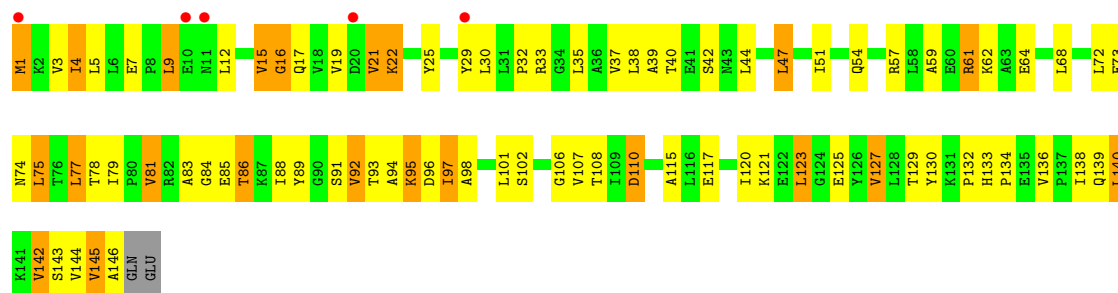
Chain BH: 4% 63% 28% 5% ..



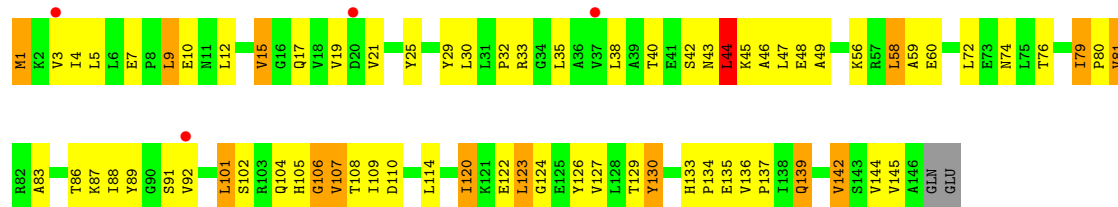
• Molecule 29: 50S Ribosomal Protein L6



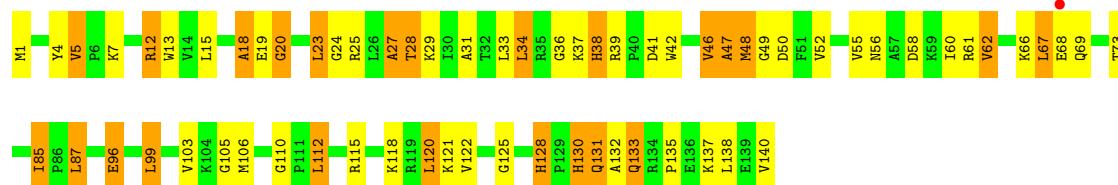
• Molecule 30: 50S Ribosomal Protein L9



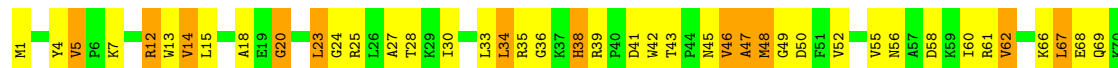
• Molecule 30: 50S Ribosomal Protein L9

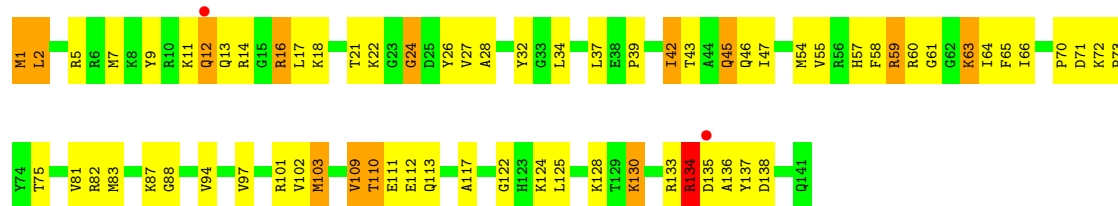


• Molecule 31: 50S Ribosomal Protein L13

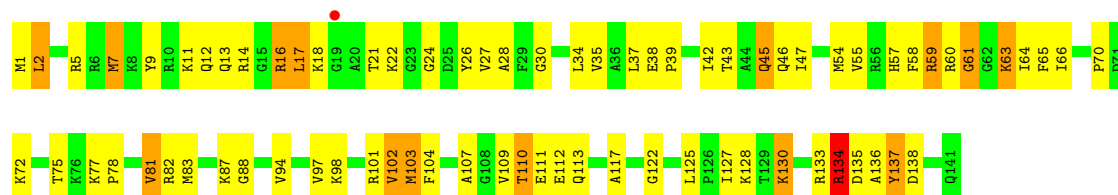


• Molecule 31: 50S Ribosomal Protein L13

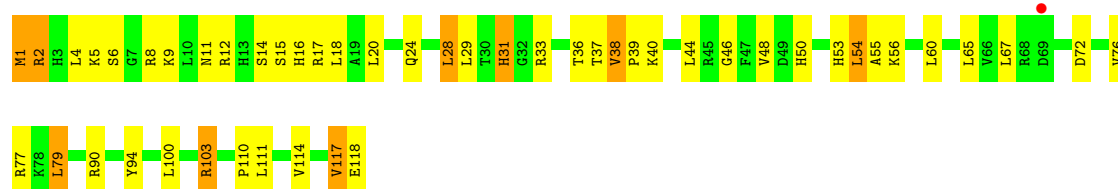




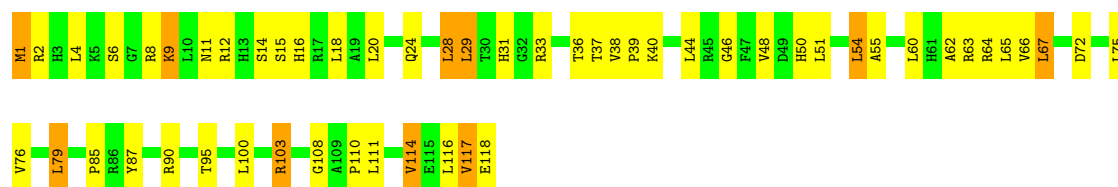
• Molecule 34: 50S Ribosomal Protein L16



• Molecule 35: 50S Ribosomal Protein L17



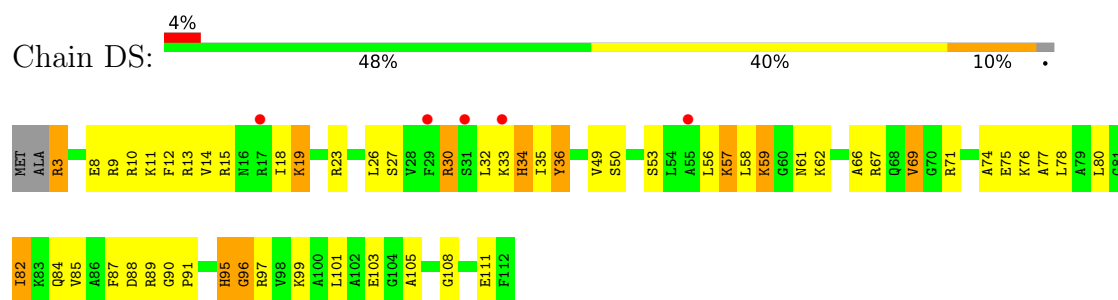
• Molecule 36: 50S Ribosomal Protein L18



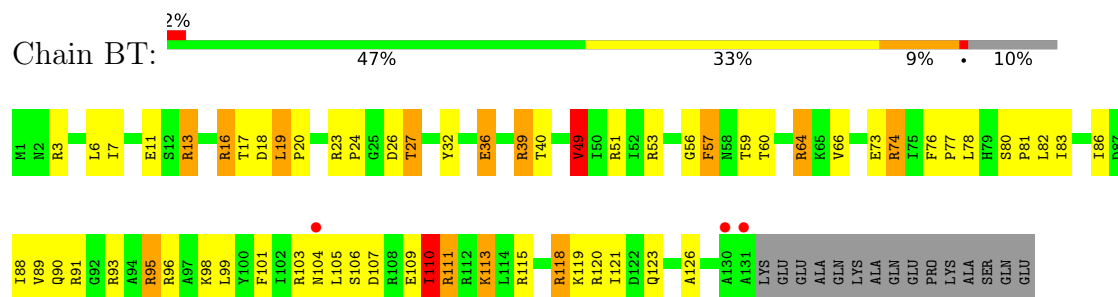
• Molecule 37: 50S Ribosomal Protein L19



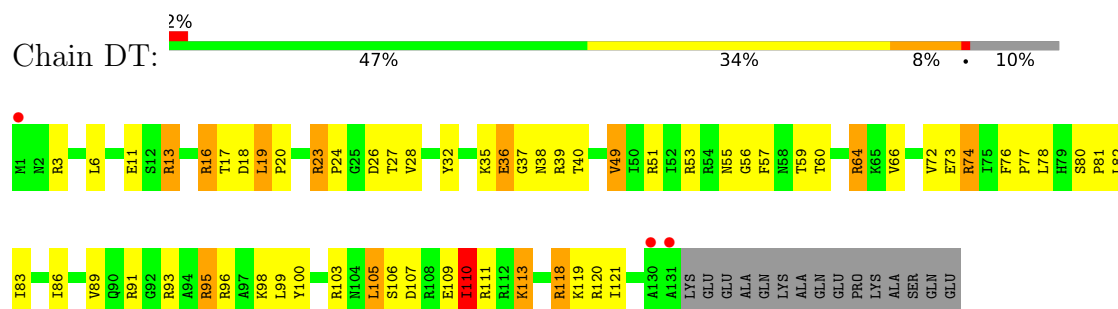
• Molecule 38: 50S Ribosomal Protein L20



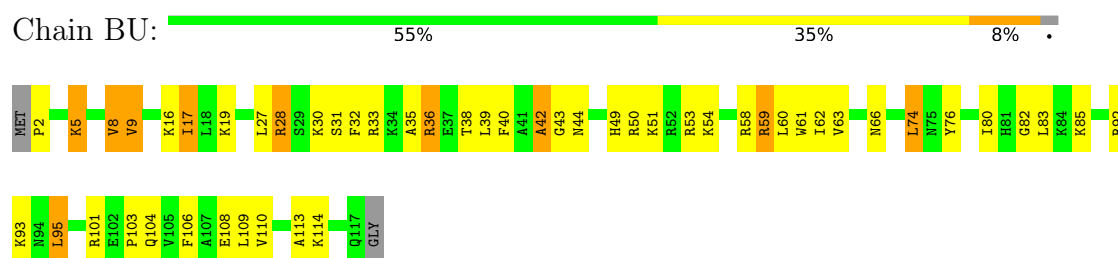
• Molecule 37: 50S Ribosomal Protein L19



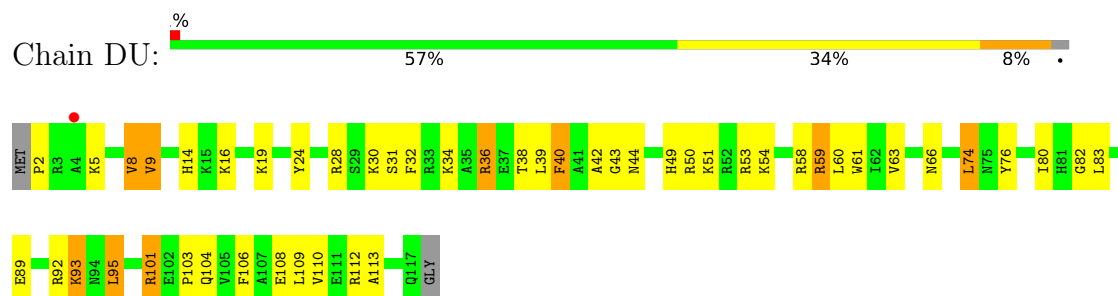
• Molecule 37: 50S Ribosomal Protein L19



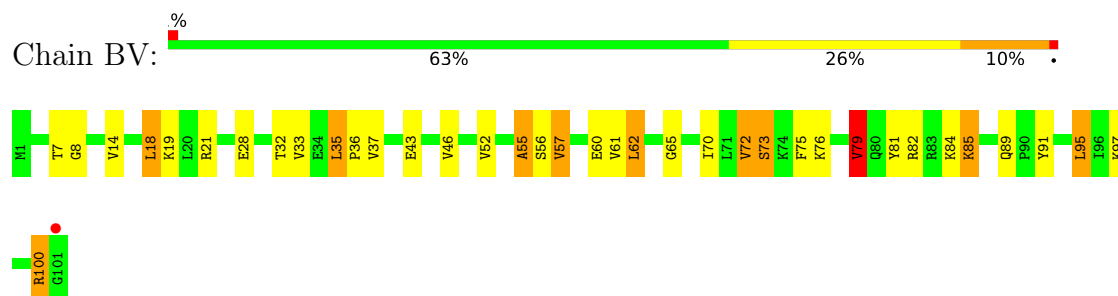
• Molecule 38: 50S Ribosomal Protein L20



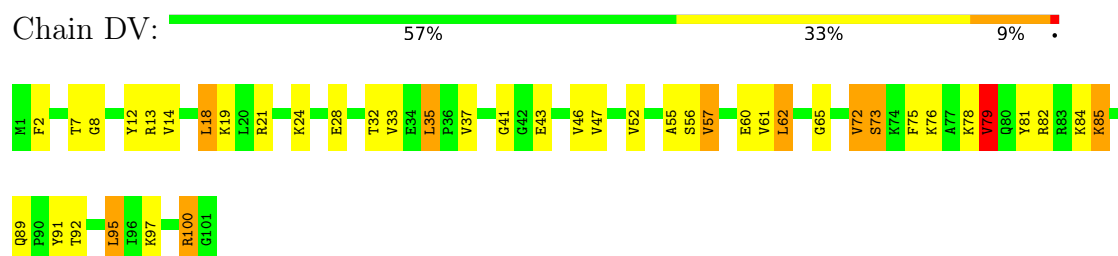
• Molecule 38: 50S Ribosomal Protein L20



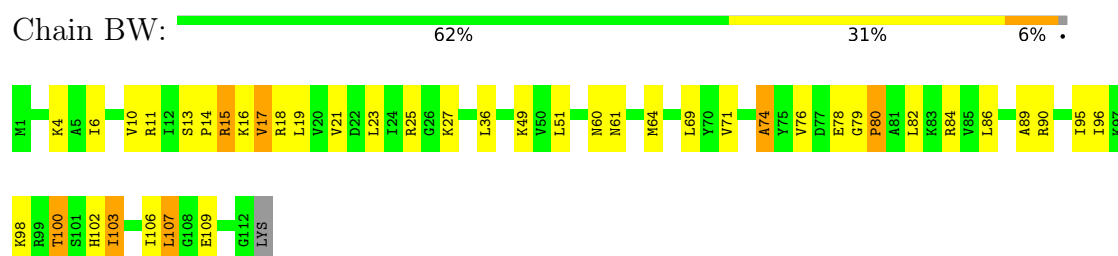
● Molecule 39: 50S Ribosomal Protein L21



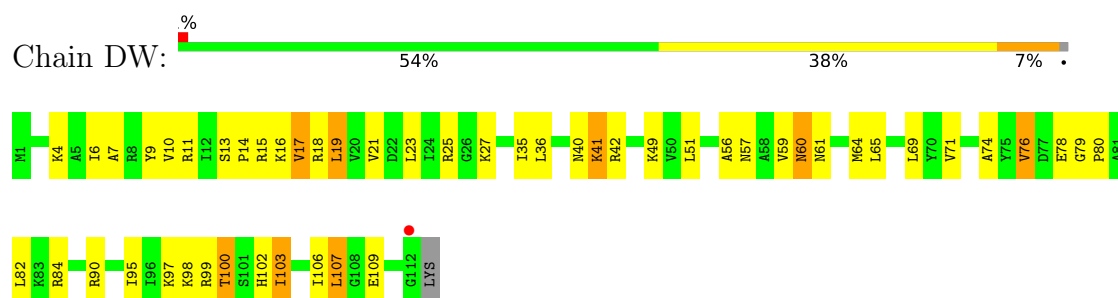
● Molecule 39: 50S Ribosomal Protein L21



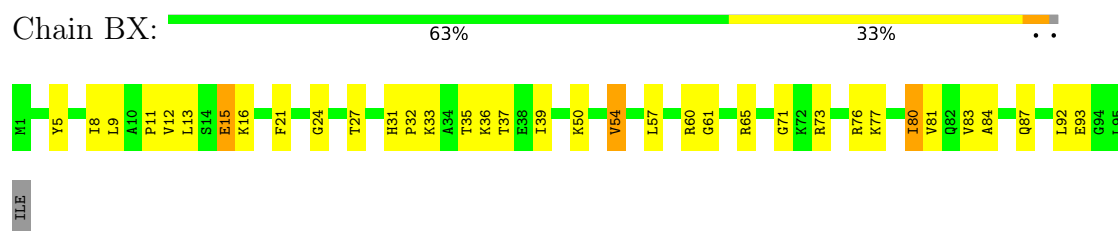
● Molecule 40: 50S Ribosomal Protein L22



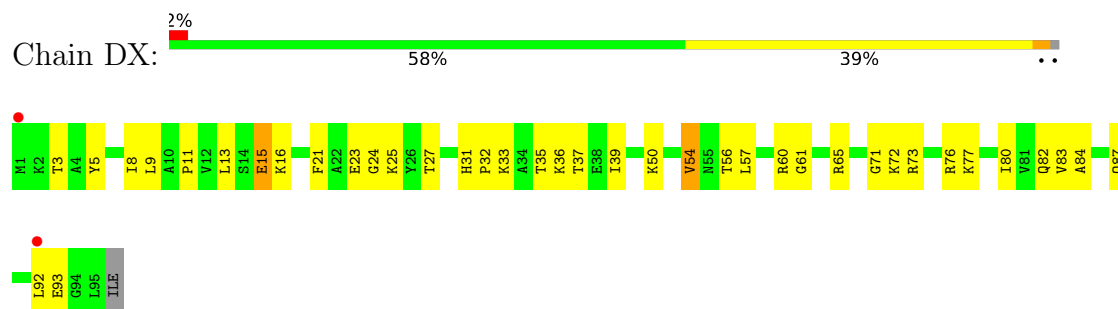
● Molecule 40: 50S Ribosomal Protein L22



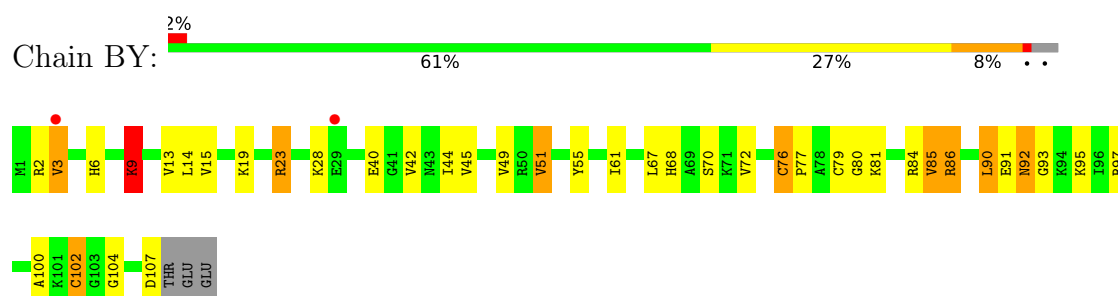
● Molecule 41: 50S Ribosomal Protein L23



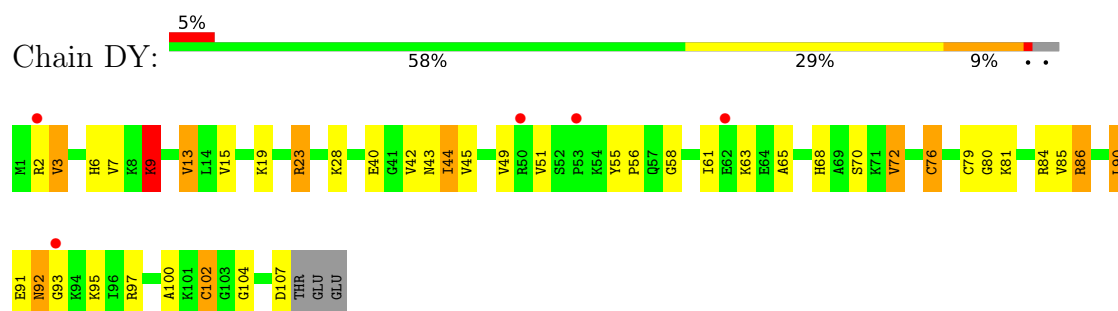
- Molecule 41: 50S Ribosomal Protein L23



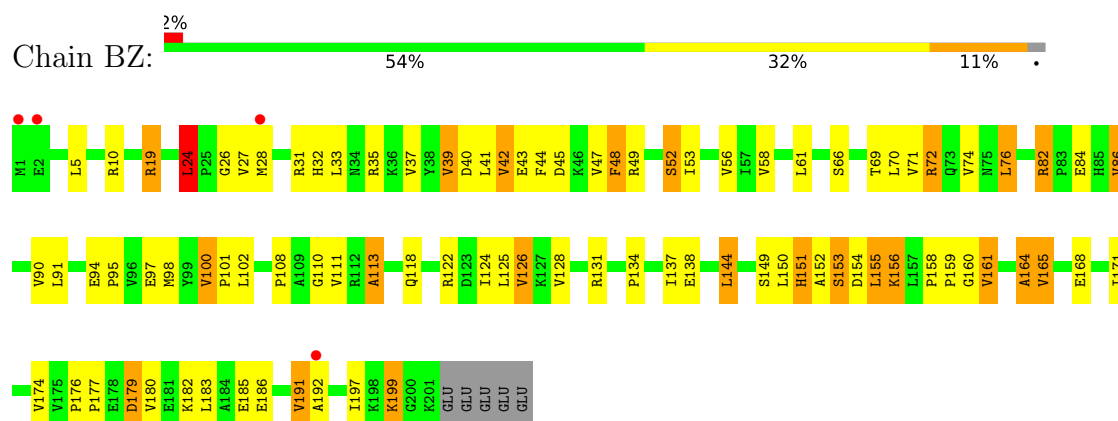
- Molecule 42: 50S Ribosomal Protein L24



- Molecule 42: 50S Ribosomal Protein L24

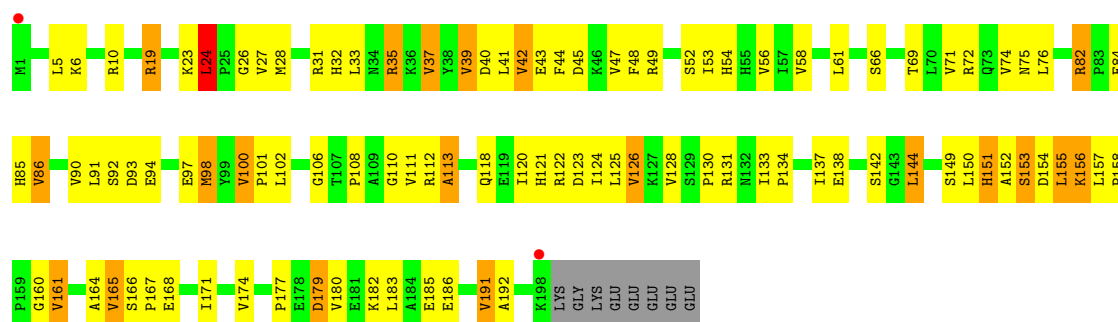


- Molecule 43: 50S Ribosomal Protein L25



- Molecule 43: 50S Ribosomal Protein L25





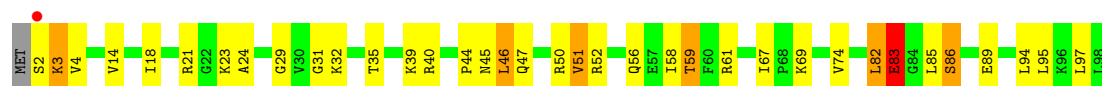
• Molecule 44: 50S Ribosomal Protein L27



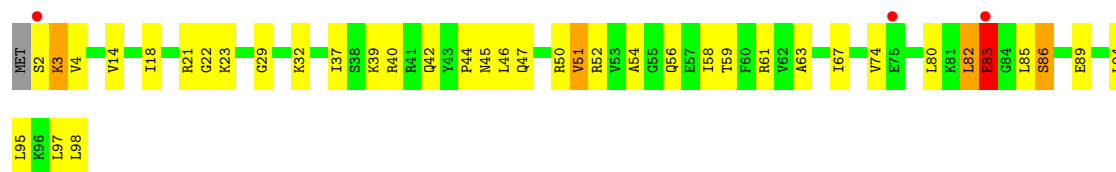
• Molecule 44: 50S Ribosomal Protein L27



• Molecule 45: 50S Ribosomal Protein L28



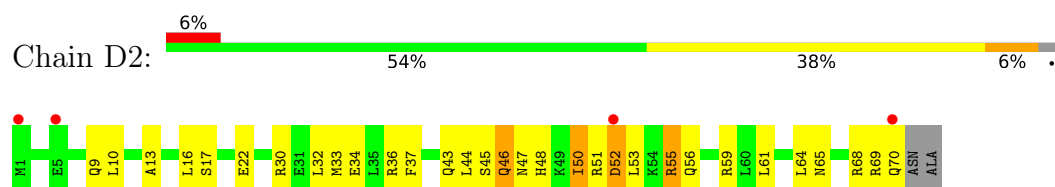
• Molecule 45: 50S Ribosomal Protein L28



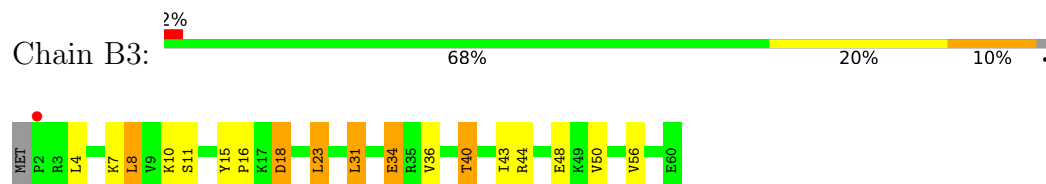
• Molecule 46: 50S Ribosomal Protein L29



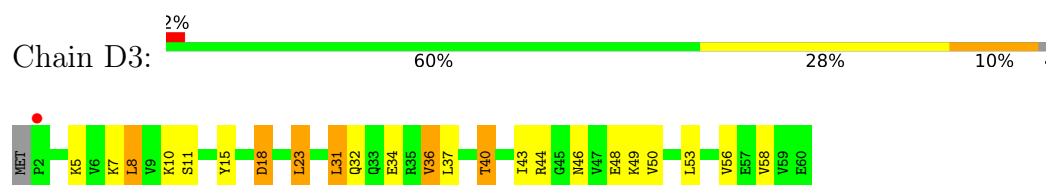
• Molecule 46: 50S Ribosomal Protein L29



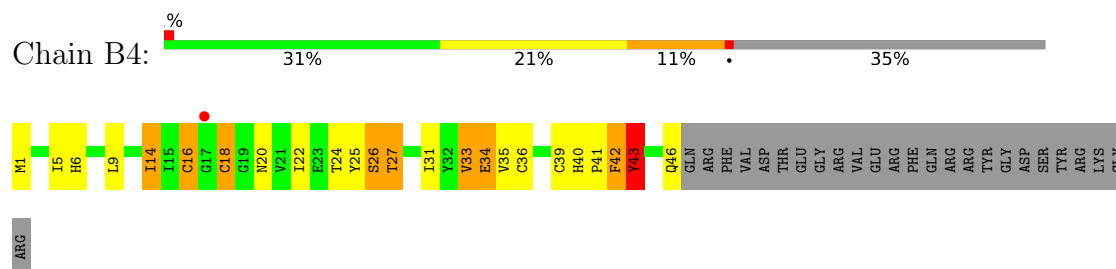
• Molecule 47: 50S Ribosomal Protein L30



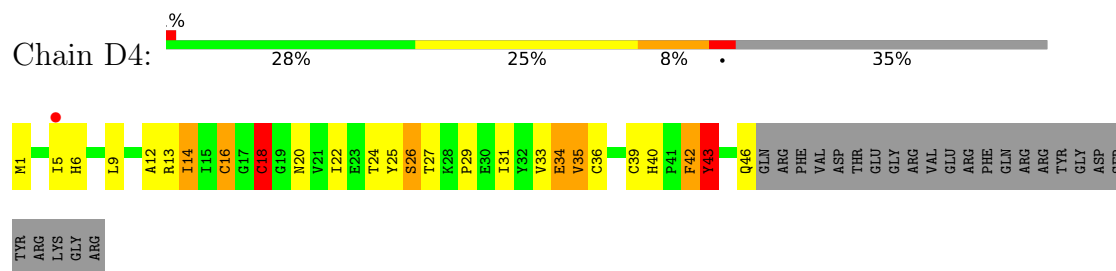
• Molecule 47: 50S Ribosomal Protein L30



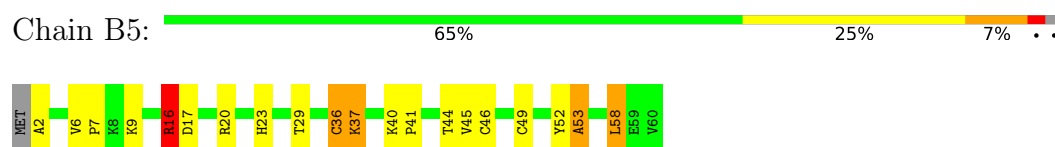
• Molecule 48: 50S Ribosomal Protein L31



• Molecule 48: 50S Ribosomal Protein L31



• Molecule 49: 50S Ribosomal Protein L32

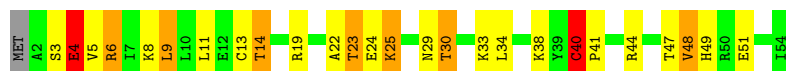


• Molecule 49: 50S Ribosomal Protein L32





- Molecule 50: 50S Ribosomal Protein L33



- Molecule 50: 50S Ribosomal Protein L33



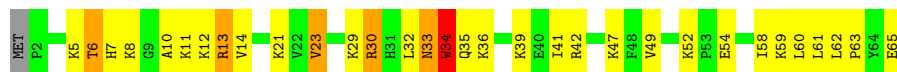
- Molecule 51: 50S Ribosomal Protein L34



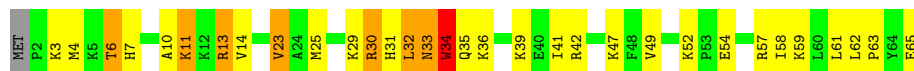
- Molecule 51: 50S Ribosomal Protein L34



- 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	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.216 , 0.258 0.213 , 0.256	Depositor DCC
R_{free} test set	49829 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	286308	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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	0.63	3/36123 (0.0%)	0.56	5/56379 (0.0%)
1	CA	0.61	3/36028 (0.0%)	0.56	4/56231 (0.0%)
2	AB	0.87	0/1822	1.25	13/2468 (0.5%)
2	CB	0.92	0/1809	1.24	15/2450 (0.6%)
3	AC	1.03	0/1474	1.37	14/2003 (0.7%)
3	CC	1.06	3/1474 (0.2%)	1.30	9/2003 (0.4%)
4	AD	0.85	1/1556 (0.1%)	1.30	17/2113 (0.8%)
4	CD	0.86	4/1556 (0.3%)	1.32	22/2113 (1.0%)
5	AE	0.76	0/1121	1.25	11/1517 (0.7%)
5	CE	0.76	0/1121	1.26	14/1517 (0.9%)
6	AF	0.75	0/790	1.17	4/1077 (0.4%)
6	CF	0.74	0/790	1.17	5/1077 (0.5%)
7	AG	1.39	2/1183 (0.2%)	1.51	23/1599 (1.4%)
7	CG	1.27	3/1183 (0.3%)	1.45	15/1599 (0.9%)
8	AH	0.72	0/1065	1.17	8/1445 (0.6%)
8	CH	0.69	0/1065	1.17	5/1445 (0.3%)
9	AI	1.28	1/867 (0.1%)	1.51	13/1180 (1.1%)
9	CI	1.43	1/867 (0.1%)	1.40	12/1180 (1.0%)
10	AJ	1.18	2/676 (0.3%)	1.51	8/924 (0.9%)
10	CJ	1.34	1/676 (0.1%)	1.47	10/924 (1.1%)
11	AK	0.76	0/843	1.19	5/1144 (0.4%)
11	CK	0.72	0/843	1.19	7/1144 (0.6%)
12	AL	0.78	0/921	1.17	6/1247 (0.5%)
12	CL	0.80	0/921	1.21	6/1247 (0.5%)
13	AM	1.49	5/814 (0.6%)	1.58	18/1107 (1.6%)
13	CM	1.42	3/814 (0.4%)	1.59	12/1107 (1.1%)
14	AN	0.91	0/487	1.32	4/649 (0.6%)
14	CN	0.93	1/487 (0.2%)	1.22	3/649 (0.5%)
15	AO	0.82	0/735	1.13	1/981 (0.1%)
15	CO	0.82	0/735	1.17	3/981 (0.3%)
16	AP	0.77	0/667	1.24	4/905 (0.4%)
16	CP	0.71	0/667	1.20	2/905 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.75	0/836	1.20	3/1117 (0.3%)
17	CQ	0.76	0/836	1.24	3/1117 (0.3%)
18	AR	0.73	0/519	1.14	4/699 (0.6%)
18	CR	0.73	0/519	1.08	2/699 (0.3%)
19	AS	1.41	2/574 (0.3%)	1.47	10/781 (1.3%)
19	CS	1.43	3/574 (0.5%)	1.51	11/781 (1.4%)
20	AT	0.75	0/666	1.18	2/880 (0.2%)
20	CT	0.82	0/715	1.30	10/947 (1.1%)
21	AU	1.01	0/203	1.30	0/266
21	CU	1.14	0/203	1.34	2/266 (0.8%)
22	AX	0.93	0/637	1.27	3/864 (0.3%)
22	CX	1.06	0/606	1.39	7/828 (0.8%)
23	BA	0.86	3/68445 (0.0%)	0.61	7/106848 (0.0%)
23	DA	0.67	0/67893	0.59	4/105980 (0.0%)
24	BB	0.65	0/2878	0.55	0/4490
24	DB	0.62	0/2878	0.55	0/4490
25	BD	1.18	6/2185 (0.3%)	1.33	15/2942 (0.5%)
25	DD	0.99	1/2186 (0.0%)	1.30	14/2944 (0.5%)
26	BE	1.16	5/1588 (0.3%)	1.34	10/2145 (0.5%)
26	DE	0.97	1/1588 (0.1%)	1.31	10/2145 (0.5%)
27	BF	1.16	3/1615 (0.2%)	1.33	17/2188 (0.8%)
27	DF	0.90	1/1615 (0.1%)	1.33	19/2188 (0.9%)
28	BG	0.76	0/1393	1.21	8/1892 (0.4%)
28	DG	0.84	0/1393	1.26	9/1892 (0.5%)
29	BH	1.00	2/1343 (0.1%)	1.28	9/1820 (0.5%)
29	DH	0.79	0/1343	1.25	6/1820 (0.3%)
30	BI	0.82	0/1052	1.29	13/1441 (0.9%)
30	DI	0.89	0/967	1.43	13/1334 (1.0%)
31	BN	1.16	3/1139 (0.3%)	1.34	14/1538 (0.9%)
31	DN	0.89	0/1139	1.38	15/1538 (1.0%)
32	BO	1.10	2/933 (0.2%)	1.35	10/1257 (0.8%)
32	DO	0.90	0/933	1.30	10/1257 (0.8%)
33	BP	1.06	0/1148	1.31	9/1529 (0.6%)
33	DP	0.86	0/1148	1.31	7/1529 (0.5%)
34	BQ	1.08	1/1143 (0.1%)	1.27	8/1527 (0.5%)
34	DQ	0.91	0/1143	1.26	10/1527 (0.7%)
35	BR	1.12	1/982 (0.1%)	1.19	2/1312 (0.2%)
35	DR	0.94	0/982	1.18	1/1312 (0.1%)
36	BS	0.88	0/875	1.20	4/1168 (0.3%)
36	DS	0.80	0/875	1.17	4/1168 (0.3%)
37	BT	1.06	3/1077 (0.3%)	1.30	13/1444 (0.9%)
37	DT	0.89	0/1077	1.26	9/1444 (0.6%)
38	BU	1.37	2/977 (0.2%)	1.19	4/1301 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	1.00	1/977 (0.1%)	1.16	4/1301 (0.3%)
39	BV	1.09	1/782 (0.1%)	1.27	4/1049 (0.4%)
39	DV	0.90	0/782	1.25	2/1049 (0.2%)
40	BW	1.40	4/891 (0.4%)	1.19	1/1197 (0.1%)
40	DW	1.20	5/891 (0.6%)	1.21	1/1197 (0.1%)
41	BX	1.16	1/756 (0.1%)	1.14	2/1016 (0.2%)
41	DX	0.94	0/756	1.15	2/1016 (0.2%)
42	BY	1.03	1/798 (0.1%)	1.30	8/1073 (0.7%)
42	DY	0.86	0/798	1.29	9/1073 (0.8%)
43	BZ	0.91	0/1569	1.31	16/2137 (0.7%)
43	DZ	0.87	1/1555 (0.1%)	1.30	12/2118 (0.6%)
44	B0	1.03	0/602	1.26	3/804 (0.4%)
44	D0	0.89	0/602	1.31	1/804 (0.1%)
45	B1	1.13	2/752 (0.3%)	1.23	4/1003 (0.4%)
45	D1	1.05	2/752 (0.3%)	1.22	4/1003 (0.4%)
46	B2	1.05	0/590	1.23	3/781 (0.4%)
46	D2	0.92	0/590	1.22	3/781 (0.4%)
47	B3	1.05	0/463	1.23	4/623 (0.6%)
47	D3	0.85	0/463	1.30	2/623 (0.3%)
48	B4	0.82	0/358	1.31	4/487 (0.8%)
48	D4	0.99	0/358	1.32	5/487 (1.0%)
49	B5	1.14	0/469	1.40	5/634 (0.8%)
49	D5	1.00	0/469	1.35	7/634 (1.1%)
50	B6	1.06	0/456	1.21	3/609 (0.5%)
50	D6	0.82	0/456	1.19	3/609 (0.5%)
51	B7	1.36	1/426 (0.2%)	1.39	3/561 (0.5%)
51	D7	1.13	2/426 (0.5%)	1.30	5/561 (0.9%)
52	B8	1.23	1/516 (0.2%)	1.51	8/679 (1.2%)
52	D8	1.00	0/516	1.44	6/679 (0.9%)
53	B9	1.05	0/300	1.23	1/395 (0.3%)
53	D9	0.89	1/300 (0.3%)	1.19	0/395
All	All	0.81	95/305420 (0.0%)	0.83	764/457343 (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	3
2	CB	0	4
3	AC	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	1
4	AD	0	1
4	CD	0	1
7	CG	0	2
9	AI	0	1
9	CI	0	1
10	AJ	0	2
10	CJ	0	2
13	AM	0	4
13	CM	0	2
14	AN	0	1
15	AO	0	1
15	CO	0	1
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
19	CS	0	1
20	AT	0	1
20	CT	0	1
23	BA	0	1
23	DA	0	1
26	BE	0	1
26	DE	0	1
27	DF	0	1
30	DI	0	1
34	BQ	0	1
34	DQ	0	1
36	BS	0	1
36	DS	0	1
41	BX	0	1
41	DX	0	1
43	BZ	0	3
43	DZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	1
48	D4	0	1
All	All	0	56

The worst 5 of 95 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	B7	30	VAL	CA-CB	-9.53	1.43	1.54
45	B1	67	ILE	CA-CB	-9.22	1.49	1.54
45	D1	67	ILE	CA-CB	-8.42	1.50	1.54
13	AM	9	ILE	CA-CB	8.13	1.64	1.54
23	BA	2055	C	P-OP1	-8.10	1.32	1.49

The worst 5 of 764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	DI	106	GLY	N-CA-C	13.70	130.21	111.03
10	AJ	52	GLY	CA-C-N	11.61	131.95	119.87
10	AJ	52	GLY	C-N-CA	11.61	131.95	119.87
52	B8	52	LYS	CA-C-N	-11.48	107.03	118.97
52	B8	52	LYS	C-N-CA	-11.48	107.03	118.97

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	129	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	19	GLU	Peptide
3	AC	51	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	32270	0	16286	1215	0
1	CA	32185	0	16244	1269	1
2	AB	1787	0	1752	128	0
2	CB	1775	0	1743	124	0
3	AC	1450	0	1314	93	0
3	CC	1450	0	1314	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1526	0	1415	74	0
4	CD	1526	0	1415	89	0
5	AE	1105	0	1130	58	0
5	CE	1105	0	1130	62	0
6	AF	777	0	737	35	0
6	CF	777	0	737	38	0
7	AG	1164	0	1106	88	0
7	CG	1164	0	1106	101	0
8	AH	1045	0	1033	49	0
8	CH	1045	0	1033	51	0
9	AI	852	0	742	85	0
9	CI	852	0	742	82	0
10	AJ	663	0	558	55	0
10	CJ	663	0	558	71	0
11	AK	828	0	822	28	0
11	CK	828	0	822	28	0
12	AL	905	0	916	41	0
12	CL	905	0	916	33	0
13	AM	804	0	752	59	0
13	CM	804	0	752	60	0
14	AN	478	0	497	35	0
14	CN	478	0	496	58	0
15	AO	724	0	749	35	0
15	CO	724	0	749	32	0
16	AP	651	0	638	33	0
16	CP	651	0	638	37	0
17	AQ	823	0	891	44	0
17	CQ	823	0	891	48	0
18	AR	514	0	530	27	0
18	CR	514	0	530	23	0
19	AS	560	0	466	46	0
19	CS	560	0	466	42	0
20	AT	665	0	731	33	0
20	CT	713	0	766	42	0
21	AU	199	0	208	32	0
21	CU	199	0	208	22	0
22	AX	631	0	540	20	0
22	CX	601	0	485	16	0
23	BA	61112	0	30809	1223	1
23	DA	60621	0	30566	1233	0
24	BB	2573	0	1306	56	0
24	DB	2573	0	1306	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BD	2135	0	2214	76	0
25	DD	2136	0	2218	81	0
26	BE	1555	0	1607	54	0
26	DE	1555	0	1607	61	0
27	BF	1580	0	1621	63	0
27	DF	1580	0	1621	63	0
28	BG	1368	0	1324	81	0
28	DG	1368	0	1324	92	0
29	BH	1317	0	1376	35	0
29	DH	1317	0	1376	37	0
30	BI	1037	0	1036	60	1
30	DI	953	0	858	44	0
31	BN	1112	0	1180	35	0
31	DN	1112	0	1180	46	0
32	BO	923	0	981	27	0
32	DO	923	0	981	28	0
33	BP	1131	0	1201	47	0
33	DP	1131	0	1201	57	0
34	BQ	1122	0	1179	47	0
34	DQ	1122	0	1179	50	0
35	BR	968	0	1033	34	0
35	DR	968	0	1033	37	0
36	BS	865	0	905	51	0
36	DS	865	0	905	51	0
37	BT	1063	0	1103	42	0
37	DT	1063	0	1103	45	0
38	BU	959	0	1019	36	0
38	DU	959	0	1019	36	0
39	BV	771	0	830	23	0
39	DV	771	0	830	26	0
40	BW	881	0	935	22	0
40	DW	881	0	935	33	0
41	BX	742	0	799	23	0
41	DX	742	0	799	28	0
42	BY	785	0	828	24	0
42	DY	785	0	828	25	0
43	BZ	1536	0	1518	53	0
43	DZ	1522	0	1511	67	0
44	B0	594	0	604	17	0
44	D0	594	0	604	16	0
45	B1	745	0	804	21	0
45	D1	745	0	804	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B2	588	0	643	15	0
46	D2	588	0	643	19	0
47	B3	458	0	503	8	0
47	D3	458	0	503	13	0
48	B4	349	0	336	25	0
48	D4	349	0	336	29	0
49	B5	455	0	472	13	0
49	D5	455	0	472	14	0
50	B6	449	0	462	18	0
50	D6	449	0	462	15	0
51	B7	418	0	467	15	0
51	D7	418	0	467	19	0
52	B8	509	0	565	18	0
52	D8	509	0	565	25	0
53	B9	297	0	316	8	0
53	D9	297	0	316	9	0
54	AA	135	0	0	0	0
54	AC	1	0	0	0	0
54	AD	1	0	0	0	0
54	AF	1	0	0	0	0
54	AQ	1	0	0	0	0
54	B0	3	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	1	0	0	0	0
54	B5	2	0	0	0	0
54	B8	2	0	0	0	0
54	B9	1	0	0	0	0
54	BA	660	0	0	0	0
54	BB	23	0	0	0	0
54	BD	3	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BG	1	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	4	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	2	0	0	0	0
54	BZ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	162	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	2	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	2	0	0	0	0
54	DA	598	0	0	0	0
54	DB	8	0	0	0	0
54	DD	2	0	0	0	0
54	DE	4	0	0	0	0
54	DF	1	0	0	0	0
54	DO	2	0	0	0	0
54	DP	1	0	0	0	0
54	DQ	2	0	0	0	0
54	DR	3	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
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	268	0	0	32	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	AX	1	0	0	0	0
56	B0	8	0	0	0	0
56	B1	2	0	0	0	0
56	B3	1	0	0	0	0
56	B5	3	0	0	0	0
56	B6	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B7	5	0	0	0	0
56	B8	10	0	0	0	0
56	B9	1	0	0	1	0
56	BA	1694	0	0	170	0
56	BB	57	0	0	3	1
56	BD	20	0	0	3	0
56	BE	11	0	0	0	0
56	BF	6	0	0	1	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	2	0	0	0	0
56	BP	11	0	0	2	0
56	BQ	5	0	0	0	0
56	BR	6	0	0	1	0
56	BT	1	0	0	0	0
56	BU	3	0	0	0	0
56	BV	3	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	4	0	0	0	0
56	CA	265	0	0	25	0
56	CC	1	0	0	2	0
56	CD	1	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	1	0
56	CL	2	0	0	1	0
56	CN	1	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D1	5	0	0	0	0
56	D3	1	0	0	0	0
56	D4	1	0	0	0	0
56	D7	3	0	0	0	0
56	D8	1	0	0	0	0
56	DA	1174	0	0	171	0
56	DB	17	0	0	0	0
56	DD	8	0	0	2	0
56	DE	11	0	0	2	0
56	DF	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DN	1	0	0	0	0
56	DO	5	0	0	1	0
56	DP	10	0	0	1	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	1	0
56	DT	2	0	0	0	0
56	DU	5	0	0	0	0
56	DV	2	0	0	1	0
56	DW	2	0	0	0	0
56	DX	1	0	0	1	0
56	DY	2	0	0	0	0
All	All	286308	0	187082	8441	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 18.

The worst 5 of 8441 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1441:G:H2'	1:AA:1459:C:N4	1.20	1.46
1:AA:1459:C:C5	1:AA:1460:A:N6	1.79	1.44
1:AA:1441:G:C2'	1:AA:1459:C:N4	1.88	1.36
1:AA:1441:G:C2'	1:AA:1459:C:H41	1.44	1.29
1:CA:1441:G:H2'	1:CA:1459:C:N4	1.50	1.25

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)
23:BA:1594:G:OP1	56:BB:323:HOH:O[1_455]	2.18	0.02
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	228/256 (89%)	199 (87%)	28 (12%)	1 (0%)	30	61
2	CB	227/256 (89%)	197 (87%)	29 (13%)	1 (0%)	30	61
3	AC	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	24	57
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	CD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	AE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18	49
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	35
7	CG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	18	49
8	AH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
8	CH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	AI	123/128 (96%)	112 (91%)	10 (8%)	1 (1%)	16	47
9	CI	123/128 (96%)	111 (90%)	11 (9%)	1 (1%)	16	47
10	AJ	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	3	18
10	CJ	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	5	25
11	AK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
11	CK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
12	AL	120/132 (91%)	110 (92%)	9 (8%)	1 (1%)	16	47
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	16	47
13	AM	112/126 (89%)	89 (80%)	21 (19%)	2 (2%)	6	28
13	CM	112/126 (89%)	87 (78%)	21 (19%)	4 (4%)	2	16
14	AN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	16
14	CN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	23
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	23
16	AP	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	9	35
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	9	35
19	CS	79/93 (85%)	65 (82%)	13 (16%)	1 (1%)	9	35
20	AT	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
20	CT	95/106 (90%)	84 (88%)	8 (8%)	3 (3%)	3	18
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	AX	93/101 (92%)	79 (85%)	13 (14%)	1 (1%)	11	39
22	CX	93/101 (92%)	84 (90%)	9 (10%)	0	100	100
25	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30	61
25	DD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	30	61
26	BE	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	12	41
26	DE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	12	41
27	BF	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
27	DF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	57
28	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	21	52
28	DG	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
29	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	52
29	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	52
30	BI	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	9	34
30	DI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	34
31	BN	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	24
31	DN	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	5	24
32	BO	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	BP	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
33	DP	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
34	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	49
35	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
35	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
36	BS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
36	DS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
37	BT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
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%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	14	44
40	DW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	12	41
42	DY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	12	41
43	BZ	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	12	41
43	DZ	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	12	41
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
44	D0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	39
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	39
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
46	D2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
47	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	B4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
48	D4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
50	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
51	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	24
51	D7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	24
52	B8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
52	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11552/12330 (94%)	10628 (92%)	855 (7%)	69 (1%)	21	52

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	CT	100	ILE
12	AL	28	LYS
14	AN	15	LYS
16	AP	79	VAL
12	CL	28	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	178/220 (81%)	133 (75%)	45 (25%)	0	2
2	CB	177/220 (80%)	135 (76%)	42 (24%)	1	3
3	AC	114/188 (61%)	79 (69%)	35 (31%)	0	0
3	CC	114/188 (61%)	86 (75%)	28 (25%)	1	3
4	AD	141/181 (78%)	118 (84%)	23 (16%)	2	11
4	CD	141/181 (78%)	119 (84%)	22 (16%)	2	12
5	AE	108/123 (88%)	82 (76%)	26 (24%)	1	3
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	76/90 (84%)	60 (79%)	16 (21%)	1	5
6	CF	76/90 (84%)	57 (75%)	19 (25%)	0	2
7	AG	103/127 (81%)	74 (72%)	29 (28%)	0	1
7	CG	103/127 (81%)	71 (69%)	32 (31%)	0	0
8	AH	103/119 (87%)	81 (79%)	22 (21%)	1	5
8	CH	103/119 (87%)	83 (81%)	20 (19%)	1	7
9	AI	62/99 (63%)	47 (76%)	15 (24%)	1	3
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1	4
10	AJ	53/92 (58%)	35 (66%)	18 (34%)	0	0
10	CJ	53/92 (58%)	37 (70%)	16 (30%)	0	0
11	AK	81/99 (82%)	68 (84%)	13 (16%)	2	12
11	CK	81/99 (82%)	68 (84%)	13 (16%)	2	12
12	AL	91/109 (84%)	73 (80%)	18 (20%)	1	6
12	CL	91/109 (84%)	75 (82%)	16 (18%)	2	9
13	AM	64/101 (63%)	43 (67%)	21 (33%)	0	0
13	CM	64/101 (63%)	48 (75%)	16 (25%)	0	2
14	AN	46/50 (92%)	35 (76%)	11 (24%)	1	3
14	CN	46/50 (92%)	32 (70%)	14 (30%)	0	0
15	AO	77/80 (96%)	65 (84%)	12 (16%)	2	12
15	CO	77/80 (96%)	64 (83%)	13 (17%)	2	10
16	AP	63/74 (85%)	45 (71%)	18 (29%)	0	1
16	CP	63/74 (85%)	45 (71%)	18 (29%)	0	1
17	AQ	94/97 (97%)	77 (82%)	17 (18%)	2	8
17	CQ	94/97 (97%)	78 (83%)	16 (17%)	2	10
18	AR	49/77 (64%)	43 (88%)	6 (12%)	5	20
18	CR	49/77 (64%)	42 (86%)	7 (14%)	3	14
19	AS	43/80 (54%)	27 (63%)	16 (37%)	0	0
19	CS	43/80 (54%)	33 (77%)	10 (23%)	1	4
20	AT	64/82 (78%)	52 (81%)	12 (19%)	1	7
20	CT	65/82 (79%)	53 (82%)	12 (18%)	1	8
21	AU	18/22 (82%)	12 (67%)	6 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	18/22 (82%)	11 (61%)	7 (39%)	0	0
22	AX	45/87 (52%)	29 (64%)	16 (36%)	0	0
22	CX	38/87 (44%)	22 (58%)	16 (42%)	0	0
25	BD	215/218 (99%)	174 (81%)	41 (19%)	1	7
25	DD	215/218 (99%)	176 (82%)	39 (18%)	2	8
26	BE	163/166 (98%)	127 (78%)	36 (22%)	1	4
26	DE	163/166 (98%)	127 (78%)	36 (22%)	1	4
27	BF	159/166 (96%)	129 (81%)	30 (19%)	1	7
27	DF	159/166 (96%)	129 (81%)	30 (19%)	1	7
28	BG	128/156 (82%)	109 (85%)	19 (15%)	3	13
28	DG	128/156 (82%)	107 (84%)	21 (16%)	2	11
29	BH	141/148 (95%)	123 (87%)	18 (13%)	4	18
29	DH	141/148 (95%)	119 (84%)	22 (16%)	2	12
30	BI	98/124 (79%)	76 (78%)	22 (22%)	1	4
30	DI	74/124 (60%)	57 (77%)	17 (23%)	1	4
31	BN	117/119 (98%)	95 (81%)	22 (19%)	1	7
31	DN	117/119 (98%)	92 (79%)	25 (21%)	1	5
32	BO	98/100 (98%)	82 (84%)	16 (16%)	2	11
32	DO	98/100 (98%)	82 (84%)	16 (16%)	2	11
33	BP	114/116 (98%)	94 (82%)	20 (18%)	2	9
33	DP	114/116 (98%)	94 (82%)	20 (18%)	2	9
34	BQ	111/111 (100%)	93 (84%)	18 (16%)	2	11
34	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	11
35	BR	101/101 (100%)	81 (80%)	20 (20%)	1	6
35	DR	101/101 (100%)	79 (78%)	22 (22%)	1	5
36	BS	84/88 (96%)	64 (76%)	20 (24%)	1	3
36	DS	84/88 (96%)	67 (80%)	17 (20%)	1	5
37	BT	110/127 (87%)	90 (82%)	20 (18%)	2	8
37	DT	110/127 (87%)	88 (80%)	22 (20%)	1	6
38	BU	93/94 (99%)	76 (82%)	17 (18%)	2	8
38	DU	93/94 (99%)	77 (83%)	16 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BV	80/82 (98%)	60 (75%)	20 (25%)	0	2
39	DV	80/82 (98%)	58 (72%)	22 (28%)	0	1
40	BW	89/92 (97%)	77 (86%)	12 (14%)	4	16
40	DW	89/92 (97%)	78 (88%)	11 (12%)	4	19
41	BX	75/78 (96%)	70 (93%)	5 (7%)	15	43
41	DX	75/78 (96%)	69 (92%)	6 (8%)	11	37
42	BY	80/91 (88%)	61 (76%)	19 (24%)	1	3
42	DY	80/91 (88%)	61 (76%)	19 (24%)	1	3
43	BZ	159/179 (89%)	132 (83%)	27 (17%)	2	10
43	DZ	159/179 (89%)	131 (82%)	28 (18%)	2	9
44	B0	59/67 (88%)	51 (86%)	8 (14%)	3	16
44	D0	59/67 (88%)	51 (86%)	8 (14%)	3	16
45	B1	78/83 (94%)	65 (83%)	13 (17%)	2	10
45	D1	78/83 (94%)	65 (83%)	13 (17%)	2	10
46	B2	65/67 (97%)	54 (83%)	11 (17%)	2	10
46	D2	65/67 (97%)	54 (83%)	11 (17%)	2	10
47	B3	49/52 (94%)	42 (86%)	7 (14%)	3	14
47	D3	49/52 (94%)	41 (84%)	8 (16%)	2	11
48	B4	39/63 (62%)	31 (80%)	8 (20%)	1	5
48	D4	39/63 (62%)	31 (80%)	8 (20%)	1	5
49	B5	50/52 (96%)	43 (86%)	7 (14%)	3	15
49	D5	50/52 (96%)	42 (84%)	8 (16%)	2	12
50	B6	50/52 (96%)	37 (74%)	13 (26%)	0	2
50	D6	50/52 (96%)	39 (78%)	11 (22%)	1	4
51	B7	41/42 (98%)	34 (83%)	7 (17%)	2	10
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2	10
52	B8	52/55 (94%)	41 (79%)	11 (21%)	1	5
52	D8	52/55 (94%)	41 (79%)	11 (21%)	1	5
53	B9	32/34 (94%)	27 (84%)	5 (16%)	2	12
53	D9	32/34 (94%)	26 (81%)	6 (19%)	1	7
All	All	8775/10240 (86%)	7015 (80%)	1760 (20%)	1	5

5 of 1760 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CB	212	GLN
13	CM	74	VAL
53	D9	2	LYS
39	DV	73	SER
3	CC	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
28	DG	108	ASN
30	DI	105	HIS
38	DU	104	GLN
30	BI	133	HIS
30	BI	74	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1499/1522 (98%)	386 (25%)	33 (2%)
1	CA	1495/1522 (98%)	397 (26%)	34 (2%)
23	BA	2833/2913 (97%)	614 (21%)	60 (2%)
23	DA	2807/2913 (96%)	604 (21%)	56 (1%)
24	BB	119/122 (97%)	25 (21%)	0
24	DB	119/122 (97%)	26 (21%)	0
All	All	8872/9114 (97%)	2052 (23%)	183 (2%)

5 of 2052 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	32	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1201	A

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Mol	Chain	Res	Type
23	DA	764	A
1	CA	1280	A
23	DA	249	C
23	DA	1049	C

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

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 1662 ligands modelled in this entry, 1662 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	1501/1522 (98%)	0.19	34 (2%) 61 39	47, 95, 155, 169	0
1	CA	1497/1522 (98%)	0.12	37 (2%) 58 37	50, 96, 158, 171	0
2	AB	230/256 (89%)	0.57	14 (6%) 27 15	87, 114, 134, 148	0
2	CB	229/256 (89%)	0.81	26 (11%) 10 5	92, 116, 136, 149	0
3	AC	206/239 (86%)	0.67	14 (6%) 23 12	85, 109, 127, 136	0
3	CC	206/239 (86%)	0.75	12 (5%) 29 16	94, 120, 143, 158	0
4	AD	208/209 (99%)	0.97	24 (11%) 9 5	75, 94, 114, 125	0
4	CD	208/209 (99%)	0.90	20 (9%) 13 7	76, 93, 114, 124	0
5	AE	148/162 (91%)	0.17	4 (2%) 56 35	66, 86, 103, 125	0
5	CE	148/162 (91%)	0.46	7 (4%) 36 19	69, 88, 104, 127	0
6	AF	100/101 (99%)	0.16	1 (1%) 79 61	67, 82, 100, 116	0
6	CF	100/101 (99%)	0.28	1 (1%) 79 61	70, 86, 103, 117	0
7	AG	155/156 (99%)	1.59	52 (33%) 1 0	113, 139, 153, 159	0
7	CG	155/156 (99%)	1.42	41 (26%) 1 1	122, 137, 149, 159	0
8	AH	138/138 (100%)	0.60	8 (5%) 29 16	71, 90, 100, 110	0
8	CH	138/138 (100%)	0.63	4 (2%) 53 32	71, 92, 103, 113	0
9	AI	125/128 (97%)	1.36	29 (23%) 2 1	110, 137, 149, 154	0
9	CI	125/128 (97%)	2.19	64 (51%) 0 0	115, 139, 152, 163	0
10	AJ	96/105 (91%)	0.98	13 (13%) 7 4	92, 126, 141, 147	0
10	CJ	96/105 (91%)	1.67	36 (37%) 1 0	108, 134, 150, 160	0
11	AK	114/129 (88%)	0.21	2 (1%) 67 47	60, 86, 108, 120	0
11	CK	114/129 (88%)	0.24	3 (2%) 57 36	63, 89, 107, 126	0
12	AL	122/132 (92%)	0.58	7 (5%) 29 16	62, 77, 95, 112	0
12	CL	122/132 (92%)	0.64	10 (8%) 17 10	63, 77, 96, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	1.37	25 (21%)	2 1	112, 139, 150, 153	0
13	CM	114/126 (90%)	1.42	30 (26%)	1 1	116, 140, 151, 160	0
14	AN	60/61 (98%)	1.33	16 (26%)	1 1	93, 118, 131, 144	0
14	CN	60/61 (98%)	1.56	16 (26%)	1 1	103, 122, 134, 139	0
15	AO	88/89 (98%)	0.29	0	100 100	63, 85, 103, 113	0
15	CO	88/89 (98%)	0.24	1 (1%)	78 59	63, 85, 105, 111	0
16	AP	82/88 (93%)	1.02	10 (12%)	8 5	76, 88, 110, 120	0
16	CP	82/88 (93%)	0.97	7 (8%)	16 9	73, 85, 105, 117	0
17	AQ	99/105 (94%)	0.41	3 (3%)	52 31	68, 82, 102, 106	0
17	CQ	99/105 (94%)	0.42	2 (2%)	65 44	69, 83, 101, 108	0
18	AR	68/88 (77%)	0.12	0	100 100	71, 82, 105, 112	0
18	CR	68/88 (77%)	0.04	0	100 100	75, 85, 105, 117	0
19	AS	81/93 (87%)	1.65	30 (37%)	1 0	113, 138, 147, 152	0
19	CS	81/93 (87%)	1.34	18 (22%)	2 1	114, 140, 150, 153	0
20	AT	87/106 (82%)	0.92	10 (11%)	9 5	75, 88, 103, 111	0
20	CT	97/106 (91%)	0.66	6 (6%)	26 14	72, 86, 105, 115	0
21	AU	23/27 (85%)	3.01	17 (73%)	0 0	128, 136, 145, 154	0
21	CU	23/27 (85%)	2.96	18 (78%)	0 0	129, 137, 148, 150	0
22	AX	95/101 (94%)	0.76	8 (8%)	17 9	69, 94, 115, 123	0
22	CX	95/101 (94%)	1.07	12 (12%)	8 4	88, 106, 129, 145	0
23	BA	2837/2913 (97%)	-0.46	27 (0%)	79 61	26, 47, 132, 176	0
23	DA	2814/2913 (96%)	-0.47	27 (0%)	79 61	28, 50, 133, 176	0
24	BB	120/122 (98%)	-0.04	1 (0%)	82 65	43, 72, 93, 110	0
24	DB	120/122 (98%)	0.34	6 (5%)	34 18	48, 81, 106, 117	0
25	BD	275/276 (99%)	-0.14	2 (0%)	84 68	29, 45, 63, 113	0
25	DD	275/276 (99%)	-0.19	1 (0%)	88 76	30, 47, 66, 116	0
26	BE	204/206 (99%)	-0.13	3 (1%)	72 52	28, 49, 72, 95	0
26	DE	204/206 (99%)	-0.21	2 (0%)	79 61	29, 50, 76, 95	0
27	BF	203/210 (96%)	-0.06	1 (0%)	87 73	29, 54, 88, 111	0
27	DF	203/210 (96%)	-0.08	0	100 100	31, 59, 90, 112	0
28	BG	181/182 (99%)	0.71	10 (5%)	30 16	76, 110, 133, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	1.14	30 (16%) 4 2	86, 117, 138, 148	0
29	BH	174/180 (96%)	0.37	7 (4%) 42 23	54, 73, 94, 110	0
29	DH	174/180 (96%)	0.52	5 (2%) 53 32	65, 82, 101, 119	0
30	BI	146/148 (98%)	0.06	5 (3%) 48 28	54, 81, 99, 115	0
30	DI	146/148 (98%)	0.35	4 (2%) 56 35	56, 89, 108, 120	0
31	BN	140/140 (100%)	-0.02	1 (0%) 84 68	38, 49, 78, 92	0
31	DN	140/140 (100%)	-0.06	1 (0%) 84 68	40, 54, 82, 96	0
32	BO	122/122 (100%)	-0.20	1 (0%) 82 65	35, 50, 69, 77	0
32	DO	122/122 (100%)	-0.32	0 100 100	36, 52, 69, 77	0
33	BP	149/150 (99%)	0.14	1 (0%) 84 68	30, 58, 89, 105	0
33	DP	149/150 (99%)	0.13	1 (0%) 84 68	31, 62, 92, 112	0
34	BQ	141/141 (100%)	0.01	2 (1%) 73 53	39, 54, 71, 83	0
34	DQ	141/141 (100%)	0.05	1 (0%) 84 68	41, 58, 77, 88	0
35	BR	118/118 (100%)	-0.17	1 (0%) 82 65	34, 44, 58, 77	0
35	DR	118/118 (100%)	-0.10	0 100 100	36, 47, 62, 78	0
36	BS	110/112 (98%)	0.20	2 (1%) 67 47	50, 69, 89, 96	0
36	DS	110/112 (98%)	0.64	5 (4%) 38 20	55, 74, 94, 102	0
37	BT	131/146 (89%)	0.03	3 (2%) 61 39	43, 55, 92, 119	0
37	DT	131/146 (89%)	-0.00	3 (2%) 61 39	46, 57, 93, 128	0
38	BU	116/118 (98%)	-0.09	0 100 100	32, 44, 62, 71	0
38	DU	116/118 (98%)	-0.05	1 (0%) 81 63	34, 48, 66, 73	0
39	BV	101/101 (100%)	-0.09	1 (0%) 79 61	29, 56, 79, 103	0
39	DV	101/101 (100%)	-0.15	0 100 100	32, 62, 85, 103	0
40	BW	112/113 (99%)	-0.28	0 100 100	33, 40, 62, 103	0
40	DW	112/113 (99%)	-0.23	1 (0%) 81 63	35, 42, 67, 105	0
41	BX	95/96 (98%)	0.07	0 100 100	38, 49, 72, 88	0
41	DX	95/96 (98%)	0.10	2 (2%) 63 42	41, 52, 77, 90	0
42	BY	107/110 (97%)	0.29	2 (1%) 66 45	47, 61, 85, 108	0
42	DY	107/110 (97%)	0.56	5 (4%) 36 19	52, 65, 89, 113	0
43	BZ	201/206 (97%)	0.28	4 (1%) 65 44	53, 76, 99, 122	0
43	DZ	198/206 (96%)	0.29	2 (1%) 79 61	62, 81, 102, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	-0.03	0 100 100	39, 48, 64, 91	0
44	D0	76/85 (89%)	0.09	0 100 100	43, 52, 66, 92	0
45	B1	97/98 (98%)	-0.04	1 (1%) 79 61	36, 48, 82, 97	0
45	D1	97/98 (98%)	-0.01	3 (3%) 51 30	36, 51, 83, 98	0
46	B2	70/72 (97%)	0.25	3 (4%) 40 22	46, 60, 76, 107	0
46	D2	70/72 (97%)	0.39	4 (5%) 29 16	50, 64, 81, 103	0
47	B3	59/60 (98%)	0.14	1 (1%) 69 48	38, 49, 86, 97	0
47	D3	59/60 (98%)	0.18	1 (1%) 69 48	41, 53, 93, 102	0
48	B4	46/71 (64%)	0.21	1 (2%) 62 41	101, 129, 144, 148	0
48	D4	46/71 (64%)	0.70	1 (2%) 62 41	113, 133, 144, 152	0
49	B5	59/60 (98%)	-0.28	0 100 100	30, 45, 66, 80	0
49	D5	59/60 (98%)	-0.23	0 100 100	32, 47, 68, 81	0
50	B6	53/54 (98%)	-0.35	0 100 100	42, 51, 70, 79	0
50	D6	53/54 (98%)	-0.19	0 100 100	43, 54, 72, 82	0
51	B7	48/49 (97%)	-0.11	2 (4%) 40 22	30, 34, 55, 80	0
51	D7	48/49 (97%)	-0.12	1 (2%) 63 42	32, 35, 58, 84	0
52	B8	64/65 (98%)	-0.07	0 100 100	38, 43, 52, 70	0
52	D8	64/65 (98%)	0.06	0 100 100	40, 45, 55, 70	0
53	B9	36/37 (97%)	0.17	0 100 100	44, 55, 62, 73	0
53	D9	36/37 (97%)	0.59	3 (8%) 17 9	47, 59, 68, 75	0
All	All	20641/21444 (96%)	0.13	884 (4%) 40 22	26, 71, 144, 176	0

The worst 5 of 884 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	CH	1	MET	8.3
9	CI	40	LEU	7.2
8	AH	1	MET	6.9
21	AU	14	TRP	6.1
7	CG	8	GLU	6.0

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(Å ²)	Q<0.9
54	MG	AA	1669	1/1	0.32	0.23	103,103,103,103	0
54	MG	DA	3276	1/1	0.47	0.52	60,60,60,60	0
54	MG	CA	1664	1/1	0.54	0.31	80,80,80,80	0
54	MG	CA	1684	1/1	0.55	0.36	91,91,91,91	0
54	MG	AA	1625	1/1	0.56	0.30	79,79,79,79	0
54	MG	CA	1633	1/1	0.57	0.29	77,77,77,77	0
54	MG	AA	1607	1/1	0.59	0.27	78,78,78,78	0
54	MG	DO	201	1/1	0.59	0.13	120,120,120,120	0
54	MG	AA	1705	1/1	0.60	0.16	97,97,97,97	0
54	MG	CA	1652	1/1	0.62	0.24	76,76,76,76	0
54	MG	BA	3037	1/1	0.63	0.32	75,75,75,75	0
54	MG	BA	3237	1/1	0.63	0.18	71,71,71,71	0
54	MG	BA	3236	1/1	0.64	0.22	66,66,66,66	0
54	MG	DA	3464	1/1	0.64	0.19	89,89,89,89	0
54	MG	BA	3038	1/1	0.64	0.39	76,76,76,76	0
54	MG	BA	3060	1/1	0.65	0.25	54,54,54,54	0
54	MG	CA	1608	1/1	0.65	0.33	93,93,93,93	0
54	MG	DA	3091	1/1	0.65	0.19	55,55,55,55	0
54	MG	DA	3268	1/1	0.66	0.38	54,54,54,54	0
54	MG	DA	3557	1/1	0.67	0.18	103,103,103,103	0
54	MG	BA	3655	1/1	0.67	0.11	104,104,104,104	0
54	MG	CA	1632	1/1	0.68	0.19	69,69,69,69	0
54	MG	BA	3113	1/1	0.68	0.19	60,60,60,60	0
54	MG	DA	3167	1/1	0.68	0.17	51,51,51,51	0
54	MG	CA	1680	1/1	0.68	0.22	78,78,78,78	0
54	MG	CA	1604	1/1	0.69	0.32	81,81,81,81	0
54	MG	AA	1712	1/1	0.69	0.29	86,86,86,86	0
54	MG	AA	1619	1/1	0.69	0.29	86,86,86,86	0
54	MG	DA	3297	1/1	0.70	0.21	78,78,78,78	0
54	MG	DA	3247	1/1	0.70	0.28	67,67,67,67	0
54	MG	DA	3532	1/1	0.70	0.11	116,116,116,116	0
54	MG	CA	1642	1/1	0.70	0.23	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3030	1/1	0.70	0.18	55,55,55,55	0
54	MG	AA	1666	1/1	0.71	0.23	74,74,74,74	0
54	MG	DA	3328	1/1	0.71	0.35	57,57,57,57	0
54	MG	DA	3187	1/1	0.71	0.12	71,71,71,71	0
54	MG	DA	3066	1/1	0.71	0.16	62,62,62,62	0
54	MG	AA	1616	1/1	0.71	0.11	92,92,92,92	0
54	MG	DA	3165	1/1	0.71	0.24	60,60,60,60	0
54	MG	AA	1618	1/1	0.72	0.21	94,94,94,94	0
54	MG	CA	1649	1/1	0.72	0.31	66,66,66,66	0
54	MG	CA	1753	1/1	0.72	0.13	86,86,86,86	0
54	MG	AA	1640	1/1	0.73	0.27	58,58,58,58	0
54	MG	AA	1620	1/1	0.73	0.29	65,65,65,65	0
54	MG	BA	3014	1/1	0.73	0.10	65,65,65,65	0
54	MG	AA	1637	1/1	0.73	0.26	84,84,84,84	0
54	MG	DA	3236	1/1	0.73	0.24	47,47,47,47	0
54	MG	CA	1626	1/1	0.73	0.32	62,62,62,62	0
54	MG	CA	1655	1/1	0.73	0.20	98,98,98,98	0
54	MG	AA	1613	1/1	0.74	0.28	65,65,65,65	0
54	MG	DA	3525	1/1	0.74	0.09	106,106,106,106	0
54	MG	CA	1717	1/1	0.74	0.12	110,110,110,110	0
54	MG	AA	1622	1/1	0.74	0.28	81,81,81,81	0
54	MG	DA	3434	1/1	0.74	0.14	60,60,60,60	0
54	MG	BA	3305	1/1	0.75	0.31	69,69,69,69	0
54	MG	BA	3512	1/1	0.75	0.17	109,109,109,109	0
54	MG	BA	3261	1/1	0.75	0.26	34,34,34,34	0
54	MG	CA	1661	1/1	0.75	0.31	67,67,67,67	0
54	MG	DA	3123	1/1	0.75	0.28	53,53,53,53	0
54	MG	CA	1677	1/1	0.76	0.14	64,64,64,64	0
54	MG	DA	3073	1/1	0.76	0.28	68,68,68,68	0
54	MG	BA	3337	1/1	0.76	0.10	49,49,49,49	0
54	MG	BA	3104	1/1	0.76	0.28	63,63,63,63	0
54	MG	CA	1692	1/1	0.76	0.37	86,86,86,86	0
54	MG	CA	1699	1/1	0.76	0.15	83,83,83,83	0
54	MG	DA	3486	1/1	0.76	0.18	64,64,64,64	0
54	MG	DA	3179	1/1	0.76	0.25	68,68,68,68	0
54	MG	BA	3287	1/1	0.76	0.17	44,44,44,44	0
54	MG	BB	219	1/1	0.76	0.10	105,105,105,105	0
54	MG	AA	1645	1/1	0.76	0.20	60,60,60,60	0
54	MG	D5	101	1/1	0.76	0.14	52,52,52,52	0
54	MG	BA	3048	1/1	0.77	0.20	68,68,68,68	0
54	MG	CA	1697	1/1	0.77	0.10	57,57,57,57	0
54	MG	DA	3189	1/1	0.77	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1614	1/1	0.77	0.24	56,56,56,56	0
54	MG	DA	3497	1/1	0.77	0.15	83,83,83,83	0
54	MG	BB	204	1/1	0.77	0.18	52,52,52,52	0
54	MG	CA	1637	1/1	0.77	0.33	73,73,73,73	0
54	MG	CA	1656	1/1	0.77	0.25	86,86,86,86	0
54	MG	DA	3582	1/1	0.77	0.16	63,63,63,63	0
54	MG	DA	3177	1/1	0.77	0.24	88,88,88,88	0
54	MG	DA	3301	1/1	0.77	0.29	50,50,50,50	0
54	MG	CA	1663	1/1	0.78	0.28	64,64,64,64	0
54	MG	BA	3079	1/1	0.78	0.17	50,50,50,50	0
54	MG	CA	1667	1/1	0.78	0.27	77,77,77,77	0
54	MG	CA	1676	1/1	0.78	0.18	73,73,73,73	0
54	MG	CA	1614	1/1	0.78	0.15	85,85,85,85	0
54	MG	DB	204	1/1	0.78	0.30	74,74,74,74	0
54	MG	CA	1737	1/1	0.78	0.12	89,89,89,89	0
54	MG	CA	1662	1/1	0.78	0.32	75,75,75,75	0
54	MG	AA	1674	1/1	0.79	0.38	63,63,63,63	0
54	MG	DA	3278	1/1	0.79	0.11	83,83,83,83	0
54	MG	AA	1702	1/1	0.79	0.14	68,68,68,68	0
54	MG	DA	3130	1/1	0.79	0.22	47,47,47,47	0
54	MG	DA	3146	1/1	0.79	0.16	44,44,44,44	0
54	MG	CA	1607	1/1	0.79	0.23	50,50,50,50	0
54	MG	CA	1735	1/1	0.79	0.26	69,69,69,69	0
54	MG	BA	3174	1/1	0.79	0.14	32,32,32,32	0
54	MG	CA	1740	1/1	0.79	0.29	68,68,68,68	0
54	MG	DA	3521	1/1	0.79	0.12	86,86,86,86	0
54	MG	BA	3513	1/1	0.79	0.14	86,86,86,86	0
54	MG	BA	3593	1/1	0.79	0.14	84,84,84,84	0
54	MG	DA	3218	1/1	0.79	0.41	62,62,62,62	0
54	MG	BA	3194	1/1	0.79	0.27	63,63,63,63	0
54	MG	BA	3301	1/1	0.79	0.40	75,75,75,75	0
54	MG	DA	3257	1/1	0.79	0.33	56,56,56,56	0
54	MG	DA	3075	1/1	0.79	0.18	58,58,58,58	0
54	MG	DA	3188	1/1	0.80	0.09	69,69,69,69	0
54	MG	BA	3232	1/1	0.80	0.17	64,64,64,64	0
54	MG	AA	1678	1/1	0.80	0.35	74,74,74,74	0
54	MG	BA	3582	1/1	0.80	0.11	79,79,79,79	0
54	MG	CA	1668	1/1	0.80	0.24	87,87,87,87	0
54	MG	AA	1692	1/1	0.80	0.18	144,144,144,144	0
54	MG	AA	1651	1/1	0.80	0.23	60,60,60,60	0
54	MG	CA	1629	1/1	0.80	0.18	87,87,87,87	0
54	MG	DA	3567	1/1	0.80	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3020	1/1	0.80	0.29	56,56,56,56	0
54	MG	BA	3367	1/1	0.80	0.15	71,71,71,71	0
54	MG	DA	3048	1/1	0.80	0.11	40,40,40,40	0
54	MG	BA	3470	1/1	0.80	0.18	60,60,60,60	0
54	MG	BA	3196	1/1	0.81	0.15	46,46,46,46	0
54	MG	AA	1663	1/1	0.81	0.40	64,64,64,64	0
54	MG	AA	1731	1/1	0.81	0.10	119,119,119,119	0
54	MG	CA	1616	1/1	0.81	0.25	58,58,58,58	0
54	MG	DA	3116	1/1	0.81	0.18	43,43,43,43	0
54	MG	CA	1756	1/1	0.81	0.21	80,80,80,80	0
54	MG	DA	3221	1/1	0.81	0.24	51,51,51,51	0
54	MG	DA	3127	1/1	0.81	0.23	56,56,56,56	0
54	MG	CA	1758	1/1	0.81	0.11	84,84,84,84	0
54	MG	DA	3254	1/1	0.81	0.26	64,64,64,64	0
54	MG	BB	212	1/1	0.81	0.20	60,60,60,60	0
54	MG	BA	3195	1/1	0.81	0.24	60,60,60,60	0
54	MG	BA	3238	1/1	0.81	0.25	53,53,53,53	0
54	MG	DA	3277	1/1	0.81	0.19	77,77,77,77	0
54	MG	DA	3172	1/1	0.81	0.21	64,64,64,64	0
54	MG	DO	202	1/1	0.81	0.12	39,39,39,39	0
54	MG	DA	3280	1/1	0.81	0.16	58,58,58,58	0
54	MG	DA	3324	1/1	0.82	0.10	51,51,51,51	0
54	MG	AA	1688	1/1	0.82	0.14	96,96,96,96	0
54	MG	DA	3400	1/1	0.82	0.19	66,66,66,66	0
54	MG	AA	1611	1/1	0.82	0.07	83,83,83,83	0
54	MG	AA	1626	1/1	0.82	0.08	71,71,71,71	0
54	MG	DA	3157	1/1	0.82	0.19	44,44,44,44	0
54	MG	DA	3058	1/1	0.82	0.20	58,58,58,58	0
54	MG	BA	3109	1/1	0.82	0.33	62,62,62,62	0
54	MG	DA	3071	1/1	0.82	0.13	44,44,44,44	0
54	MG	CA	1601	1/1	0.82	0.19	45,45,45,45	0
54	MG	AA	1635	1/1	0.82	0.15	61,61,61,61	0
54	MG	DA	3184	1/1	0.82	0.09	46,46,46,46	0
54	MG	CA	1660	1/1	0.82	0.31	70,70,70,70	0
54	MG	DA	3282	1/1	0.82	0.17	64,64,64,64	0
54	MG	AA	1684	1/1	0.82	0.32	60,60,60,60	0
54	MG	CA	1636	1/1	0.82	0.32	59,59,59,59	0
54	MG	DA	3321	1/1	0.82	0.24	51,51,51,51	0
54	MG	CA	1641	1/1	0.83	0.19	52,52,52,52	0
54	MG	DA	3131	1/1	0.83	0.22	56,56,56,56	0
54	MG	BA	3146	1/1	0.83	0.22	65,65,65,65	0
54	MG	DA	3238	1/1	0.83	0.32	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	AA	1604	1/1	0.83	0.17	73,73,73,73	0
54	MG	DA	3481	1/1	0.83	0.27	61,61,61,61	0
54	MG	DA	3164	1/1	0.83	0.22	56,56,56,56	0
54	MG	DA	3496	1/1	0.83	0.14	66,66,66,66	0
54	MG	DA	3059	1/1	0.83	0.10	45,45,45,45	0
54	MG	CA	1739	1/1	0.83	0.13	87,87,87,87	0
54	MG	DA	3275	1/1	0.83	0.17	47,47,47,47	0
54	MG	DA	3168	1/1	0.83	0.24	42,42,42,42	0
54	MG	CA	1683	1/1	0.83	0.27	100,100,100,100	0
54	MG	DA	3564	1/1	0.83	0.16	61,61,61,61	0
54	MG	CA	1742	1/1	0.83	0.09	113,113,113,113	0
54	MG	BA	3123	1/1	0.83	0.17	43,43,43,43	0
54	MG	CA	1653	1/1	0.83	0.36	57,57,57,57	0
54	MG	BS	201	1/1	0.83	0.19	49,49,49,49	0
54	MG	CE	201	1/1	0.83	0.29	77,77,77,77	0
54	MG	CA	1640	1/1	0.83	0.25	82,82,82,82	0
54	MG	BA	3231	1/1	0.84	0.19	47,47,47,47	0
54	MG	AA	1726	1/1	0.84	0.15	86,86,86,86	0
54	MG	DA	3147	1/1	0.84	0.26	54,54,54,54	0
54	MG	BA	3399	1/1	0.84	0.10	43,43,43,43	0
54	MG	CA	1646	1/1	0.84	0.24	59,59,59,59	0
54	MG	DA	3283	1/1	0.84	0.21	61,61,61,61	0
54	MG	DA	3002	1/1	0.84	0.12	69,69,69,69	0
54	MG	BA	3438	1/1	0.84	0.13	65,65,65,65	0
54	MG	AA	1632	1/1	0.84	0.20	71,71,71,71	0
54	MG	CA	1685	1/1	0.84	0.45	71,71,71,71	0
54	MG	DA	3049	1/1	0.84	0.15	49,49,49,49	0
54	MG	CA	1686	1/1	0.84	0.18	61,61,61,61	0
54	MG	BA	3063	1/1	0.84	0.20	54,54,54,54	0
54	MG	DA	3062	1/1	0.84	0.26	49,49,49,49	0
54	MG	DA	3478	1/1	0.84	0.18	87,87,87,87	0
54	MG	DA	3063	1/1	0.84	0.33	60,60,60,60	0
54	MG	CA	1693	1/1	0.84	0.41	59,59,59,59	0
54	MG	DA	3193	1/1	0.84	0.14	40,40,40,40	0
54	MG	DA	3212	1/1	0.84	0.32	75,75,75,75	0
54	MG	AA	1608	1/1	0.84	0.35	67,67,67,67	0
54	MG	CA	1625	1/1	0.84	0.32	63,63,63,63	0
54	MG	BA	3239	1/1	0.84	0.27	67,67,67,67	0
54	MG	DA	3546	1/1	0.84	0.22	64,64,64,64	0
54	MG	BA	3100	1/1	0.84	0.10	42,42,42,42	0
54	MG	DA	3096	1/1	0.84	0.44	59,59,59,59	0
54	MG	AA	1624	1/1	0.84	0.35	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3569	1/1	0.84	0.10	104,104,104,104	0
54	MG	AA	1673	1/1	0.84	0.39	60,60,60,60	0
54	MG	DA	3258	1/1	0.84	0.24	52,52,52,52	0
54	MG	DA	3265	1/1	0.84	0.22	44,44,44,44	0
54	MG	BA	3197	1/1	0.84	0.24	41,41,41,41	0
54	MG	BA	3307	1/1	0.84	0.12	44,44,44,44	0
54	MG	AA	1699	1/1	0.85	0.10	99,99,99,99	0
54	MG	DA	3125	1/1	0.85	0.20	50,50,50,50	0
54	MG	BA	3128	1/1	0.85	0.18	49,49,49,49	0
54	MG	DA	3231	1/1	0.85	0.17	36,36,36,36	0
54	MG	DA	3401	1/1	0.85	0.14	108,108,108,108	0
54	MG	DA	3232	1/1	0.85	0.39	57,57,57,57	0
54	MG	BA	3094	1/1	0.85	0.21	54,54,54,54	0
54	MG	BA	3347	1/1	0.85	0.11	94,94,94,94	0
54	MG	BA	3039	1/1	0.85	0.12	32,32,32,32	0
54	MG	BA	3368	1/1	0.85	0.11	53,53,53,53	0
54	MG	BA	3384	1/1	0.85	0.07	88,88,88,88	0
54	MG	BA	3189	1/1	0.85	0.16	41,41,41,41	0
54	MG	DA	3262	1/1	0.85	0.20	53,53,53,53	0
54	MG	BA	3102	1/1	0.85	0.29	44,44,44,44	0
54	MG	BA	3241	1/1	0.85	0.19	65,65,65,65	0
54	MG	CA	1624	1/1	0.85	0.31	63,63,63,63	0
54	MG	CA	1716	1/1	0.85	0.13	102,102,102,102	0
54	MG	DA	3561	1/1	0.85	0.13	71,71,71,71	0
54	MG	AA	1686	1/1	0.85	0.12	68,68,68,68	0
54	MG	BA	3264	1/1	0.85	0.30	41,41,41,41	0
54	MG	BA	3273	1/1	0.85	0.33	37,37,37,37	0
54	MG	AA	1660	1/1	0.85	0.36	80,80,80,80	0
54	MG	AA	1671	1/1	0.85	0.22	67,67,67,67	0
54	MG	DB	207	1/1	0.85	0.20	57,57,57,57	0
54	MG	BA	3658	1/1	0.85	0.11	114,114,114,114	0
54	MG	CA	1672	1/1	0.85	0.19	66,66,66,66	0
54	MG	DA	3303	1/1	0.85	0.33	34,34,34,34	0
54	MG	DA	3153	1/1	0.86	0.17	58,58,58,58	0
54	MG	BA	3258	1/1	0.86	0.28	55,55,55,55	0
54	MG	BA	3185	1/1	0.86	0.25	51,51,51,51	0
54	MG	AA	1661	1/1	0.86	0.21	55,55,55,55	0
54	MG	BA	3015	1/1	0.86	0.22	48,48,48,48	0
54	MG	DA	3287	1/1	0.86	0.23	57,57,57,57	0
54	MG	DA	3028	1/1	0.86	0.21	67,67,67,67	0
54	MG	BA	3280	1/1	0.86	0.26	46,46,46,46	0
54	MG	DA	3040	1/1	0.86	0.16	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	DA	3310	1/1	0.86	0.27	28,28,28,28	0
54	MG	DA	3316	1/1	0.86	0.27	69,69,69,69	0
54	MG	BA	3016	1/1	0.86	0.11	47,47,47,47	0
54	MG	DA	3181	1/1	0.86	0.18	49,49,49,49	0
54	MG	DA	3326	1/1	0.86	0.16	46,46,46,46	0
54	MG	BA	3288	1/1	0.86	0.11	66,66,66,66	0
54	MG	DA	3185	1/1	0.86	0.14	57,57,57,57	0
54	MG	BA	3030	1/1	0.86	0.08	48,48,48,48	0
54	MG	AA	1679	1/1	0.86	0.17	44,44,44,44	0
54	MG	BB	206	1/1	0.86	0.17	57,57,57,57	0
54	MG	BB	207	1/1	0.86	0.18	52,52,52,52	0
54	MG	DA	3196	1/1	0.86	0.36	58,58,58,58	0
54	MG	AA	1636	1/1	0.86	0.18	79,79,79,79	0
54	MG	AA	1650	1/1	0.86	0.33	53,53,53,53	0
54	MG	CA	1707	1/1	0.86	0.11	94,94,94,94	0
54	MG	BA	3340	1/1	0.86	0.09	79,79,79,79	0
54	MG	AA	1668	1/1	0.86	0.33	62,62,62,62	0
54	MG	CA	1720	1/1	0.86	0.15	89,89,89,89	0
54	MG	DA	3537	1/1	0.86	0.08	63,63,63,63	0
54	MG	CA	1721	1/1	0.86	0.24	64,64,64,64	0
54	MG	DA	3548	1/1	0.86	0.08	89,89,89,89	0
54	MG	AA	1676	1/1	0.86	0.20	59,59,59,59	0
54	MG	BA	3002	1/1	0.86	0.29	51,51,51,51	0
54	MG	BA	3162	1/1	0.86	0.11	42,42,42,42	0
54	MG	BA	3394	1/1	0.86	0.10	50,50,50,50	0
54	MG	BA	3067	1/1	0.86	0.15	43,43,43,43	0
54	MG	DA	3133	1/1	0.86	0.21	36,36,36,36	0
54	MG	DA	3145	1/1	0.86	0.18	61,61,61,61	0
54	MG	DA	3270	1/1	0.86	0.11	64,64,64,64	0
54	MG	DA	3274	1/1	0.86	0.24	61,61,61,61	0
54	MG	CA	1620	1/1	0.86	0.17	58,58,58,58	0
54	MG	BA	3433	1/1	0.86	0.11	55,55,55,55	0
54	MG	DA	3141	1/1	0.87	0.26	60,60,60,60	0
54	MG	CA	1754	1/1	0.87	0.16	74,74,74,74	0
54	MG	BA	3589	1/1	0.87	0.14	94,94,94,94	0
54	MG	CA	1757	1/1	0.87	0.09	80,80,80,80	0
54	MG	CA	1669	1/1	0.87	0.29	76,76,76,76	0
54	MG	DA	3155	1/1	0.87	0.08	64,64,64,64	0
54	MG	CA	1670	1/1	0.87	0.35	73,73,73,73	0
54	MG	DA	3001	1/1	0.87	0.20	48,48,48,48	0
54	MG	BA	3243	1/1	0.87	0.28	42,42,42,42	0
54	MG	DA	3298	1/1	0.87	0.08	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	DA	3299	1/1	0.87	0.29	65,65,65,65	0
54	MG	DA	3011	1/1	0.87	0.20	42,42,42,42	0
54	MG	DA	3016	1/1	0.87	0.24	62,62,62,62	0
54	MG	BA	3252	1/1	0.87	0.26	36,36,36,36	0
54	MG	BA	3072	1/1	0.87	0.23	59,59,59,59	0
54	MG	BA	3660	1/1	0.87	0.11	104,104,104,104	0
54	MG	CA	1634	1/1	0.87	0.16	64,64,64,64	0
54	MG	DA	3045	1/1	0.87	0.12	38,38,38,38	0
54	MG	BA	3073	1/1	0.87	0.24	52,52,52,52	0
54	MG	DA	3398	1/1	0.87	0.13	88,88,88,88	0
54	MG	BA	3025	1/1	0.87	0.10	48,48,48,48	0
54	MG	DA	3055	1/1	0.87	0.19	56,56,56,56	0
54	MG	DA	3424	1/1	0.87	0.07	52,52,52,52	0
54	MG	BA	3026	1/1	0.87	0.18	52,52,52,52	0
54	MG	DA	3460	1/1	0.87	0.12	65,65,65,65	0
54	MG	BA	3275	1/1	0.87	0.23	26,26,26,26	0
54	MG	BA	3097	1/1	0.87	0.12	47,47,47,47	0
54	MG	DA	3201	1/1	0.87	0.16	49,49,49,49	0
54	MG	DA	3206	1/1	0.87	0.36	52,52,52,52	0
54	MG	DA	3209	1/1	0.87	0.21	51,51,51,51	0
54	MG	BG	201	1/1	0.87	0.22	60,60,60,60	0
54	MG	DA	3515	1/1	0.87	0.12	37,37,37,37	0
54	MG	DA	3216	1/1	0.87	0.14	51,51,51,51	0
54	MG	DA	3522	1/1	0.87	0.16	61,61,61,61	0
54	MG	CA	1648	1/1	0.87	0.30	60,60,60,60	0
54	MG	BQ	203	1/1	0.87	0.11	73,73,73,73	0
54	MG	BA	3404	1/1	0.87	0.10	45,45,45,45	0
54	MG	DA	3540	1/1	0.87	0.07	53,53,53,53	0
54	MG	BA	3421	1/1	0.87	0.13	68,68,68,68	0
54	MG	DA	3235	1/1	0.87	0.15	54,54,54,54	0
54	MG	DA	3082	1/1	0.87	0.20	36,36,36,36	0
54	MG	CA	1718	1/1	0.87	0.10	83,83,83,83	0
54	MG	AA	1623	1/1	0.87	0.16	74,74,74,74	0
54	MG	DA	3102	1/1	0.87	0.28	40,40,40,40	0
54	MG	BA	3183	1/1	0.87	0.19	29,29,29,29	0
54	MG	BA	3298	1/1	0.87	0.24	54,54,54,54	0
54	MG	CA	1609	1/1	0.87	0.24	70,70,70,70	0
54	MG	BA	3062	1/1	0.87	0.19	45,45,45,45	0
54	MG	AA	1709	1/1	0.87	0.12	101,101,101,101	0
54	MG	BA	3532	1/1	0.87	0.12	79,79,79,79	0
54	MG	AA	1646	1/1	0.87	0.29	59,59,59,59	0
54	MG	DA	3162	1/1	0.88	0.19	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1649	1/1	0.88	0.26	43,43,43,43	0
54	MG	BA	3547	1/1	0.88	0.12	105,105,105,105	0
54	MG	CA	1679	1/1	0.88	0.26	59,59,59,59	0
54	MG	DA	3296	1/1	0.88	0.22	67,67,67,67	0
54	MG	BA	3306	1/1	0.88	0.09	55,55,55,55	0
54	MG	CA	1681	1/1	0.88	0.09	82,82,82,82	0
54	MG	DA	3046	1/1	0.88	0.13	42,42,42,42	0
54	MG	BA	3205	1/1	0.88	0.12	54,54,54,54	0
54	MG	BA	3313	1/1	0.88	0.11	37,37,37,37	0
54	MG	BA	3642	1/1	0.88	0.10	139,139,139,139	0
54	MG	BA	3251	1/1	0.88	0.19	27,27,27,27	0
54	MG	BA	3207	1/1	0.88	0.09	33,33,33,33	0
54	MG	DA	3060	1/1	0.88	0.14	41,41,41,41	0
54	MG	BA	3344	1/1	0.88	0.19	61,61,61,61	0
54	MG	DA	3327	1/1	0.88	0.14	52,52,52,52	0
54	MG	CA	1639	1/1	0.88	0.21	76,76,76,76	0
54	MG	DA	3353	1/1	0.88	0.15	61,61,61,61	0
54	MG	BA	3212	1/1	0.88	0.28	68,68,68,68	0
54	MG	BA	3223	1/1	0.88	0.23	60,60,60,60	0
54	MG	BA	3263	1/1	0.88	0.15	36,36,36,36	0
54	MG	DA	3410	1/1	0.88	0.08	86,86,86,86	0
54	MG	DA	3416	1/1	0.88	0.13	66,66,66,66	0
54	MG	DA	3208	1/1	0.88	0.28	53,53,53,53	0
54	MG	BB	210	1/1	0.88	0.09	60,60,60,60	0
54	MG	BA	3369	1/1	0.88	0.08	52,52,52,52	0
54	MG	BA	3126	1/1	0.88	0.15	41,41,41,41	0
54	MG	DA	3093	1/1	0.88	0.21	56,56,56,56	0
54	MG	DA	3219	1/1	0.88	0.17	38,38,38,38	0
54	MG	BE	302	1/1	0.88	0.07	41,41,41,41	0
54	MG	DA	3222	1/1	0.88	0.29	68,68,68,68	0
54	MG	DA	3100	1/1	0.88	0.21	38,38,38,38	0
54	MG	AA	1606	1/1	0.88	0.41	79,79,79,79	0
54	MG	DA	3115	1/1	0.88	0.27	59,59,59,59	0
54	MG	BA	3234	1/1	0.88	0.18	69,69,69,69	0
54	MG	BA	3400	1/1	0.88	0.19	47,47,47,47	0
54	MG	DA	3239	1/1	0.88	0.25	58,58,58,58	0
54	MG	CA	1657	1/1	0.88	0.10	61,61,61,61	0
54	MG	DA	3251	1/1	0.88	0.14	40,40,40,40	0
54	MG	BA	3276	1/1	0.88	0.15	23,23,23,23	0
54	MG	BA	3279	1/1	0.88	0.24	27,27,27,27	0
54	MG	DA	3552	1/1	0.88	0.17	35,35,35,35	0
54	MG	BA	3192	1/1	0.88	0.18	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	BA	3107	1/1	0.88	0.28	60,60,60,60	0
54	MG	BA	3442	1/1	0.88	0.09	76,76,76,76	0
54	MG	CA	1612	1/1	0.88	0.15	65,65,65,65	0
54	MG	AQ	201	1/1	0.88	0.19	58,58,58,58	0
54	MG	DA	3273	1/1	0.88	0.22	50,50,50,50	0
54	MG	AA	1664	1/1	0.88	0.24	57,57,57,57	0
54	MG	DA	3148	1/1	0.88	0.12	48,48,48,48	0
54	MG	DF	301	1/1	0.88	0.19	50,50,50,50	0
54	MG	BA	3240	1/1	0.88	0.32	71,71,71,71	0
54	MG	CA	1621	1/1	0.88	0.21	64,64,64,64	0
54	MG	D0	101	1/1	0.88	0.13	41,41,41,41	0
54	MG	CA	1674	1/1	0.88	0.17	74,74,74,74	0
54	MG	DA	3267	1/1	0.89	0.26	54,54,54,54	0
54	MG	BA	3216	1/1	0.89	0.14	43,43,43,43	0
54	MG	CA	1729	1/1	0.89	0.10	81,81,81,81	0
54	MG	BA	3222	1/1	0.89	0.16	60,60,60,60	0
54	MG	DA	3129	1/1	0.89	0.16	61,61,61,61	0
54	MG	BA	3010	1/1	0.89	0.22	39,39,39,39	0
54	MG	BA	3397	1/1	0.89	0.09	86,86,86,86	0
54	MG	BA	3225	1/1	0.89	0.18	44,44,44,44	0
54	MG	DA	3134	1/1	0.89	0.17	62,62,62,62	0
54	MG	CA	1654	1/1	0.89	0.20	65,65,65,65	0
54	MG	DA	3281	1/1	0.89	0.09	42,42,42,42	0
54	MG	DA	3144	1/1	0.89	0.29	42,42,42,42	0
54	MG	BA	3013	1/1	0.89	0.09	49,49,49,49	0
54	MG	BA	3171	1/1	0.89	0.14	31,31,31,31	0
54	MG	DA	3288	1/1	0.89	0.17	39,39,39,39	0
54	MG	DA	3295	1/1	0.89	0.21	59,59,59,59	0
54	MG	B0	101	1/1	0.89	0.19	39,39,39,39	0
54	MG	B1	101	1/1	0.89	0.18	45,45,45,45	0
54	MG	BA	3409	1/1	0.89	0.09	68,68,68,68	0
54	MG	CA	1602	1/1	0.89	0.35	62,62,62,62	0
54	MG	CQ	201	1/1	0.89	0.34	62,62,62,62	0
54	MG	BA	3233	1/1	0.89	0.31	41,41,41,41	0
54	MG	DA	3308	1/1	0.89	0.17	33,33,33,33	0
54	MG	DA	3309	1/1	0.89	0.24	28,28,28,28	0
54	MG	AA	1603	1/1	0.89	0.23	79,79,79,79	0
54	MG	BA	3101	1/1	0.89	0.12	37,37,37,37	0
54	MG	DA	3012	1/1	0.89	0.16	30,30,30,30	0
54	MG	DA	3015	1/1	0.89	0.23	38,38,38,38	0
54	MG	DA	3170	1/1	0.89	0.11	56,56,56,56	0
54	MG	BA	3290	1/1	0.89	0.13	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	AA	1633	1/1	0.89	0.21	62,62,62,62	0
54	MG	DA	3329	1/1	0.89	0.13	41,41,41,41	0
54	MG	DA	3331	1/1	0.89	0.23	71,71,71,71	0
54	MG	DA	3332	1/1	0.89	0.20	53,53,53,53	0
54	MG	DA	3024	1/1	0.89	0.27	47,47,47,47	0
54	MG	DA	3372	1/1	0.89	0.10	41,41,41,41	0
54	MG	BA	3300	1/1	0.89	0.22	48,48,48,48	0
54	MG	CA	1615	1/1	0.89	0.20	65,65,65,65	0
54	MG	DA	3035	1/1	0.89	0.24	60,60,60,60	0
54	MG	AA	1602	1/1	0.89	0.22	89,89,89,89	0
54	MG	CA	1675	1/1	0.89	0.42	61,61,61,61	0
54	MG	BA	3304	1/1	0.89	0.12	54,54,54,54	0
54	MG	AC	301	1/1	0.89	0.09	57,57,57,57	0
54	MG	DA	3435	1/1	0.89	0.28	57,57,57,57	0
54	MG	DA	3438	1/1	0.89	0.09	90,90,90,90	0
54	MG	DA	3453	1/1	0.89	0.09	79,79,79,79	0
54	MG	AA	1659	1/1	0.89	0.46	70,70,70,70	0
54	MG	DA	3197	1/1	0.89	0.26	49,49,49,49	0
54	MG	BA	3112	1/1	0.89	0.15	55,55,55,55	0
54	MG	BA	3001	1/1	0.89	0.11	43,43,43,43	0
54	MG	CA	1627	1/1	0.89	0.20	55,55,55,55	0
54	MG	DA	3488	1/1	0.89	0.08	58,58,58,58	0
54	MG	CA	1628	1/1	0.89	0.20	75,75,75,75	0
54	MG	BA	3245	1/1	0.89	0.25	23,23,23,23	0
54	MG	CA	1630	1/1	0.89	0.33	72,72,72,72	0
54	MG	BA	3249	1/1	0.89	0.22	25,25,25,25	0
54	MG	BA	3032	1/1	0.89	0.13	40,40,40,40	0
54	MG	AA	1615	1/1	0.89	0.19	54,54,54,54	0
54	MG	CA	1698	1/1	0.89	0.09	47,47,47,47	0
54	MG	DA	3535	1/1	0.89	0.23	64,64,64,64	0
54	MG	DA	3223	1/1	0.89	0.25	54,54,54,54	0
54	MG	DA	3225	1/1	0.89	0.28	51,51,51,51	0
54	MG	DA	3081	1/1	0.89	0.12	58,58,58,58	0
54	MG	BB	202	1/1	0.89	0.15	43,43,43,43	0
54	MG	BA	3352	1/1	0.89	0.10	81,81,81,81	0
54	MG	DA	3555	1/1	0.89	0.09	56,56,56,56	0
54	MG	DA	3092	1/1	0.89	0.19	41,41,41,41	0
54	MG	CA	1712	1/1	0.89	0.12	87,87,87,87	0
54	MG	CA	1714	1/1	0.89	0.10	87,87,87,87	0
54	MG	DA	3241	1/1	0.89	0.09	35,35,35,35	0
54	MG	BA	3082	1/1	0.89	0.21	36,36,36,36	0
54	MG	DA	3248	1/1	0.89	0.13	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	3587	1/1	0.89	0.13	95,95,95,95	0
54	MG	DB	202	1/1	0.89	0.27	50,50,50,50	0
54	MG	BA	3131	1/1	0.89	0.24	62,62,62,62	0
54	MG	DA	3252	1/1	0.89	0.38	59,59,59,59	0
54	MG	DA	3103	1/1	0.89	0.30	54,54,54,54	0
54	MG	DA	3114	1/1	0.89	0.18	30,30,30,30	0
54	MG	BB	208	1/1	0.89	0.12	43,43,43,43	0
54	MG	BB	209	1/1	0.89	0.20	60,60,60,60	0
54	MG	DA	3119	1/1	0.89	0.30	48,48,48,48	0
55	ZN	D4	101	1/1	0.89	0.12	214,214,214,214	0
54	MG	DA	3160	1/1	0.90	0.08	42,42,42,42	0
54	MG	DA	3161	1/1	0.90	0.17	39,39,39,39	0
54	MG	DA	3294	1/1	0.90	0.14	42,42,42,42	0
54	MG	DA	3019	1/1	0.90	0.11	40,40,40,40	0
54	MG	BA	3114	1/1	0.90	0.08	63,63,63,63	0
54	MG	BA	3217	1/1	0.90	0.12	41,41,41,41	0
54	MG	AA	1695	1/1	0.90	0.12	74,74,74,74	0
54	MG	AA	1697	1/1	0.90	0.10	106,106,106,106	0
54	MG	DA	3169	1/1	0.90	0.09	45,45,45,45	0
54	MG	BA	3029	1/1	0.90	0.09	32,32,32,32	0
54	MG	BA	3226	1/1	0.90	0.09	50,50,50,50	0
54	MG	DA	3042	1/1	0.90	0.15	33,33,33,33	0
54	MG	DA	3044	1/1	0.90	0.16	46,46,46,46	0
54	MG	BA	3076	1/1	0.90	0.18	44,44,44,44	0
54	MG	DA	3320	1/1	0.90	0.18	38,38,38,38	0
54	MG	BA	3132	1/1	0.90	0.10	33,33,33,33	0
54	MG	BA	3137	1/1	0.90	0.17	38,38,38,38	0
54	MG	CA	1618	1/1	0.90	0.27	64,64,64,64	0
54	MG	DA	3052	1/1	0.90	0.29	52,52,52,52	0
54	MG	CA	1682	1/1	0.90	0.22	58,58,58,58	0
54	MG	AA	1677	1/1	0.90	0.15	62,62,62,62	0
54	MG	BA	3554	1/1	0.90	0.08	88,88,88,88	0
54	MG	BA	3570	1/1	0.90	0.10	78,78,78,78	0
54	MG	DA	3198	1/1	0.90	0.27	57,57,57,57	0
54	MG	BA	3581	1/1	0.90	0.09	86,86,86,86	0
54	MG	CA	1689	1/1	0.90	0.24	61,61,61,61	0
54	MG	AA	1665	1/1	0.90	0.18	51,51,51,51	0
54	MG	BA	3090	1/1	0.90	0.18	62,62,62,62	0
54	MG	DA	3211	1/1	0.90	0.25	48,48,48,48	0
54	MG	CA	1694	1/1	0.90	0.06	62,62,62,62	0
54	MG	BA	3173	1/1	0.90	0.25	32,32,32,32	0
54	MG	DA	3076	1/1	0.90	0.18	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	BA	3597	1/1	0.90	0.15	84,84,84,84	0
54	MG	BA	3600	1/1	0.90	0.07	81,81,81,81	0
54	MG	DA	3447	1/1	0.90	0.11	74,74,74,74	0
54	MG	DA	3452	1/1	0.90	0.07	90,90,90,90	0
54	MG	DA	3088	1/1	0.90	0.25	55,55,55,55	0
54	MG	BA	3035	1/1	0.90	0.20	45,45,45,45	0
54	MG	BA	3646	1/1	0.90	0.08	142,142,142,142	0
54	MG	DA	3228	1/1	0.90	0.34	40,40,40,40	0
54	MG	BA	3009	1/1	0.90	0.21	45,45,45,45	0
54	MG	DA	3483	1/1	0.90	0.17	59,59,59,59	0
54	MG	DA	3095	1/1	0.90	0.25	53,53,53,53	0
54	MG	CA	1635	1/1	0.90	0.12	60,60,60,60	0
54	MG	BA	3336	1/1	0.90	0.05	45,45,45,45	0
54	MG	BA	3099	1/1	0.90	0.10	46,46,46,46	0
54	MG	DA	3499	1/1	0.90	0.10	67,67,67,67	0
54	MG	BA	3186	1/1	0.90	0.22	26,26,26,26	0
54	MG	BB	203	1/1	0.90	0.21	70,70,70,70	0
54	MG	AA	1672	1/1	0.90	0.28	46,46,46,46	0
54	MG	CA	1733	1/1	0.90	0.13	82,82,82,82	0
54	MG	AA	1629	1/1	0.90	0.23	44,44,44,44	0
54	MG	CA	1645	1/1	0.90	0.36	60,60,60,60	0
54	MG	BA	3250	1/1	0.90	0.23	26,26,26,26	0
54	MG	DA	3255	1/1	0.90	0.07	58,58,58,58	0
54	MG	DA	3256	1/1	0.90	0.33	52,52,52,52	0
54	MG	BA	3353	1/1	0.90	0.12	91,91,91,91	0
54	MG	BA	3364	1/1	0.90	0.08	81,81,81,81	0
54	MG	DA	3261	1/1	0.90	0.22	44,44,44,44	0
54	MG	AA	1642	1/1	0.90	0.31	54,54,54,54	0
54	MG	BA	3052	1/1	0.90	0.24	52,52,52,52	0
54	MG	BA	3056	1/1	0.90	0.13	57,57,57,57	0
54	MG	BE	301	1/1	0.90	0.28	34,34,34,34	0
54	MG	DA	3140	1/1	0.90	0.21	64,64,64,64	0
54	MG	AA	1675	1/1	0.90	0.17	76,76,76,76	0
54	MG	BE	305	1/1	0.90	0.12	60,60,60,60	0
54	MG	DA	3590	1/1	0.90	0.12	82,82,82,82	0
54	MG	BA	3111	1/1	0.90	0.36	56,56,56,56	0
54	MG	BQ	201	1/1	0.90	0.15	51,51,51,51	0
54	MG	AA	1627	1/1	0.90	0.19	59,59,59,59	0
54	MG	DE	301	1/1	0.90	0.14	41,41,41,41	0
54	MG	BA	3269	1/1	0.90	0.24	35,35,35,35	0
54	MG	DA	3151	1/1	0.90	0.15	43,43,43,43	0
54	MG	BA	3271	1/1	0.90	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3018	1/1	0.90	0.23	40,40,40,40	0
54	MG	BA	3407	1/1	0.90	0.10	47,47,47,47	0
54	MG	DA	3285	1/1	0.90	0.13	64,64,64,64	0
54	MG	BA	3120	1/1	0.91	0.14	51,51,51,51	0
54	MG	BA	3081	1/1	0.91	0.21	42,42,42,42	0
54	MG	DA	3067	1/1	0.91	0.25	49,49,49,49	0
54	MG	BQ	202	1/1	0.91	0.08	34,34,34,34	0
54	MG	BA	3524	1/1	0.91	0.08	38,38,38,38	0
54	MG	CA	1650	1/1	0.91	0.29	60,60,60,60	0
54	MG	DA	3195	1/1	0.91	0.25	48,48,48,48	0
54	MG	BA	3310	1/1	0.91	0.21	23,23,23,23	0
54	MG	BA	3040	1/1	0.91	0.12	30,30,30,30	0
54	MG	BA	3085	1/1	0.91	0.22	52,52,52,52	0
54	MG	CA	1734	1/1	0.91	0.16	66,66,66,66	0
54	MG	DA	3089	1/1	0.91	0.17	52,52,52,52	0
54	MG	DA	3207	1/1	0.91	0.21	54,54,54,54	0
54	MG	B3	101	1/1	0.91	0.14	51,51,51,51	0
54	MG	AA	1634	1/1	0.91	0.17	56,56,56,56	0
54	MG	DA	3210	1/1	0.91	0.23	53,53,53,53	0
54	MG	BA	3579	1/1	0.91	0.07	100,100,100,100	0
54	MG	BA	3254	1/1	0.91	0.23	25,25,25,25	0
54	MG	DA	3367	1/1	0.91	0.15	30,30,30,30	0
54	MG	CA	1605	1/1	0.91	0.30	67,67,67,67	0
54	MG	DA	3382	1/1	0.91	0.13	53,53,53,53	0
54	MG	DA	3387	1/1	0.91	0.08	60,60,60,60	0
54	MG	DA	3098	1/1	0.91	0.08	37,37,37,37	0
54	MG	BA	3257	1/1	0.91	0.26	23,23,23,23	0
54	MG	BA	3049	1/1	0.91	0.23	53,53,53,53	0
54	MG	CA	1755	1/1	0.91	0.06	129,129,129,129	0
54	MG	DA	3107	1/1	0.91	0.16	54,54,54,54	0
54	MG	AA	1704	1/1	0.91	0.07	86,86,86,86	0
54	MG	DA	3426	1/1	0.91	0.12	81,81,81,81	0
54	MG	DA	3227	1/1	0.91	0.17	52,52,52,52	0
54	MG	BA	3139	1/1	0.91	0.34	46,46,46,46	0
54	MG	BA	3141	1/1	0.91	0.15	36,36,36,36	0
54	MG	BA	3621	1/1	0.91	0.23	52,52,52,52	0
54	MG	DA	3233	1/1	0.91	0.08	38,38,38,38	0
54	MG	DA	3120	1/1	0.91	0.21	43,43,43,43	0
54	MG	BA	3637	1/1	0.91	0.14	108,108,108,108	0
54	MG	AA	1601	1/1	0.91	0.27	55,55,55,55	0
54	MG	DA	3466	1/1	0.91	0.08	68,68,68,68	0
54	MG	AA	1652	1/1	0.91	0.33	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	3647	1/1	0.91	0.07	70,70,70,70	0
54	MG	DA	3482	1/1	0.91	0.13	56,56,56,56	0
54	MG	DA	3246	1/1	0.91	0.32	68,68,68,68	0
54	MG	BA	3654	1/1	0.91	0.07	126,126,126,126	0
54	MG	BA	3164	1/1	0.91	0.31	50,50,50,50	0
54	MG	BA	3230	1/1	0.91	0.13	30,30,30,30	0
54	MG	BA	3061	1/1	0.91	0.29	54,54,54,54	0
54	MG	DA	3139	1/1	0.91	0.45	59,59,59,59	0
54	MG	BA	3031	1/1	0.91	0.14	44,44,44,44	0
54	MG	DA	3517	1/1	0.91	0.21	66,66,66,66	0
54	MG	DA	3021	1/1	0.91	0.16	51,51,51,51	0
54	MG	DA	3023	1/1	0.91	0.11	43,43,43,43	0
54	MG	AA	1656	1/1	0.91	0.31	59,59,59,59	0
54	MG	DA	3528	1/1	0.91	0.08	124,124,124,124	0
54	MG	DA	3259	1/1	0.91	0.18	43,43,43,43	0
54	MG	BA	3283	1/1	0.91	0.33	21,21,21,21	0
54	MG	BA	3177	1/1	0.91	0.23	57,57,57,57	0
54	MG	DA	3031	1/1	0.91	0.29	53,53,53,53	0
54	MG	DA	3544	1/1	0.91	0.07	72,72,72,72	0
54	MG	DA	3150	1/1	0.91	0.22	42,42,42,42	0
54	MG	DA	3032	1/1	0.91	0.14	49,49,49,49	0
54	MG	DA	3033	1/1	0.91	0.18	66,66,66,66	0
54	MG	BA	3033	1/1	0.91	0.13	36,36,36,36	0
54	MG	AA	1658	1/1	0.91	0.33	57,57,57,57	0
54	MG	CA	1688	1/1	0.91	0.30	54,54,54,54	0
54	MG	AA	1647	1/1	0.91	0.21	55,55,55,55	0
54	MG	BA	3074	1/1	0.91	0.20	53,53,53,53	0
54	MG	BA	3191	1/1	0.91	0.16	40,40,40,40	0
54	MG	CA	1638	1/1	0.91	0.17	52,52,52,52	0
54	MG	CA	1695	1/1	0.91	0.06	50,50,50,50	0
54	MG	AA	1643	1/1	0.91	0.23	47,47,47,47	0
54	MG	DA	3597	1/1	0.91	0.11	93,93,93,93	0
54	MG	DB	201	1/1	0.91	0.17	43,43,43,43	0
54	MG	BA	3456	1/1	0.91	0.13	32,32,32,32	0
54	MG	DA	3284	1/1	0.91	0.11	55,55,55,55	0
54	MG	DA	3056	1/1	0.91	0.12	43,43,43,43	0
54	MG	AA	1670	1/1	0.91	0.20	53,53,53,53	0
54	MG	DA	3176	1/1	0.91	0.41	70,70,70,70	0
54	MG	DA	3290	1/1	0.91	0.32	58,58,58,58	0
54	MG	CA	1704	1/1	0.91	0.10	92,92,92,92	0
54	MG	DQ	202	1/1	0.91	0.07	33,33,33,33	0
54	MG	DA	3178	1/1	0.91	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	BA	3486	1/1	0.91	0.10	75,75,75,75	0
54	MG	CA	1643	1/1	0.91	0.25	70,70,70,70	0
54	MG	BA	3219	1/1	0.92	0.18	46,46,46,46	0
54	MG	BA	3553	1/1	0.92	0.07	89,89,89,89	0
54	MG	BA	3335	1/1	0.92	0.08	66,66,66,66	0
54	MG	CA	1611	1/1	0.92	0.21	43,43,43,43	0
54	MG	BA	3559	1/1	0.92	0.08	71,71,71,71	0
54	MG	AA	1648	1/1	0.92	0.28	44,44,44,44	0
54	MG	BA	3572	1/1	0.92	0.12	63,63,63,63	0
54	MG	BA	3259	1/1	0.92	0.25	27,27,27,27	0
54	MG	BA	3045	1/1	0.92	0.15	45,45,45,45	0
54	MG	DA	3171	1/1	0.92	0.14	61,61,61,61	0
54	MG	BA	3108	1/1	0.92	0.14	51,51,51,51	0
54	MG	DA	3304	1/1	0.92	0.27	29,29,29,29	0
54	MG	DA	3305	1/1	0.92	0.14	35,35,35,35	0
54	MG	DA	3306	1/1	0.92	0.17	29,29,29,29	0
54	MG	CA	1687	1/1	0.92	0.12	62,62,62,62	0
54	MG	BA	3027	1/1	0.92	0.13	38,38,38,38	0
54	MG	BA	3266	1/1	0.92	0.32	22,22,22,22	0
54	MG	DA	3312	1/1	0.92	0.32	29,29,29,29	0
54	MG	BA	3267	1/1	0.92	0.20	36,36,36,36	0
54	MG	DA	3318	1/1	0.92	0.24	58,58,58,58	0
54	MG	DA	3319	1/1	0.92	0.34	57,57,57,57	0
54	MG	DA	3180	1/1	0.92	0.15	49,49,49,49	0
54	MG	BA	3358	1/1	0.92	0.08	55,55,55,55	0
54	MG	DA	3322	1/1	0.92	0.18	49,49,49,49	0
54	MG	BA	3601	1/1	0.92	0.09	76,76,76,76	0
54	MG	BA	3360	1/1	0.92	0.05	35,35,35,35	0
54	MG	BA	3363	1/1	0.92	0.10	64,64,64,64	0
54	MG	BA	3638	1/1	0.92	0.11	67,67,67,67	0
54	MG	CA	1631	1/1	0.92	0.17	48,48,48,48	0
54	MG	DA	3190	1/1	0.92	0.15	59,59,59,59	0
54	MG	DA	3191	1/1	0.92	0.12	51,51,51,51	0
54	MG	DA	3345	1/1	0.92	0.18	54,54,54,54	0
54	MG	DA	3192	1/1	0.92	0.09	50,50,50,50	0
54	MG	BA	3268	1/1	0.92	0.24	27,27,27,27	0
54	MG	DA	3370	1/1	0.92	0.07	32,32,32,32	0
54	MG	BA	3110	1/1	0.92	0.35	66,66,66,66	0
54	MG	DA	3070	1/1	0.92	0.31	57,57,57,57	0
54	MG	BA	3078	1/1	0.92	0.17	30,30,30,30	0
54	MG	DA	3072	1/1	0.92	0.28	50,50,50,50	0
54	MG	DA	3199	1/1	0.92	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3649	1/1	0.92	0.10	125,125,125,125	0
54	MG	AA	1654	1/1	0.92	0.38	59,59,59,59	0
54	MG	BA	3370	1/1	0.92	0.15	41,41,41,41	0
54	MG	DA	3077	1/1	0.92	0.23	49,49,49,49	0
54	MG	BA	3012	1/1	0.92	0.29	27,27,27,27	0
54	MG	AA	1610	1/1	0.92	0.14	56,56,56,56	0
54	MG	DA	3086	1/1	0.92	0.21	48,48,48,48	0
54	MG	DA	3437	1/1	0.92	0.07	85,85,85,85	0
54	MG	BA	3059	1/1	0.92	0.11	48,48,48,48	0
54	MG	BA	3086	1/1	0.92	0.33	57,57,57,57	0
54	MG	CA	1730	1/1	0.92	0.06	62,62,62,62	0
54	MG	CA	1731	1/1	0.92	0.07	74,74,74,74	0
54	MG	DA	3459	1/1	0.92	0.06	53,53,53,53	0
54	MG	DA	3220	1/1	0.92	0.22	51,51,51,51	0
54	MG	CA	1732	1/1	0.92	0.07	110,110,110,110	0
54	MG	BA	3125	1/1	0.92	0.22	45,45,45,45	0
54	MG	BA	3403	1/1	0.92	0.08	67,67,67,67	0
54	MG	CA	1644	1/1	0.92	0.24	53,53,53,53	0
54	MG	BA	3285	1/1	0.92	0.15	38,38,38,38	0
54	MG	BA	3286	1/1	0.92	0.18	52,52,52,52	0
54	MG	DA	3229	1/1	0.92	0.19	44,44,44,44	0
54	MG	DA	3230	1/1	0.92	0.16	45,45,45,45	0
54	MG	BA	3408	1/1	0.92	0.12	50,50,50,50	0
54	MG	BA	3088	1/1	0.92	0.10	33,33,33,33	0
54	MG	DA	3110	1/1	0.92	0.24	53,53,53,53	0
54	MG	DA	3510	1/1	0.92	0.08	74,74,74,74	0
54	MG	DA	3111	1/1	0.92	0.15	50,50,50,50	0
54	MG	DA	3112	1/1	0.92	0.18	51,51,51,51	0
54	MG	DA	3113	1/1	0.92	0.20	59,59,59,59	0
54	MG	CA	1746	1/1	0.92	0.06	97,97,97,97	0
54	MG	CA	1750	1/1	0.92	0.07	78,78,78,78	0
54	MG	CA	1751	1/1	0.92	0.18	61,61,61,61	0
54	MG	AD	302	1/1	0.92	0.27	77,77,77,77	0
54	MG	BA	3427	1/1	0.92	0.12	89,89,89,89	0
54	MG	DA	3122	1/1	0.92	0.23	49,49,49,49	0
54	MG	AF	201	1/1	0.92	0.11	62,62,62,62	0
54	MG	BA	3292	1/1	0.92	0.30	70,70,70,70	0
54	MG	AA	1628	1/1	0.92	0.17	68,68,68,68	0
54	MG	AA	1609	1/1	0.92	0.23	51,51,51,51	0
54	MG	CA	1759	1/1	0.92	0.11	69,69,69,69	0
54	MG	BA	3461	1/1	0.92	0.11	79,79,79,79	0
54	MG	BA	3246	1/1	0.92	0.33	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3023	1/1	0.92	0.10	52,52,52,52	0
54	MG	DA	3563	1/1	0.92	0.09	70,70,70,70	0
54	MG	BA	3209	1/1	0.92	0.22	56,56,56,56	0
54	MG	DA	3264	1/1	0.92	0.22	61,61,61,61	0
54	MG	DA	3009	1/1	0.92	0.23	46,46,46,46	0
54	MG	BV	201	1/1	0.92	0.08	67,67,67,67	0
54	MG	DA	3583	1/1	0.92	0.10	65,65,65,65	0
54	MG	DA	3142	1/1	0.92	0.17	37,37,37,37	0
54	MG	DA	3143	1/1	0.92	0.20	60,60,60,60	0
54	MG	DA	3271	1/1	0.92	0.19	57,57,57,57	0
54	MG	BA	3140	1/1	0.92	0.37	36,36,36,36	0
54	MG	BA	3516	1/1	0.92	0.16	63,63,63,63	0
54	MG	DB	203	1/1	0.92	0.21	58,58,58,58	0
54	MG	BA	3068	1/1	0.92	0.13	50,50,50,50	0
54	MG	AA	1723	1/1	0.92	0.06	112,112,112,112	0
54	MG	BA	3539	1/1	0.92	0.08	47,47,47,47	0
54	MG	DE	304	1/1	0.92	0.14	42,42,42,42	0
54	MG	BA	3543	1/1	0.92	0.09	119,119,119,119	0
54	MG	CA	1673	1/1	0.92	0.43	57,57,57,57	0
54	MG	BA	3544	1/1	0.92	0.10	46,46,46,46	0
54	MG	DQ	201	1/1	0.92	0.05	40,40,40,40	0
54	MG	CA	1606	1/1	0.92	0.20	59,59,59,59	0
54	MG	DA	3156	1/1	0.92	0.17	35,35,35,35	0
54	MG	DA	3029	1/1	0.92	0.11	40,40,40,40	0
54	MG	D8	101	1/1	0.92	0.12	48,48,48,48	0
54	MG	D8	102	1/1	0.92	0.18	45,45,45,45	0
54	MG	DA	3159	1/1	0.92	0.14	45,45,45,45	0
54	MG	DA	3084	1/1	0.93	0.15	37,37,37,37	0
54	MG	BA	3648	1/1	0.93	0.08	91,91,91,91	0
54	MG	BA	3393	1/1	0.93	0.09	37,37,37,37	0
54	MG	BA	3159	1/1	0.93	0.20	46,46,46,46	0
54	MG	AA	1720	1/1	0.93	0.10	68,68,68,68	0
54	MG	BA	3656	1/1	0.93	0.08	68,68,68,68	0
54	MG	AA	1638	1/1	0.93	0.11	53,53,53,53	0
54	MG	AA	1662	1/1	0.93	0.22	58,58,58,58	0
54	MG	CA	1736	1/1	0.93	0.10	70,70,70,70	0
54	MG	DA	3097	1/1	0.93	0.19	23,23,23,23	0
54	MG	DA	3330	1/1	0.93	0.08	37,37,37,37	0
54	MG	BA	3172	1/1	0.93	0.30	47,47,47,47	0
54	MG	AA	1617	1/1	0.93	0.14	45,45,45,45	0
54	MG	BA	3017	1/1	0.93	0.13	31,31,31,31	0
54	MG	BB	205	1/1	0.93	0.20	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	3358	1/1	0.93	0.08	39,39,39,39	0
54	MG	AA	1734	1/1	0.93	0.07	96,96,96,96	0
54	MG	DA	3368	1/1	0.93	0.09	52,52,52,52	0
54	MG	DA	3108	1/1	0.93	0.11	42,42,42,42	0
54	MG	DA	3371	1/1	0.93	0.14	43,43,43,43	0
54	MG	BA	3021	1/1	0.93	0.05	44,44,44,44	0
54	MG	DA	3374	1/1	0.93	0.21	37,37,37,37	0
54	MG	BA	3295	1/1	0.93	0.21	54,54,54,54	0
54	MG	DA	3383	1/1	0.93	0.07	54,54,54,54	0
54	MG	BA	3296	1/1	0.93	0.07	43,43,43,43	0
54	MG	DA	3391	1/1	0.93	0.07	37,37,37,37	0
54	MG	BA	3297	1/1	0.93	0.10	46,46,46,46	0
54	MG	BB	211	1/1	0.93	0.07	47,47,47,47	0
54	MG	DA	3226	1/1	0.93	0.29	55,55,55,55	0
54	MG	DA	3408	1/1	0.93	0.07	51,51,51,51	0
54	MG	AA	1657	1/1	0.93	0.23	58,58,58,58	0
54	MG	DA	3411	1/1	0.93	0.07	49,49,49,49	0
54	MG	BB	216	1/1	0.93	0.08	82,82,82,82	0
54	MG	AA	1680	1/1	0.93	0.16	72,72,72,72	0
54	MG	BA	3443	1/1	0.93	0.14	47,47,47,47	0
54	MG	BA	3444	1/1	0.93	0.09	53,53,53,53	0
54	MG	BA	3446	1/1	0.93	0.09	30,30,30,30	0
54	MG	BF	301	1/1	0.93	0.15	33,33,33,33	0
54	MG	BF	302	1/1	0.93	0.09	42,42,42,42	0
54	MG	DA	3004	1/1	0.93	0.07	88,88,88,88	0
54	MG	DA	3008	1/1	0.93	0.17	58,58,58,58	0
54	MG	BA	3057	1/1	0.93	0.19	51,51,51,51	0
54	MG	DA	3457	1/1	0.93	0.07	64,64,64,64	0
54	MG	CA	1665	1/1	0.93	0.13	84,84,84,84	0
54	MG	BA	3302	1/1	0.93	0.15	47,47,47,47	0
54	MG	DA	3138	1/1	0.93	0.24	41,41,41,41	0
54	MG	BA	3467	1/1	0.93	0.15	30,30,30,30	0
54	MG	BA	3303	1/1	0.93	0.19	64,64,64,64	0
54	MG	BA	3124	1/1	0.93	0.08	33,33,33,33	0
54	MG	AA	1682	1/1	0.93	0.20	76,76,76,76	0
54	MG	BA	3091	1/1	0.93	0.22	40,40,40,40	0
54	MG	AA	1605	1/1	0.93	0.19	66,66,66,66	0
54	MG	BA	3308	1/1	0.93	0.09	52,52,52,52	0
54	MG	DA	3026	1/1	0.93	0.11	39,39,39,39	0
54	MG	AA	1706	1/1	0.93	0.07	91,91,91,91	0
54	MG	DA	3260	1/1	0.93	0.11	41,41,41,41	0
54	MG	BA	3536	1/1	0.93	0.08	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3513	1/1	0.93	0.07	34,34,34,34	0
54	MG	DA	3149	1/1	0.93	0.10	53,53,53,53	0
54	MG	CA	1603	1/1	0.93	0.24	56,56,56,56	0
54	MG	AA	1630	1/1	0.93	0.18	39,39,39,39	0
54	MG	DA	3266	1/1	0.93	0.24	47,47,47,47	0
54	MG	DA	3523	1/1	0.93	0.06	74,74,74,74	0
54	MG	DA	3152	1/1	0.93	0.22	61,61,61,61	0
54	MG	BA	3316	1/1	0.93	0.13	45,45,45,45	0
54	MG	BA	3317	1/1	0.93	0.09	34,34,34,34	0
54	MG	BA	3199	1/1	0.93	0.18	41,41,41,41	0
54	MG	BA	3552	1/1	0.93	0.11	82,82,82,82	0
54	MG	BA	3203	1/1	0.93	0.24	55,55,55,55	0
54	MG	CA	1610	1/1	0.93	0.26	60,60,60,60	0
54	MG	DA	3545	1/1	0.93	0.09	82,82,82,82	0
54	MG	BA	3204	1/1	0.93	0.10	38,38,38,38	0
54	MG	BA	3135	1/1	0.93	0.18	45,45,45,45	0
54	MG	DA	3163	1/1	0.93	0.29	30,30,30,30	0
54	MG	DA	3554	1/1	0.93	0.07	47,47,47,47	0
54	MG	BA	3007	1/1	0.93	0.21	28,28,28,28	0
54	MG	CA	1691	1/1	0.93	0.27	51,51,51,51	0
54	MG	AA	1653	1/1	0.93	0.16	49,49,49,49	0
54	MG	DA	3053	1/1	0.93	0.12	40,40,40,40	0
54	MG	AA	1713	1/1	0.93	0.07	91,91,91,91	0
54	MG	BA	3215	1/1	0.93	0.15	50,50,50,50	0
54	MG	DA	3568	1/1	0.93	0.05	78,78,78,78	0
54	MG	AA	1717	1/1	0.93	0.09	93,93,93,93	0
54	MG	DA	3580	1/1	0.93	0.17	52,52,52,52	0
54	MG	BA	3145	1/1	0.93	0.12	44,44,44,44	0
54	MG	DA	3289	1/1	0.93	0.33	54,54,54,54	0
54	MG	DA	3584	1/1	0.93	0.22	48,48,48,48	0
54	MG	DA	3586	1/1	0.93	0.06	49,49,49,49	0
54	MG	DA	3175	1/1	0.93	0.16	44,44,44,44	0
54	MG	BA	3105	1/1	0.93	0.24	28,28,28,28	0
54	MG	DA	3596	1/1	0.93	0.07	125,125,125,125	0
54	MG	BA	3220	1/1	0.93	0.20	31,31,31,31	0
54	MG	DA	3598	1/1	0.93	0.11	76,76,76,76	0
54	MG	CA	1702	1/1	0.93	0.07	64,64,64,64	0
54	MG	BA	3221	1/1	0.93	0.32	57,57,57,57	0
54	MG	CA	1705	1/1	0.93	0.07	96,96,96,96	0
54	MG	DA	3069	1/1	0.93	0.35	42,42,42,42	0
54	MG	DB	206	1/1	0.93	0.26	58,58,58,58	0
54	MG	BA	3147	1/1	0.93	0.21	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	3274	1/1	0.93	0.20	26,26,26,26	0
54	MG	DE	303	1/1	0.93	0.16	45,45,45,45	0
54	MG	BA	3150	1/1	0.93	0.10	42,42,42,42	0
54	MG	BA	3375	1/1	0.93	0.07	34,34,34,34	0
54	MG	BA	3154	1/1	0.93	0.23	50,50,50,50	0
54	MG	BA	3645	1/1	0.93	0.07	102,102,102,102	0
54	MG	DP	201	1/1	0.93	0.10	54,54,54,54	0
54	MG	BA	3385	1/1	0.93	0.09	63,63,63,63	0
54	MG	BA	3389	1/1	0.93	0.15	46,46,46,46	0
54	MG	DA	3311	1/1	0.93	0.27	26,26,26,26	0
54	MG	CA	1727	1/1	0.93	0.17	46,46,46,46	0
54	MG	DA	3313	1/1	0.93	0.23	29,29,29,29	0
54	MG	DA	3194	1/1	0.93	0.14	37,37,37,37	0
54	MG	DA	3317	1/1	0.93	0.06	47,47,47,47	0
54	MG	DA	3323	1/1	0.94	0.12	40,40,40,40	0
54	MG	DA	3068	1/1	0.94	0.12	33,33,33,33	0
54	MG	DA	3325	1/1	0.94	0.10	38,38,38,38	0
54	MG	BA	3019	1/1	0.94	0.19	34,34,34,34	0
54	MG	BA	3020	1/1	0.94	0.10	82,82,82,82	0
54	MG	BA	3208	1/1	0.94	0.08	38,38,38,38	0
54	MG	BA	3075	1/1	0.94	0.20	46,46,46,46	0
54	MG	BA	3577	1/1	0.94	0.06	77,77,77,77	0
54	MG	DA	3074	1/1	0.94	0.08	54,54,54,54	0
54	MG	CA	1706	1/1	0.94	0.07	103,103,103,103	0
54	MG	DA	3342	1/1	0.94	0.10	38,38,38,38	0
54	MG	BA	3359	1/1	0.94	0.08	70,70,70,70	0
54	MG	BA	3004	1/1	0.94	0.07	76,76,76,76	0
54	MG	DA	3079	1/1	0.94	0.14	47,47,47,47	0
54	MG	DA	3364	1/1	0.94	0.09	32,32,32,32	0
54	MG	DA	3202	1/1	0.94	0.15	66,66,66,66	0
54	MG	DA	3205	1/1	0.94	0.22	47,47,47,47	0
54	MG	CA	1713	1/1	0.94	0.09	73,73,73,73	0
54	MG	BA	3152	1/1	0.94	0.29	54,54,54,54	0
54	MG	BA	3272	1/1	0.94	0.27	31,31,31,31	0
54	MG	CA	1623	1/1	0.94	0.24	43,43,43,43	0
54	MG	DA	3087	1/1	0.94	0.16	54,54,54,54	0
54	MG	BA	3590	1/1	0.94	0.20	31,31,31,31	0
54	MG	BA	3592	1/1	0.94	0.07	47,47,47,47	0
54	MG	BA	3366	1/1	0.94	0.18	83,83,83,83	0
54	MG	DA	3396	1/1	0.94	0.09	52,52,52,52	0
54	MG	BA	3153	1/1	0.94	0.29	51,51,51,51	0
54	MG	BA	3598	1/1	0.94	0.07	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	3094	1/1	0.94	0.09	56,56,56,56	0
54	MG	BA	3005	1/1	0.94	0.15	60,60,60,60	0
54	MG	AA	1707	1/1	0.94	0.08	102,102,102,102	0
54	MG	BA	3160	1/1	0.94	0.20	39,39,39,39	0
54	MG	BA	3633	1/1	0.94	0.07	43,43,43,43	0
54	MG	BA	3050	1/1	0.94	0.11	35,35,35,35	0
54	MG	BA	3377	1/1	0.94	0.10	32,32,32,32	0
54	MG	DA	3433	1/1	0.94	0.07	47,47,47,47	0
54	MG	BA	3382	1/1	0.94	0.05	100,100,100,100	0
54	MG	DA	3104	1/1	0.94	0.16	34,34,34,34	0
54	MG	BA	3008	1/1	0.94	0.13	28,28,28,28	0
54	MG	CA	1738	1/1	0.94	0.10	112,112,112,112	0
54	MG	DA	3442	1/1	0.94	0.09	82,82,82,82	0
54	MG	BA	3281	1/1	0.94	0.18	24,24,24,24	0
54	MG	BA	3282	1/1	0.94	0.20	27,27,27,27	0
54	MG	BA	3390	1/1	0.94	0.07	62,62,62,62	0
54	MG	DA	3455	1/1	0.94	0.05	68,68,68,68	0
54	MG	BA	3165	1/1	0.94	0.25	51,51,51,51	0
54	MG	DA	3237	1/1	0.94	0.20	62,62,62,62	0
54	MG	CA	1749	1/1	0.94	0.15	61,61,61,61	0
54	MG	BA	3651	1/1	0.94	0.15	87,87,87,87	0
54	MG	BA	3166	1/1	0.94	0.26	36,36,36,36	0
54	MG	DA	3471	1/1	0.94	0.10	31,31,31,31	0
54	MG	DA	3476	1/1	0.94	0.07	66,66,66,66	0
54	MG	DA	3245	1/1	0.94	0.26	57,57,57,57	0
54	MG	DA	3118	1/1	0.94	0.25	43,43,43,43	0
54	MG	BA	3119	1/1	0.94	0.20	42,42,42,42	0
54	MG	BA	3053	1/1	0.94	0.30	57,57,57,57	0
54	MG	DA	3484	1/1	0.94	0.05	64,64,64,64	0
54	MG	DA	3485	1/1	0.94	0.12	58,58,58,58	0
54	MG	DA	3249	1/1	0.94	0.17	49,49,49,49	0
54	MG	DA	3487	1/1	0.94	0.06	48,48,48,48	0
54	MG	BA	3657	1/1	0.94	0.21	65,65,65,65	0
54	MG	DA	3491	1/1	0.94	0.18	44,44,44,44	0
54	MG	BA	3122	1/1	0.94	0.19	49,49,49,49	0
54	MG	DA	3253	1/1	0.94	0.14	50,50,50,50	0
54	MG	BA	3054	1/1	0.94	0.10	34,34,34,34	0
54	MG	DA	3505	1/1	0.94	0.07	91,91,91,91	0
54	MG	DA	3506	1/1	0.94	0.09	96,96,96,96	0
54	MG	BA	3175	1/1	0.94	0.07	43,43,43,43	0
54	MG	BA	3293	1/1	0.94	0.05	48,48,48,48	0
54	MG	BA	3176	1/1	0.94	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	AA	1708	1/1	0.94	0.19	91,91,91,91	0
54	MG	DA	3132	1/1	0.94	0.26	49,49,49,49	0
54	MG	BA	3178	1/1	0.94	0.37	43,43,43,43	0
54	MG	AA	1683	1/1	0.94	0.39	58,58,58,58	0
54	MG	BA	3299	1/1	0.94	0.21	66,66,66,66	0
54	MG	DA	3526	1/1	0.94	0.07	98,98,98,98	0
54	MG	DA	3007	1/1	0.94	0.20	48,48,48,48	0
54	MG	DA	3530	1/1	0.94	0.09	132,132,132,132	0
54	MG	BA	3435	1/1	0.94	0.08	48,48,48,48	0
54	MG	CA	1658	1/1	0.94	0.12	58,58,58,58	0
54	MG	DA	3010	1/1	0.94	0.11	42,42,42,42	0
54	MG	BA	3436	1/1	0.94	0.09	70,70,70,70	0
54	MG	AA	1644	1/1	0.94	0.28	39,39,39,39	0
54	MG	AA	1641	1/1	0.94	0.23	42,42,42,42	0
54	MG	DA	3272	1/1	0.94	0.27	30,30,30,30	0
54	MG	BB	213	1/1	0.94	0.08	38,38,38,38	0
54	MG	DA	3550	1/1	0.94	0.09	58,58,58,58	0
54	MG	BB	215	1/1	0.94	0.12	65,65,65,65	0
54	MG	DA	3553	1/1	0.94	0.10	54,54,54,54	0
54	MG	BA	3187	1/1	0.94	0.27	42,42,42,42	0
54	MG	CA	1666	1/1	0.94	0.20	64,64,64,64	0
54	MG	BA	3129	1/1	0.94	0.27	37,37,37,37	0
54	MG	DA	3559	1/1	0.94	0.05	79,79,79,79	0
54	MG	BA	3244	1/1	0.94	0.07	30,30,30,30	0
54	MG	DA	3279	1/1	0.94	0.15	44,44,44,44	0
54	MG	DA	3025	1/1	0.94	0.22	49,49,49,49	0
54	MG	DA	3565	1/1	0.94	0.08	34,34,34,34	0
54	MG	AA	1639	1/1	0.94	0.22	67,67,67,67	0
54	MG	DA	3154	1/1	0.94	0.24	26,26,26,26	0
54	MG	AA	1719	1/1	0.94	0.05	144,144,144,144	0
54	MG	BA	3193	1/1	0.94	0.30	35,35,35,35	0
54	MG	BA	3133	1/1	0.94	0.23	53,53,53,53	0
54	MG	AA	1681	1/1	0.94	0.20	50,50,50,50	0
54	MG	BA	3492	1/1	0.94	0.15	27,27,27,27	0
54	MG	BA	3036	1/1	0.94	0.15	36,36,36,36	0
54	MG	AA	1612	1/1	0.94	0.13	86,86,86,86	0
54	MG	BA	3514	1/1	0.94	0.08	61,61,61,61	0
54	MG	BT	202	1/1	0.94	0.13	52,52,52,52	0
54	MG	DA	3043	1/1	0.94	0.17	54,54,54,54	0
54	MG	BA	3515	1/1	0.94	0.08	72,72,72,72	0
54	MG	BW	202	1/1	0.94	0.07	33,33,33,33	0
54	MG	BA	3256	1/1	0.94	0.23	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3523	1/1	0.94	0.05	110,110,110,110	0
54	MG	B2	101	1/1	0.94	0.07	45,45,45,45	0
54	MG	DB	205	1/1	0.94	0.15	55,55,55,55	0
54	MG	DA	3051	1/1	0.94	0.12	38,38,38,38	0
54	MG	DA	3174	1/1	0.94	0.17	51,51,51,51	0
54	MG	DB	208	1/1	0.94	0.06	104,104,104,104	0
54	MG	BA	3318	1/1	0.94	0.14	35,35,35,35	0
54	MG	BA	3320	1/1	0.94	0.09	42,42,42,42	0
54	MG	BA	3329	1/1	0.94	0.14	74,74,74,74	0
54	MG	BA	3332	1/1	0.94	0.07	50,50,50,50	0
54	MG	CA	1690	1/1	0.94	0.23	64,64,64,64	0
54	MG	BA	3540	1/1	0.94	0.07	35,35,35,35	0
54	MG	BA	3070	1/1	0.94	0.14	37,37,37,37	0
54	MG	DA	3182	1/1	0.94	0.24	46,46,46,46	0
54	MG	DA	3061	1/1	0.94	0.10	32,32,32,32	0
54	MG	BA	3201	1/1	0.94	0.26	31,31,31,31	0
54	MG	D0	102	1/1	0.94	0.17	72,72,72,72	0
54	MG	DA	3186	1/1	0.94	0.16	54,54,54,54	0
54	MG	BA	3202	1/1	0.94	0.16	48,48,48,48	0
54	MG	BA	3003	1/1	0.94	0.18	74,74,74,74	0
55	ZN	AD	301	1/1	0.94	0.19	74,74,74,74	0
55	ZN	B4	101	1/1	0.94	0.08	199,199,199,199	0
55	ZN	CD	301	1/1	0.94	0.17	71,71,71,71	0
54	MG	BA	3143	1/1	0.94	0.08	30,30,30,30	0
54	MG	BA	3206	1/1	0.95	0.19	49,49,49,49	0
54	MG	DA	3354	1/1	0.95	0.08	49,49,49,49	0
54	MG	BA	3167	1/1	0.95	0.24	31,31,31,31	0
54	MG	DA	3361	1/1	0.95	0.06	30,30,30,30	0
54	MG	BA	3585	1/1	0.95	0.06	52,52,52,52	0
54	MG	BA	3587	1/1	0.95	0.09	60,60,60,60	0
54	MG	BA	3169	1/1	0.95	0.13	31,31,31,31	0
54	MG	BA	3255	1/1	0.95	0.15	25,25,25,25	0
54	MG	BA	3034	1/1	0.95	0.13	41,41,41,41	0
54	MG	BA	3210	1/1	0.95	0.14	40,40,40,40	0
54	MG	DA	3213	1/1	0.95	0.20	48,48,48,48	0
54	MG	DA	3379	1/1	0.95	0.07	59,59,59,59	0
54	MG	DA	3214	1/1	0.95	0.15	37,37,37,37	0
54	MG	DA	3215	1/1	0.95	0.14	49,49,49,49	0
54	MG	BA	3024	1/1	0.95	0.08	41,41,41,41	0
54	MG	DA	3217	1/1	0.95	0.27	32,32,32,32	0
54	MG	DA	3393	1/1	0.95	0.08	41,41,41,41	0
54	MG	BA	3406	1/1	0.95	0.06	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3213	1/1	0.95	0.09	43,43,43,43	0
54	MG	BA	3260	1/1	0.95	0.18	30,30,30,30	0
54	MG	BA	3608	1/1	0.95	0.10	71,71,71,71	0
54	MG	BA	3616	1/1	0.95	0.14	131,131,131,131	0
54	MG	BA	3084	1/1	0.95	0.25	59,59,59,59	0
54	MG	DA	3224	1/1	0.95	0.27	32,32,32,32	0
54	MG	BA	3411	1/1	0.95	0.07	63,63,63,63	0
54	MG	BA	3412	1/1	0.95	0.08	78,78,78,78	0
54	MG	BA	3413	1/1	0.95	0.10	57,57,57,57	0
54	MG	BA	3420	1/1	0.95	0.07	61,61,61,61	0
54	MG	BA	3311	1/1	0.95	0.09	24,24,24,24	0
54	MG	BA	3424	1/1	0.95	0.11	72,72,72,72	0
54	MG	BA	3134	1/1	0.95	0.26	41,41,41,41	0
54	MG	DA	3109	1/1	0.95	0.11	59,59,59,59	0
54	MG	DA	3439	1/1	0.95	0.08	57,57,57,57	0
54	MG	DA	3441	1/1	0.95	0.13	48,48,48,48	0
54	MG	AA	1724	1/1	0.95	0.09	74,74,74,74	0
54	MG	DA	3445	1/1	0.95	0.09	42,42,42,42	0
54	MG	DA	3446	1/1	0.95	0.11	42,42,42,42	0
54	MG	AA	1687	1/1	0.95	0.14	62,62,62,62	0
54	MG	DA	3449	1/1	0.95	0.15	42,42,42,42	0
54	MG	DA	3450	1/1	0.95	0.06	67,67,67,67	0
54	MG	BA	3087	1/1	0.95	0.24	46,46,46,46	0
54	MG	CA	1752	1/1	0.95	0.06	71,71,71,71	0
54	MG	DA	3454	1/1	0.95	0.05	64,64,64,64	0
54	MG	BA	3319	1/1	0.95	0.12	54,54,54,54	0
54	MG	BA	3439	1/1	0.95	0.13	59,59,59,59	0
54	MG	DA	3240	1/1	0.95	0.24	53,53,53,53	0
54	MG	AA	1631	1/1	0.95	0.21	41,41,41,41	0
54	MG	DA	3244	1/1	0.95	0.29	33,33,33,33	0
54	MG	DA	3465	1/1	0.95	0.05	75,75,75,75	0
54	MG	BA	3182	1/1	0.95	0.21	37,37,37,37	0
54	MG	DA	3469	1/1	0.95	0.06	56,56,56,56	0
54	MG	DA	3470	1/1	0.95	0.06	47,47,47,47	0
54	MG	BA	3270	1/1	0.95	0.32	25,25,25,25	0
54	MG	BA	3659	1/1	0.95	0.05	81,81,81,81	0
54	MG	DA	3477	1/1	0.95	0.05	53,53,53,53	0
54	MG	BA	3445	1/1	0.95	0.08	31,31,31,31	0
54	MG	CA	1760	1/1	0.95	0.06	87,87,87,87	0
54	MG	DA	3250	1/1	0.95	0.12	49,49,49,49	0
54	MG	CA	1761	1/1	0.95	0.15	65,65,65,65	0
54	MG	DA	3126	1/1	0.95	0.33	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	BB	201	1/1	0.95	0.17	57,57,57,57	0
54	MG	AA	1690	1/1	0.95	0.07	72,72,72,72	0
54	MG	BA	3449	1/1	0.95	0.17	29,29,29,29	0
54	MG	BA	3142	1/1	0.95	0.20	42,42,42,42	0
54	MG	DA	3489	1/1	0.95	0.07	79,79,79,79	0
54	MG	BA	3459	1/1	0.95	0.08	38,38,38,38	0
54	MG	DA	3493	1/1	0.95	0.10	63,63,63,63	0
54	MG	DA	3006	1/1	0.95	0.20	38,38,38,38	0
54	MG	BA	3058	1/1	0.95	0.08	32,32,32,32	0
54	MG	DA	3136	1/1	0.95	0.31	62,62,62,62	0
54	MG	DA	3137	1/1	0.95	0.06	38,38,38,38	0
54	MG	BA	3465	1/1	0.95	0.09	44,44,44,44	0
54	MG	DA	3508	1/1	0.95	0.08	60,60,60,60	0
54	MG	DA	3263	1/1	0.95	0.21	40,40,40,40	0
54	MG	BA	3338	1/1	0.95	0.12	62,62,62,62	0
54	MG	CA	1659	1/1	0.95	0.21	48,48,48,48	0
54	MG	DA	3516	1/1	0.95	0.09	32,32,32,32	0
54	MG	BA	3469	1/1	0.95	0.09	40,40,40,40	0
54	MG	BA	3339	1/1	0.95	0.08	70,70,70,70	0
54	MG	BA	3227	1/1	0.95	0.11	32,32,32,32	0
54	MG	DA	3269	1/1	0.95	0.34	47,47,47,47	0
54	MG	BA	3092	1/1	0.95	0.29	26,26,26,26	0
54	MG	DA	3017	1/1	0.95	0.12	50,50,50,50	0
54	MG	BA	3500	1/1	0.95	0.08	44,44,44,44	0
54	MG	BA	3504	1/1	0.95	0.08	65,65,65,65	0
54	MG	BA	3507	1/1	0.95	0.13	41,41,41,41	0
54	MG	DA	3022	1/1	0.95	0.12	34,34,34,34	0
54	MG	BA	3188	1/1	0.95	0.26	39,39,39,39	0
54	MG	DA	3538	1/1	0.95	0.06	87,87,87,87	0
54	MG	BB	223	1/1	0.95	0.06	133,133,133,133	0
54	MG	DA	3541	1/1	0.95	0.05	130,130,130,130	0
54	MG	BA	3278	1/1	0.95	0.25	30,30,30,30	0
54	MG	BA	3118	1/1	0.95	0.17	44,44,44,44	0
54	MG	DA	3027	1/1	0.95	0.17	56,56,56,56	0
54	MG	CA	1671	1/1	0.95	0.31	49,49,49,49	0
54	MG	BA	3190	1/1	0.95	0.13	27,27,27,27	0
54	MG	BA	3011	1/1	0.95	0.18	26,26,26,26	0
54	MG	BA	3520	1/1	0.95	0.06	95,95,95,95	0
54	MG	BA	3235	1/1	0.95	0.13	50,50,50,50	0
54	MG	BA	3095	1/1	0.95	0.18	48,48,48,48	0
54	MG	BA	3529	1/1	0.95	0.06	65,65,65,65	0
54	MG	DA	3036	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	DA	3038	1/1	0.95	0.08	37,37,37,37	0
54	MG	DA	3562	1/1	0.95	0.07	58,58,58,58	0
54	MG	CA	1678	1/1	0.95	0.11	55,55,55,55	0
54	MG	DA	3041	1/1	0.95	0.28	36,36,36,36	0
54	MG	BA	3121	1/1	0.95	0.15	36,36,36,36	0
54	MG	BQ	204	1/1	0.95	0.06	43,43,43,43	0
54	MG	BA	3096	1/1	0.95	0.29	47,47,47,47	0
54	MG	BA	3538	1/1	0.95	0.08	66,66,66,66	0
54	MG	DA	3300	1/1	0.95	0.14	41,41,41,41	0
54	MG	AA	1735	1/1	0.95	0.07	110,110,110,110	0
54	MG	BA	3155	1/1	0.95	0.06	41,41,41,41	0
54	MG	BA	3157	1/1	0.95	0.27	48,48,48,48	0
54	MG	B0	102	1/1	0.95	0.09	54,54,54,54	0
54	MG	B0	103	1/1	0.95	0.07	89,89,89,89	0
54	MG	DA	3589	1/1	0.95	0.06	75,75,75,75	0
54	MG	DA	3307	1/1	0.95	0.20	35,35,35,35	0
54	MG	DA	3591	1/1	0.95	0.08	66,66,66,66	0
54	MG	BA	3077	1/1	0.95	0.09	42,42,42,42	0
54	MG	DA	3054	1/1	0.95	0.20	46,46,46,46	0
54	MG	BA	3374	1/1	0.95	0.06	34,34,34,34	0
54	MG	AA	1685	1/1	0.95	0.07	71,71,71,71	0
54	MG	B5	103	1/1	0.95	0.10	57,57,57,57	0
54	MG	DA	3183	1/1	0.95	0.23	26,26,26,26	0
54	MG	DA	3314	1/1	0.95	0.21	43,43,43,43	0
54	MG	B9	102	1/1	0.95	0.13	28,28,28,28	0
54	MG	BA	3294	1/1	0.95	0.10	39,39,39,39	0
54	MG	AA	1667	1/1	0.95	0.19	38,38,38,38	0
54	MG	BA	3555	1/1	0.95	0.07	47,47,47,47	0
54	MG	BA	3557	1/1	0.95	0.09	78,78,78,78	0
54	MG	DE	302	1/1	0.95	0.26	21,21,21,21	0
54	MG	DA	3065	1/1	0.95	0.18	53,53,53,53	0
54	MG	BA	3127	1/1	0.95	0.23	38,38,38,38	0
54	MG	BA	3562	1/1	0.95	0.08	59,59,59,59	0
54	MG	CA	1700	1/1	0.95	0.09	70,70,70,70	0
54	MG	BA	3565	1/1	0.95	0.06	68,68,68,68	0
54	MG	CA	1703	1/1	0.95	0.15	56,56,56,56	0
54	MG	BA	3247	1/1	0.95	0.32	26,26,26,26	0
54	MG	BA	3386	1/1	0.95	0.09	40,40,40,40	0
54	MG	DR	202	1/1	0.95	0.24	34,34,34,34	0
54	MG	BA	3574	1/1	0.95	0.17	33,33,33,33	0
54	MG	BA	3080	1/1	0.95	0.08	39,39,39,39	0
54	MG	D1	101	1/1	0.95	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1708	1/1	0.95	0.07	80,80,80,80	0
54	MG	DA	3200	1/1	0.95	0.15	34,34,34,34	0
54	MG	DA	3337	1/1	0.95	0.15	30,30,30,30	0
54	MG	DA	3340	1/1	0.95	0.09	45,45,45,45	0
55	ZN	AN	101	1/1	0.95	0.06	117,117,117,117	0
54	MG	DA	3341	1/1	0.95	0.11	43,43,43,43	0
54	MG	CA	1711	1/1	0.95	0.06	103,103,103,103	0
54	MG	BA	3103	1/1	0.95	0.20	29,29,29,29	0
54	MG	BA	3333	1/1	0.96	0.12	40,40,40,40	0
54	MG	BA	3116	1/1	0.96	0.07	53,53,53,53	0
54	MG	DA	3013	1/1	0.96	0.12	37,37,37,37	0
54	MG	DA	3436	1/1	0.96	0.10	81,81,81,81	0
54	MG	BB	222	1/1	0.96	0.09	80,80,80,80	0
54	MG	BA	3542	1/1	0.96	0.05	83,83,83,83	0
54	MG	BD	301	1/1	0.96	0.13	49,49,49,49	0
54	MG	DA	3018	1/1	0.96	0.18	54,54,54,54	0
54	MG	BA	3117	1/1	0.96	0.14	39,39,39,39	0
54	MG	DA	3443	1/1	0.96	0.06	75,75,75,75	0
54	MG	AA	1727	1/1	0.96	0.06	61,61,61,61	0
54	MG	AA	1729	1/1	0.96	0.06	80,80,80,80	0
54	MG	BA	3551	1/1	0.96	0.10	82,82,82,82	0
54	MG	BA	3214	1/1	0.96	0.16	52,52,52,52	0
54	MG	BA	3417	1/1	0.96	0.07	48,48,48,48	0
54	MG	BP	201	1/1	0.96	0.06	45,45,45,45	0
54	MG	BA	3418	1/1	0.96	0.06	49,49,49,49	0
54	MG	BA	3419	1/1	0.96	0.27	21,21,21,21	0
54	MG	BA	3181	1/1	0.96	0.07	38,38,38,38	0
54	MG	BA	3558	1/1	0.96	0.19	28,28,28,28	0
54	MG	DA	3458	1/1	0.96	0.05	62,62,62,62	0
54	MG	AA	1655	1/1	0.96	0.29	43,43,43,43	0
54	MG	BA	3422	1/1	0.96	0.10	76,76,76,76	0
54	MG	BA	3563	1/1	0.96	0.06	70,70,70,70	0
54	MG	BA	3564	1/1	0.96	0.10	59,59,59,59	0
54	MG	BA	3345	1/1	0.96	0.14	71,71,71,71	0
54	MG	BA	3566	1/1	0.96	0.10	44,44,44,44	0
54	MG	DA	3037	1/1	0.96	0.12	43,43,43,43	0
54	MG	BA	3567	1/1	0.96	0.06	54,54,54,54	0
54	MG	DA	3472	1/1	0.96	0.14	50,50,50,50	0
54	MG	DA	3473	1/1	0.96	0.12	38,38,38,38	0
54	MG	BA	3569	1/1	0.96	0.05	69,69,69,69	0
54	MG	DA	3158	1/1	0.96	0.18	46,46,46,46	0
54	MG	BA	3425	1/1	0.96	0.10	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	3480	1/1	0.96	0.12	52,52,52,52	0
54	MG	BA	3346	1/1	0.96	0.06	52,52,52,52	0
54	MG	BA	3291	1/1	0.96	0.07	39,39,39,39	0
54	MG	B8	102	1/1	0.96	0.05	61,61,61,61	0
54	MG	BA	3148	1/1	0.96	0.23	47,47,47,47	0
54	MG	BA	3578	1/1	0.96	0.08	44,44,44,44	0
54	MG	DA	3047	1/1	0.96	0.14	38,38,38,38	0
54	MG	BA	3218	1/1	0.96	0.05	55,55,55,55	0
54	MG	BA	3580	1/1	0.96	0.10	49,49,49,49	0
54	MG	DA	3050	1/1	0.96	0.23	34,34,34,34	0
54	MG	CA	1696	1/1	0.96	0.30	61,61,61,61	0
54	MG	DA	3492	1/1	0.96	0.05	56,56,56,56	0
54	MG	DA	3286	1/1	0.96	0.20	33,33,33,33	0
54	MG	DA	3494	1/1	0.96	0.08	37,37,37,37	0
54	MG	BA	3437	1/1	0.96	0.10	49,49,49,49	0
54	MG	BA	3149	1/1	0.96	0.36	57,57,57,57	0
54	MG	BA	3584	1/1	0.96	0.05	42,42,42,42	0
54	MG	DA	3500	1/1	0.96	0.07	74,74,74,74	0
54	MG	DA	3503	1/1	0.96	0.10	34,34,34,34	0
54	MG	BA	3098	1/1	0.96	0.11	40,40,40,40	0
54	MG	DA	3292	1/1	0.96	0.13	33,33,33,33	0
54	MG	DA	3293	1/1	0.96	0.23	33,33,33,33	0
54	MG	DA	3509	1/1	0.96	0.06	37,37,37,37	0
54	MG	BA	3440	1/1	0.96	0.09	46,46,46,46	0
54	MG	AA	1732	1/1	0.96	0.05	94,94,94,94	0
54	MG	DA	3514	1/1	0.96	0.11	42,42,42,42	0
54	MG	BA	3028	1/1	0.96	0.10	22,22,22,22	0
54	MG	BA	3043	1/1	0.96	0.06	39,39,39,39	0
54	MG	BA	3224	1/1	0.96	0.16	50,50,50,50	0
54	MG	DA	3520	1/1	0.96	0.17	56,56,56,56	0
54	MG	BA	3596	1/1	0.96	0.05	48,48,48,48	0
54	MG	BA	3262	1/1	0.96	0.16	27,27,27,27	0
54	MG	BA	3448	1/1	0.96	0.07	38,38,38,38	0
54	MG	DA	3524	1/1	0.96	0.12	79,79,79,79	0
54	MG	DA	3302	1/1	0.96	0.26	21,21,21,21	0
54	MG	CA	1617	1/1	0.96	0.06	87,87,87,87	0
54	MG	AA	1711	1/1	0.96	0.15	46,46,46,46	0
54	MG	BA	3452	1/1	0.96	0.07	64,64,64,64	0
54	MG	BA	3156	1/1	0.96	0.21	39,39,39,39	0
54	MG	DA	3533	1/1	0.96	0.08	89,89,89,89	0
54	MG	CA	1622	1/1	0.96	0.21	47,47,47,47	0
54	MG	BA	3609	1/1	0.96	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3612	1/1	0.96	0.08	59,59,59,59	0
54	MG	BA	3265	1/1	0.96	0.22	29,29,29,29	0
54	MG	BA	3046	1/1	0.96	0.07	36,36,36,36	0
54	MG	BA	3627	1/1	0.96	0.06	50,50,50,50	0
54	MG	BA	3083	1/1	0.96	0.09	43,43,43,43	0
54	MG	BA	3064	1/1	0.96	0.23	34,34,34,34	0
54	MG	DA	3078	1/1	0.96	0.16	48,48,48,48	0
54	MG	BA	3378	1/1	0.96	0.10	25,25,25,25	0
54	MG	DA	3080	1/1	0.96	0.22	44,44,44,44	0
54	MG	BA	3640	1/1	0.96	0.05	116,116,116,116	0
54	MG	BA	3641	1/1	0.96	0.12	72,72,72,72	0
54	MG	DA	3083	1/1	0.96	0.15	37,37,37,37	0
54	MG	BA	3106	1/1	0.96	0.20	52,52,52,52	0
54	MG	DA	3558	1/1	0.96	0.07	36,36,36,36	0
54	MG	DA	3203	1/1	0.96	0.24	33,33,33,33	0
54	MG	DA	3560	1/1	0.96	0.08	57,57,57,57	0
54	MG	DA	3085	1/1	0.96	0.11	43,43,43,43	0
54	MG	BA	3644	1/1	0.96	0.06	88,88,88,88	0
54	MG	BA	3472	1/1	0.96	0.13	26,26,26,26	0
54	MG	BA	3477	1/1	0.96	0.07	53,53,53,53	0
54	MG	BA	3478	1/1	0.96	0.06	41,41,41,41	0
54	MG	BA	3163	1/1	0.96	0.25	23,23,23,23	0
54	MG	CA	1741	1/1	0.96	0.17	79,79,79,79	0
54	MG	BA	3066	1/1	0.96	0.26	39,39,39,39	0
54	MG	DA	3573	1/1	0.96	0.20	31,31,31,31	0
54	MG	DA	3578	1/1	0.96	0.11	29,29,29,29	0
54	MG	CA	1745	1/1	0.96	0.16	116,116,116,116	0
54	MG	DA	3333	1/1	0.96	0.09	37,37,37,37	0
54	MG	BA	3496	1/1	0.96	0.08	39,39,39,39	0
54	MG	CA	1747	1/1	0.96	0.07	95,95,95,95	0
54	MG	BA	3499	1/1	0.96	0.09	60,60,60,60	0
54	MG	BA	3006	1/1	0.96	0.13	25,25,25,25	0
54	MG	DA	3588	1/1	0.96	0.07	34,34,34,34	0
54	MG	DA	3099	1/1	0.96	0.14	36,36,36,36	0
54	MG	DA	3347	1/1	0.96	0.11	35,35,35,35	0
54	MG	DA	3348	1/1	0.96	0.07	41,41,41,41	0
54	MG	DA	3593	1/1	0.96	0.06	83,83,83,83	0
54	MG	DA	3595	1/1	0.96	0.10	58,58,58,58	0
54	MG	DA	3352	1/1	0.96	0.06	33,33,33,33	0
54	MG	BA	3502	1/1	0.96	0.08	34,34,34,34	0
54	MG	DA	3101	1/1	0.96	0.18	39,39,39,39	0
54	MG	BA	3503	1/1	0.96	0.06	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	3360	1/1	0.96	0.06	37,37,37,37	0
54	MG	AA	1722	1/1	0.96	0.06	66,66,66,66	0
54	MG	BA	3069	1/1	0.96	0.26	42,42,42,42	0
54	MG	CA	1647	1/1	0.96	0.13	86,86,86,86	0
54	MG	BA	3391	1/1	0.96	0.07	39,39,39,39	0
54	MG	BA	3392	1/1	0.96	0.09	110,110,110,110	0
54	MG	AA	1621	1/1	0.96	0.26	62,62,62,62	0
54	MG	DD	302	1/1	0.96	0.29	38,38,38,38	0
54	MG	CA	1651	1/1	0.96	0.19	46,46,46,46	0
54	MG	DA	3373	1/1	0.96	0.14	32,32,32,32	0
54	MG	BA	3170	1/1	0.96	0.09	29,29,29,29	0
54	MG	AA	1693	1/1	0.96	0.06	51,51,51,51	0
54	MG	CA	1762	1/1	0.96	0.10	156,156,156,156	0
54	MG	BA	3398	1/1	0.96	0.08	52,52,52,52	0
54	MG	BA	3522	1/1	0.96	0.09	74,74,74,74	0
54	MG	DA	3234	1/1	0.96	0.25	41,41,41,41	0
54	MG	AA	1725	1/1	0.96	0.07	56,56,56,56	0
54	MG	BA	3328	1/1	0.96	0.16	30,30,30,30	0
54	MG	DR	201	1/1	0.96	0.16	40,40,40,40	0
54	MG	DA	3397	1/1	0.96	0.07	34,34,34,34	0
54	MG	DA	3003	1/1	0.96	0.10	46,46,46,46	0
54	MG	BA	3525	1/1	0.96	0.07	35,35,35,35	0
54	MG	BA	3528	1/1	0.96	0.07	39,39,39,39	0
54	MG	DA	3406	1/1	0.96	0.05	58,58,58,58	0
54	MG	BA	3401	1/1	0.96	0.06	58,58,58,58	0
54	MG	AA	1689	1/1	0.96	0.06	99,99,99,99	0
54	MG	DA	3243	1/1	0.96	0.14	28,28,28,28	0
54	MG	DA	3414	1/1	0.96	0.10	51,51,51,51	0
54	MG	BA	3330	1/1	0.96	0.06	34,34,34,34	0
54	MG	DA	3128	1/1	0.96	0.20	45,45,45,45	0
54	MG	BA	3115	1/1	0.96	0.21	45,45,45,45	0
54	MG	BA	3351	1/1	0.97	0.07	60,60,60,60	0
54	MG	DA	3315	1/1	0.97	0.05	31,31,31,31	0
54	MG	BA	3460	1/1	0.97	0.13	61,61,61,61	0
54	MG	DA	3039	1/1	0.97	0.12	28,28,28,28	0
54	MG	BA	3180	1/1	0.97	0.15	41,41,41,41	0
54	MG	BA	3462	1/1	0.97	0.05	43,43,43,43	0
54	MG	BA	3284	1/1	0.97	0.25	24,24,24,24	0
54	MG	BA	3356	1/1	0.97	0.05	29,29,29,29	0
54	MG	BA	3042	1/1	0.97	0.13	40,40,40,40	0
54	MG	BA	3136	1/1	0.97	0.20	45,45,45,45	0
54	MG	BA	3314	1/1	0.97	0.11	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	3490	1/1	0.97	0.06	33,33,33,33	0
54	MG	BA	3474	1/1	0.97	0.06	37,37,37,37	0
54	MG	CA	1722	1/1	0.97	0.12	71,71,71,71	0
54	MG	CA	1724	1/1	0.97	0.07	49,49,49,49	0
54	MG	CA	1725	1/1	0.97	0.08	65,65,65,65	0
54	MG	DA	3495	1/1	0.97	0.07	83,83,83,83	0
54	MG	CA	1726	1/1	0.97	0.15	52,52,52,52	0
54	MG	BA	3476	1/1	0.97	0.10	49,49,49,49	0
54	MG	AA	1710	1/1	0.97	0.06	79,79,79,79	0
54	MG	BB	217	1/1	0.97	0.07	67,67,67,67	0
54	MG	BA	3410	1/1	0.97	0.08	77,77,77,77	0
54	MG	BA	3479	1/1	0.97	0.08	32,32,32,32	0
54	MG	DA	3339	1/1	0.97	0.04	44,44,44,44	0
54	MG	DA	3057	1/1	0.97	0.06	35,35,35,35	0
54	MG	BA	3482	1/1	0.97	0.10	27,27,27,27	0
54	MG	BA	3184	1/1	0.97	0.17	40,40,40,40	0
54	MG	DA	3511	1/1	0.97	0.05	49,49,49,49	0
54	MG	DA	3343	1/1	0.97	0.05	37,37,37,37	0
54	MG	BD	302	1/1	0.97	0.06	28,28,28,28	0
54	MG	BA	3488	1/1	0.97	0.10	24,24,24,24	0
54	MG	BA	3138	1/1	0.97	0.15	42,42,42,42	0
54	MG	DA	3349	1/1	0.97	0.06	35,35,35,35	0
54	MG	DA	3518	1/1	0.97	0.05	69,69,69,69	0
54	MG	DA	3519	1/1	0.97	0.10	52,52,52,52	0
54	MG	BA	3583	1/1	0.97	0.12	34,34,34,34	0
54	MG	DA	3064	1/1	0.97	0.22	48,48,48,48	0
54	MG	AA	1718	1/1	0.97	0.04	96,96,96,96	0
54	MG	DA	3356	1/1	0.97	0.09	60,60,60,60	0
54	MG	BA	3414	1/1	0.97	0.07	29,29,29,29	0
54	MG	BA	3586	1/1	0.97	0.05	63,63,63,63	0
54	MG	BA	3415	1/1	0.97	0.06	33,33,33,33	0
54	MG	DA	3527	1/1	0.97	0.05	91,91,91,91	0
54	MG	AA	1700	1/1	0.97	0.06	42,42,42,42	0
54	MG	DA	3366	1/1	0.97	0.09	31,31,31,31	0
54	MG	DA	3531	1/1	0.97	0.07	91,91,91,91	0
54	MG	BA	3321	1/1	0.97	0.07	32,32,32,32	0
54	MG	BA	3093	1/1	0.97	0.13	42,42,42,42	0
54	MG	BA	3371	1/1	0.97	0.04	33,33,33,33	0
54	MG	DA	3536	1/1	0.97	0.08	51,51,51,51	0
54	MG	BR	201	1/1	0.97	0.07	29,29,29,29	0
54	MG	DA	3166	1/1	0.97	0.15	45,45,45,45	0
54	MG	BA	3510	1/1	0.97	0.05	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	BT	201	1/1	0.97	0.04	53,53,53,53	0
54	MG	DA	3543	1/1	0.97	0.08	53,53,53,53	0
54	MG	BA	3373	1/1	0.97	0.07	44,44,44,44	0
54	MG	BA	3130	1/1	0.97	0.08	43,43,43,43	0
54	MG	BW	201	1/1	0.97	0.15	32,32,32,32	0
54	MG	DA	3386	1/1	0.97	0.05	39,39,39,39	0
54	MG	DA	3549	1/1	0.97	0.12	45,45,45,45	0
54	MG	BA	3248	1/1	0.97	0.26	27,27,27,27	0
54	MG	BZ	301	1/1	0.97	0.17	55,55,55,55	0
54	MG	DA	3392	1/1	0.97	0.09	35,35,35,35	0
54	MG	AA	1714	1/1	0.97	0.13	57,57,57,57	0
54	MG	BA	3604	1/1	0.97	0.06	50,50,50,50	0
54	MG	DA	3556	1/1	0.97	0.06	56,56,56,56	0
54	MG	BA	3426	1/1	0.97	0.08	37,37,37,37	0
54	MG	BA	3228	1/1	0.97	0.30	37,37,37,37	0
54	MG	DA	3399	1/1	0.97	0.06	51,51,51,51	0
54	MG	BA	3429	1/1	0.97	0.08	47,47,47,47	0
54	MG	BA	3432	1/1	0.97	0.04	67,67,67,67	0
54	MG	DA	3403	1/1	0.97	0.04	34,34,34,34	0
54	MG	B5	102	1/1	0.97	0.08	52,52,52,52	0
54	MG	BA	3618	1/1	0.97	0.07	52,52,52,52	0
54	MG	B8	101	1/1	0.97	0.09	51,51,51,51	0
54	MG	DA	3090	1/1	0.97	0.24	53,53,53,53	0
54	MG	DA	3413	1/1	0.97	0.07	56,56,56,56	0
54	MG	BA	3229	1/1	0.97	0.10	41,41,41,41	0
54	MG	DA	3571	1/1	0.97	0.07	55,55,55,55	0
54	MG	BA	3622	1/1	0.97	0.10	45,45,45,45	0
54	MG	DA	3417	1/1	0.97	0.07	31,31,31,31	0
54	MG	DA	3418	1/1	0.97	0.11	31,31,31,31	0
54	MG	DA	3419	1/1	0.97	0.05	44,44,44,44	0
54	MG	DA	3421	1/1	0.97	0.06	93,93,93,93	0
54	MG	BA	3623	1/1	0.97	0.07	73,73,73,73	0
54	MG	BA	3144	1/1	0.97	0.25	46,46,46,46	0
54	MG	DA	3429	1/1	0.97	0.04	56,56,56,56	0
54	MG	DA	3431	1/1	0.97	0.06	59,59,59,59	0
54	MG	DA	3432	1/1	0.97	0.07	70,70,70,70	0
54	MG	BA	3527	1/1	0.97	0.12	29,29,29,29	0
54	MG	BA	3253	1/1	0.97	0.27	19,19,19,19	0
54	MG	BA	3211	1/1	0.97	0.06	26,26,26,26	0
54	MG	BA	3388	1/1	0.97	0.05	47,47,47,47	0
54	MG	BA	3533	1/1	0.97	0.11	61,61,61,61	0
54	MG	BA	3534	1/1	0.97	0.11	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	BA	3643	1/1	0.97	0.09	59,59,59,59	0
54	MG	DA	3440	1/1	0.97	0.10	42,42,42,42	0
54	MG	BA	3277	1/1	0.97	0.26	22,22,22,22	0
54	MG	BA	3537	1/1	0.97	0.08	31,31,31,31	0
54	MG	AA	1716	1/1	0.97	0.10	116,116,116,116	0
54	MG	DA	3291	1/1	0.97	0.18	53,53,53,53	0
54	MG	DA	3106	1/1	0.97	0.20	37,37,37,37	0
54	MG	BA	3341	1/1	0.97	0.05	44,44,44,44	0
54	MG	DA	3448	1/1	0.97	0.04	42,42,42,42	0
54	MG	DD	301	1/1	0.97	0.15	47,47,47,47	0
54	MG	BA	3343	1/1	0.97	0.05	73,73,73,73	0
54	MG	BA	3161	1/1	0.97	0.18	40,40,40,40	0
54	MG	DA	3451	1/1	0.97	0.06	103,103,103,103	0
54	MG	BA	3022	1/1	0.97	0.06	46,46,46,46	0
54	MG	DA	3204	1/1	0.97	0.27	43,43,43,43	0
54	MG	BA	3652	1/1	0.97	0.05	97,97,97,97	0
54	MG	BA	3653	1/1	0.97	0.10	104,104,104,104	0
54	MG	DA	3456	1/1	0.97	0.06	42,42,42,42	0
54	MG	BA	3395	1/1	0.97	0.10	60,60,60,60	0
54	MG	BA	3396	1/1	0.97	0.06	29,29,29,29	0
54	MG	BA	3550	1/1	0.97	0.04	87,87,87,87	0
54	MG	BA	3041	1/1	0.97	0.23	40,40,40,40	0
54	MG	DA	3462	1/1	0.97	0.06	51,51,51,51	0
54	MG	DR	203	1/1	0.97	0.21	51,51,51,51	0
54	MG	DA	3463	1/1	0.97	0.04	69,69,69,69	0
54	MG	DA	3117	1/1	0.97	0.12	47,47,47,47	0
54	MG	CA	1701	1/1	0.97	0.09	72,72,72,72	0
54	MG	BA	3450	1/1	0.97	0.06	38,38,38,38	0
54	MG	BA	3179	1/1	0.97	0.21	37,37,37,37	0
54	MG	BA	3455	1/1	0.97	0.11	22,22,22,22	0
54	MG	BA	3348	1/1	0.97	0.05	59,59,59,59	0
54	MG	DA	3124	1/1	0.97	0.26	37,37,37,37	0
55	ZN	BY	201	1/1	0.97	0.04	69,69,69,69	0
54	MG	DA	3034	1/1	0.97	0.04	32,32,32,32	0
54	MG	BA	3556	1/1	0.97	0.13	57,57,57,57	0
55	ZN	DY	201	1/1	0.97	0.04	94,94,94,94	0
54	MG	BA	3457	1/1	0.97	0.09	27,27,27,27	0
55	ZN	D9	101	1/1	0.97	0.07	65,65,65,65	0
54	MG	BA	3541	1/1	0.98	0.07	42,42,42,42	0
54	MG	DA	3334	1/1	0.98	0.07	52,52,52,52	0
54	MG	DA	3335	1/1	0.98	0.07	36,36,36,36	0
54	MG	DA	3135	1/1	0.98	0.27	47,47,47,47	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	0.98	0.11	42,42,42,42	0
54	MG	CA	1613	1/1	0.98	0.20	66,66,66,66	0
54	MG	BA	3466	1/1	0.98	0.10	39,39,39,39	0
54	MG	AA	1721	1/1	0.98	0.04	62,62,62,62	0
54	MG	BA	3047	1/1	0.98	0.13	35,35,35,35	0
54	MG	BA	3545	1/1	0.98	0.04	43,43,43,43	0
54	MG	DA	3344	1/1	0.98	0.04	30,30,30,30	0
54	MG	BA	3546	1/1	0.98	0.12	73,73,73,73	0
54	MG	DA	3346	1/1	0.98	0.06	35,35,35,35	0
54	MG	CA	1619	1/1	0.98	0.05	50,50,50,50	0
54	MG	DA	3242	1/1	0.98	0.23	34,34,34,34	0
54	MG	CA	1710	1/1	0.98	0.10	48,48,48,48	0
54	MG	DA	3498	1/1	0.98	0.04	28,28,28,28	0
54	MG	DA	3350	1/1	0.98	0.03	47,47,47,47	0
54	MG	DA	3351	1/1	0.98	0.05	40,40,40,40	0
54	MG	DA	3501	1/1	0.98	0.04	58,58,58,58	0
54	MG	DA	3502	1/1	0.98	0.05	37,37,37,37	0
54	MG	BA	3381	1/1	0.98	0.05	66,66,66,66	0
54	MG	DA	3504	1/1	0.98	0.05	63,63,63,63	0
54	MG	BA	3548	1/1	0.98	0.05	29,29,29,29	0
54	MG	BA	3549	1/1	0.98	0.04	55,55,55,55	0
54	MG	DA	3507	1/1	0.98	0.07	80,80,80,80	0
54	MG	DA	3355	1/1	0.98	0.09	49,49,49,49	0
54	MG	BA	3471	1/1	0.98	0.08	27,27,27,27	0
54	MG	DA	3357	1/1	0.98	0.06	36,36,36,36	0
54	MG	CA	1715	1/1	0.98	0.05	103,103,103,103	0
54	MG	BA	3650	1/1	0.98	0.12	88,88,88,88	0
54	MG	BA	3342	1/1	0.98	0.05	32,32,32,32	0
54	MG	DA	3363	1/1	0.98	0.14	26,26,26,26	0
54	MG	BA	3473	1/1	0.98	0.10	30,30,30,30	0
54	MG	DA	3365	1/1	0.98	0.04	40,40,40,40	0
54	MG	AA	1694	1/1	0.98	0.04	80,80,80,80	0
54	MG	AA	1730	1/1	0.98	0.04	51,51,51,51	0
54	MG	BA	3158	1/1	0.98	0.09	40,40,40,40	0
54	MG	DA	3369	1/1	0.98	0.04	50,50,50,50	0
54	MG	AA	1701	1/1	0.98	0.04	48,48,48,48	0
54	MG	BA	3051	1/1	0.98	0.13	48,48,48,48	0
54	MG	BA	3481	1/1	0.98	0.07	25,25,25,25	0
54	MG	BA	3242	1/1	0.98	0.13	38,38,38,38	0
54	MG	CA	1728	1/1	0.98	0.07	60,60,60,60	0
54	MG	DA	3375	1/1	0.98	0.06	31,31,31,31	0
54	MG	DA	3378	1/1	0.98	0.10	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	DA	3529	1/1	0.98	0.05	56,56,56,56	0
54	MG	BA	3560	1/1	0.98	0.04	74,74,74,74	0
54	MG	DA	3381	1/1	0.98	0.03	42,42,42,42	0
54	MG	BA	3483	1/1	0.98	0.07	28,28,28,28	0
54	MG	BA	3484	1/1	0.98	0.09	27,27,27,27	0
54	MG	DA	3534	1/1	0.98	0.07	28,28,28,28	0
54	MG	DA	3384	1/1	0.98	0.05	45,45,45,45	0
54	MG	BA	3430	1/1	0.98	0.05	49,49,49,49	0
54	MG	BA	3431	1/1	0.98	0.05	71,71,71,71	0
54	MG	DA	3388	1/1	0.98	0.13	43,43,43,43	0
54	MG	DA	3539	1/1	0.98	0.06	67,67,67,67	0
54	MG	BA	3490	1/1	0.98	0.04	28,28,28,28	0
54	MG	BA	3350	1/1	0.98	0.06	40,40,40,40	0
54	MG	DA	3542	1/1	0.98	0.05	83,83,83,83	0
54	MG	BA	3568	1/1	0.98	0.07	39,39,39,39	0
54	MG	DA	3395	1/1	0.98	0.05	39,39,39,39	0
54	MG	BA	3493	1/1	0.98	0.05	40,40,40,40	0
54	MG	BA	3494	1/1	0.98	0.05	34,34,34,34	0
54	MG	BA	3571	1/1	0.98	0.07	44,44,44,44	0
54	MG	AA	1698	1/1	0.98	0.07	69,69,69,69	0
54	MG	BA	3573	1/1	0.98	0.11	23,23,23,23	0
54	MG	DA	3551	1/1	0.98	0.07	62,62,62,62	0
54	MG	DA	3173	1/1	0.98	0.15	52,52,52,52	0
54	MG	DA	3402	1/1	0.98	0.04	44,44,44,44	0
54	MG	AA	1733	1/1	0.98	0.04	78,78,78,78	0
54	MG	DA	3405	1/1	0.98	0.05	32,32,32,32	0
54	MG	CA	1743	1/1	0.98	0.07	61,61,61,61	0
54	MG	CA	1744	1/1	0.98	0.04	83,83,83,83	0
54	MG	DA	3409	1/1	0.98	0.04	73,73,73,73	0
54	MG	BB	214	1/1	0.98	0.06	40,40,40,40	0
54	MG	BA	3575	1/1	0.98	0.06	41,41,41,41	0
54	MG	DA	3412	1/1	0.98	0.04	58,58,58,58	0
54	MG	BA	3576	1/1	0.98	0.07	21,21,21,21	0
54	MG	BA	3323	1/1	0.98	0.06	23,23,23,23	0
54	MG	DA	3415	1/1	0.98	0.04	43,43,43,43	0
54	MG	BB	218	1/1	0.98	0.05	45,45,45,45	0
54	MG	BA	3354	1/1	0.98	0.04	37,37,37,37	0
54	MG	BB	221	1/1	0.98	0.03	50,50,50,50	0
54	MG	BA	3355	1/1	0.98	0.06	29,29,29,29	0
54	MG	DA	3570	1/1	0.98	0.10	28,28,28,28	0
54	MG	BA	3324	1/1	0.98	0.05	42,42,42,42	0
54	MG	DA	3572	1/1	0.98	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3422	1/1	0.98	0.07	43,43,43,43	0
54	MG	BA	3505	1/1	0.98	0.12	41,41,41,41	0
54	MG	DA	3579	1/1	0.98	0.05	57,57,57,57	0
54	MG	BA	3506	1/1	0.98	0.06	30,30,30,30	0
54	MG	DA	3427	1/1	0.98	0.04	59,59,59,59	0
54	MG	BD	303	1/1	0.98	0.14	35,35,35,35	0
54	MG	BA	3325	1/1	0.98	0.05	40,40,40,40	0
54	MG	BA	3509	1/1	0.98	0.08	50,50,50,50	0
54	MG	BA	3441	1/1	0.98	0.07	56,56,56,56	0
54	MG	BA	3326	1/1	0.98	0.04	49,49,49,49	0
54	MG	BA	3089	1/1	0.98	0.17	41,41,41,41	0
54	MG	BA	3588	1/1	0.98	0.03	64,64,64,64	0
54	MG	BA	3361	1/1	0.98	0.04	59,59,59,59	0
54	MG	DA	3592	1/1	0.98	0.04	83,83,83,83	0
54	MG	AA	1703	1/1	0.98	0.04	66,66,66,66	0
54	MG	BA	3151	1/1	0.98	0.24	33,33,33,33	0
54	MG	BA	3518	1/1	0.98	0.08	50,50,50,50	0
54	MG	BA	3594	1/1	0.98	0.05	86,86,86,86	0
54	MG	DA	3005	1/1	0.98	0.10	77,77,77,77	0
54	MG	BA	3595	1/1	0.98	0.16	27,27,27,27	0
54	MG	DA	3444	1/1	0.98	0.04	41,41,41,41	0
54	MG	BA	3447	1/1	0.98	0.04	29,29,29,29	0
54	MG	BA	3405	1/1	0.98	0.07	61,61,61,61	0
54	MG	DA	3105	1/1	0.98	0.18	46,46,46,46	0
54	MG	BA	3331	1/1	0.98	0.06	48,48,48,48	0
54	MG	BA	3599	1/1	0.98	0.06	30,30,30,30	0
54	MG	BA	3055	1/1	0.98	0.15	53,53,53,53	0
54	MG	BA	3451	1/1	0.98	0.06	28,28,28,28	0
54	MG	AA	1691	1/1	0.98	0.07	43,43,43,43	0
54	MG	BA	3605	1/1	0.98	0.06	55,55,55,55	0
54	MG	BA	3607	1/1	0.98	0.07	99,99,99,99	0
54	MG	BA	3453	1/1	0.98	0.04	46,46,46,46	0
54	MG	BA	3334	1/1	0.98	0.04	51,51,51,51	0
54	MG	BA	3610	1/1	0.98	0.05	63,63,63,63	0
54	MG	BA	3611	1/1	0.98	0.04	44,44,44,44	0
54	MG	BA	3530	1/1	0.98	0.09	56,56,56,56	0
54	MG	BA	3613	1/1	0.98	0.04	65,65,65,65	0
54	MG	DA	3461	1/1	0.98	0.08	41,41,41,41	0
54	MG	BA	3615	1/1	0.98	0.04	52,52,52,52	0
54	MG	BA	3531	1/1	0.98	0.04	89,89,89,89	0
54	MG	DA	3121	1/1	0.98	0.10	34,34,34,34	0
54	MG	BA	3617	1/1	0.98	0.05	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3198	1/1	0.98	0.15	44,44,44,44	0
54	MG	DA	3468	1/1	0.98	0.03	53,53,53,53	0
54	MG	BA	3620	1/1	0.98	0.04	68,68,68,68	0
54	MG	BA	3168	1/1	0.98	0.20	28,28,28,28	0
54	MG	BA	3372	1/1	0.98	0.03	49,49,49,49	0
54	MG	BA	3200	1/1	0.98	0.16	31,31,31,31	0
54	MG	BA	3626	1/1	0.98	0.09	64,64,64,64	0
54	MG	DA	3475	1/1	0.98	0.06	30,30,30,30	0
54	MG	BA	3289	1/1	0.98	0.14	34,34,34,34	0
54	MG	BA	3309	1/1	0.98	0.06	31,31,31,31	0
54	MG	BA	3464	1/1	0.98	0.06	39,39,39,39	0
54	MG	DA	3479	1/1	0.98	0.05	62,62,62,62	0
54	MG	BA	3376	1/1	0.98	0.04	26,26,26,26	0
54	MG	BA	3639	1/1	0.98	0.15	65,65,65,65	0
54	MG	DA	3394	1/1	0.99	0.03	47,47,47,47	0
54	MG	BE	303	1/1	0.99	0.07	26,26,26,26	0
54	MG	BE	304	1/1	0.99	0.10	25,25,25,25	0
54	MG	BA	3428	1/1	0.99	0.05	56,56,56,56	0
54	MG	DA	3474	1/1	0.99	0.03	30,30,30,30	0
54	MG	BA	3365	1/1	0.99	0.03	69,69,69,69	0
54	MG	BA	3315	1/1	0.99	0.07	31,31,31,31	0
54	MG	BA	3508	1/1	0.99	0.09	29,29,29,29	0
54	MG	BA	3475	1/1	0.99	0.06	39,39,39,39	0
54	MG	BA	3379	1/1	0.99	0.04	22,22,22,22	0
54	MG	BA	3511	1/1	0.99	0.07	32,32,32,32	0
54	MG	DA	3404	1/1	0.99	0.10	36,36,36,36	0
54	MG	BA	3380	1/1	0.99	0.06	26,26,26,26	0
54	MG	DA	3336	1/1	0.99	0.10	41,41,41,41	0
54	MG	DA	3407	1/1	0.99	0.06	70,70,70,70	0
54	MG	AA	1728	1/1	0.99	0.07	53,53,53,53	0
54	MG	BA	3591	1/1	0.99	0.03	34,34,34,34	0
54	MG	DA	3566	1/1	0.99	0.05	54,54,54,54	0
54	MG	CA	1748	1/1	0.99	0.04	58,58,58,58	0
54	MG	BA	3454	1/1	0.99	0.05	25,25,25,25	0
54	MG	BA	3480	1/1	0.99	0.06	31,31,31,31	0
54	MG	BA	3434	1/1	0.99	0.05	62,62,62,62	0
54	MG	BA	3517	1/1	0.99	0.05	26,26,26,26	0
54	MG	BA	3044	1/1	0.99	0.08	33,33,33,33	0
54	MG	BA	3519	1/1	0.99	0.03	64,64,64,64	0
54	MG	DA	3574	1/1	0.99	0.03	41,41,41,41	0
54	MG	DA	3575	1/1	0.99	0.08	35,35,35,35	0
54	MG	DA	3576	1/1	0.99	0.04	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	DA	3577	1/1	0.99	0.04	57,57,57,57	0
54	MG	BA	3416	1/1	0.99	0.03	25,25,25,25	0
54	MG	BA	3521	1/1	0.99	0.04	40,40,40,40	0
54	MG	BA	3458	1/1	0.99	0.05	35,35,35,35	0
54	MG	DA	3581	1/1	0.99	0.03	52,52,52,52	0
54	MG	DA	3420	1/1	0.99	0.06	37,37,37,37	0
54	MG	BA	3561	1/1	0.99	0.07	54,54,54,54	0
54	MG	BA	3602	1/1	0.99	0.05	56,56,56,56	0
54	MG	DA	3585	1/1	0.99	0.05	33,33,33,33	0
54	MG	DA	3423	1/1	0.99	0.05	32,32,32,32	0
54	MG	BA	3603	1/1	0.99	0.03	40,40,40,40	0
54	MG	DA	3425	1/1	0.99	0.03	47,47,47,47	0
54	MG	BA	3485	1/1	0.99	0.03	32,32,32,32	0
54	MG	BA	3383	1/1	0.99	0.05	70,70,70,70	0
54	MG	DA	3428	1/1	0.99	0.03	68,68,68,68	0
54	MG	BA	3065	1/1	0.99	0.06	41,41,41,41	0
54	MG	DA	3430	1/1	0.99	0.04	30,30,30,30	0
54	MG	DA	3594	1/1	0.99	0.09	58,58,58,58	0
54	MG	BA	3526	1/1	0.99	0.07	22,22,22,22	0
54	MG	BA	3489	1/1	0.99	0.06	23,23,23,23	0
54	MG	BA	3071	1/1	0.99	0.13	34,34,34,34	0
54	MG	CA	1709	1/1	0.99	0.09	63,63,63,63	0
54	MG	DA	3512	1/1	0.99	0.04	42,42,42,42	0
54	MG	DA	3359	1/1	0.99	0.04	33,33,33,33	0
54	MG	BA	3491	1/1	0.99	0.04	28,28,28,28	0
54	MG	BA	3312	1/1	0.99	0.05	51,51,51,51	0
54	MG	DA	3362	1/1	0.99	0.04	26,26,26,26	0
54	MG	BA	3387	1/1	0.99	0.06	63,63,63,63	0
54	MG	BA	3614	1/1	0.99	0.03	66,66,66,66	0
54	MG	BA	3349	1/1	0.99	0.03	36,36,36,36	0
54	MG	BA	3495	1/1	0.99	0.04	35,35,35,35	0
54	MG	BA	3423	1/1	0.99	0.05	33,33,33,33	0
54	MG	BA	3535	1/1	0.99	0.09	55,55,55,55	0
54	MG	BA	3619	1/1	0.99	0.04	64,64,64,64	0
54	MG	CA	1719	1/1	0.99	0.02	54,54,54,54	0
54	MG	DA	3014	1/1	0.99	0.13	31,31,31,31	0
54	MG	BA	3497	1/1	0.99	0.16	61,61,61,61	0
54	MG	BA	3498	1/1	0.99	0.07	32,32,32,32	0
54	MG	AA	1696	1/1	0.99	0.07	66,66,66,66	0
54	MG	CA	1723	1/1	0.99	0.07	55,55,55,55	0
54	MG	DA	3376	1/1	0.99	0.05	30,30,30,30	0
54	MG	BA	3468	1/1	0.99	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3624	1/1	0.99	0.04	36,36,36,36	0
54	MG	DA	3380	1/1	0.99	0.04	42,42,42,42	0
54	MG	BA	3625	1/1	0.99	0.04	53,53,53,53	0
54	MG	BB	220	1/1	0.99	0.10	60,60,60,60	0
54	MG	BA	3362	1/1	0.99	0.04	43,43,43,43	0
54	MG	BA	3322	1/1	0.99	0.03	37,37,37,37	0
54	MG	DA	3385	1/1	0.99	0.07	49,49,49,49	0
54	MG	BA	3628	1/1	0.99	0.06	35,35,35,35	0
54	MG	BA	3629	1/1	0.99	0.04	24,24,24,24	0
54	MG	BA	3630	1/1	0.99	0.04	34,34,34,34	0
54	MG	DA	3389	1/1	0.99	0.04	51,51,51,51	0
54	MG	DA	3390	1/1	0.99	0.06	47,47,47,47	0
54	MG	BA	3631	1/1	0.99	0.05	26,26,26,26	0
55	ZN	B5	101	1/1	0.99	0.02	45,45,45,45	0
55	ZN	B9	101	1/1	0.99	0.02	50,50,50,50	0
54	MG	DA	3467	1/1	0.99	0.05	43,43,43,43	0
55	ZN	CN	101	1/1	0.99	0.05	107,107,107,107	0
54	MG	AA	1715	1/1	0.99	0.05	61,61,61,61	0
54	MG	DA	3547	1/1	0.99	0.09	29,29,29,29	0
55	ZN	D6	101	1/1	0.99	0.03	63,63,63,63	0
54	MG	BA	3634	1/1	0.99	0.08	53,53,53,53	0
54	MG	BA	3463	1/1	1.00	0.02	28,28,28,28	0
54	MG	DA	3377	1/1	1.00	0.02	33,33,33,33	0
54	MG	BA	3327	1/1	1.00	0.06	23,23,23,23	0
54	MG	BA	3357	1/1	1.00	0.05	25,25,25,25	0
55	ZN	B6	101	1/1	1.00	0.01	48,48,48,48	0
54	MG	BA	3501	1/1	1.00	0.06	29,29,29,29	0
54	MG	BA	3632	1/1	1.00	0.02	54,54,54,54	0
54	MG	BA	3402	1/1	1.00	0.03	54,54,54,54	0
54	MG	BA	3487	1/1	1.00	0.07	20,20,20,20	0
54	MG	BA	3635	1/1	1.00	0.02	23,23,23,23	0
55	ZN	D5	102	1/1	1.00	0.02	69,69,69,69	0
54	MG	BA	3636	1/1	1.00	0.03	28,28,28,28	0
54	MG	BA	3606	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.